Supplementary Information (SI)

Eliminating Transition State Calculations for Faster and More Accurate Reactivity Prediction in Sulfa-Michael Additions Relevant to Human Health and the Environment

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1. Full Computational Methods

Kinetic glutathione assay data (log($k_{\text{GSH}}$)) for 23 1,4 Michael acceptors (MAs) was taken from work published by Bohme et al., providing experimental rate data for: nine esters, seven aldehydes and seven ketones (see section 3, Table S1). Minor truncation was performed on two compounds. 1-pentene-3-one was truncated to methyl vinyl ketone and trans-2-pentenal to but-2-enal. Conformational searches and redundant conformer eliminations were performed on all 23 MAs using Schrödinger’s MacroModel (Ver. 12.3). Molecular energies were calculated with the OPLS3e force field and the Polak-Ribière conjugate gradient (PRCG) algorithm was used for the optimization procedures.

In 2011, it was reported by Krenske et al that the rate-determining step in the addition of thiols to α,β-unsaturated ketones is the addition of methanethiolate to the corresponding enone. This paper also reported that M06-2X and a large basis set (triple-ζ) gave thermodynamic data within 1 kcal mol$^{-1}$ of CBS-QB3 benchmark data. Therefore, structures obtained from MacroModel were optimised using DFT calculations performed with Gaussian 16 (Rev. A.03) at the M06-2X/def2-TZVPP level of theory under the IEF-PCM implicit solvation model (water), which has been used extensively for modelling organic chemical reactions. In line with previous studies, and to ensure computational feasibility, methanethiolate was used as a model nucleophile in all calculations. Following DFT calculations, reactant and intermediate structures were optimised with the SQM AM1 method. Corrections to the free energy were obtained with GoodVibes using the quasi-harmonic approximation as described by Grimme. In GoodVibes, a vibrational scaling factor of 1, a temperature of 298.15 K, and a concentration of 1 mol dm$^{-3}$ were used. Electronic supplementary information was created using ESIGen.

All regression models were developed via the Scikit-learn python package. The 23 compounds were split at a 75:25 ratio into a training set of 17 compounds and a test set of 6 compounds and the training set used to fit an ordinary least squares linear regression model. This model was validated externally based on the log($k_{\text{GSH}}$) values predicted using the test set. 2-fold cross validation was also performed within the training set in order to test the stability of the model and to identify any overfitting. Thus, the performance of a model could be assessed by its mean absolute error (MAE) for both external validation (test set predictions) and cross validation (training set). Pearson correlation coefficients ($r^2$) were also calculated between the predicted and experimental log($k_{\text{GSH}}$) for each model, providing a further source of external validation (test set predictions, see section 2 below). Due to the small size of the dataset (n=23), MAEs and $r^2$ scores were calculated at 20 different random 75:25 train-test splitting’s of the data and the scores averaged. For each model, a single train-test splitting was then located with individual MAEs and $r^2$ scores that closely matched the average scores. This ensured that the scores presented matched the average performance of the model. The average scores are included in the supplementary information, whilst the scores for the individual models are presented in the manuscript.
2. Full Regression Metrics

Linear regression of log\(k_{\text{GSH}}\) with the activation energy derived from transition state structures (M06-2X/def2-TZVPP-IEFPCM(water)).

Averaged over 20 train-test splits:
- Average MAE: 0.70
- Average 2-Fold MAE: 0.69
- Average r\(^2\): 0.65

Representative train-test split:
- MAE: 0.69
- 2-Fold MAE: 0.67
- r\(^2\): 0.49

Linear regression of log\(k_{\text{GSH}}\) with the intermediate energy differences (M06-2X/def2-TZVPP-IEFPCM(water)).

Averaged over 20 train-test splits:
- Average MAE: 0.48
- Average 2-Fold MAE: 0.50
- Average r\(^2\): 0.81

Representative train-test split:
- MAE: 0.48
- 2-Fold MAE: 0.45
- r\(^2\): 0.76

Linear regression of log\(k_{\text{GSH}}\) with key atomic charges of the MA (M06-2X/def2-TZVPP-IEFPCM(water)).

Averaged over 20 train-test splits:
- Average MAE: 0.32
- Average 2-Fold MAE: 0.41
- Average r\(^2\): 0.89

Representative train-test split:
- MAE: 0.35
- 2-Fold MAE: 0.41
- r\(^2\): 0.88

Linear regression of log\(k_{\text{GSH}}\) with key atomic charges of the MA (AM1).

Averaged over 20 train-test splits:
- Average MAE: 0.33
- Average 2-Fold MAE: 0.40
- Average r\(^2\): 0.90

Representative train-test split:
- MAE: 0.37
- 2-Fold MAE: 0.33
- r\(^2\): 0.89
Multivariate Models

Except where noted, the following features were extracted for all MAs, intermediates, and TSs. Multivariate linear regression models were developed by combining up to 5 features from each subset (MAs, intermediates, TSs), fitting a model, and generating metrics (repeated over 20 train-test splits and averaged). No mixing of features occurred. For example, models were not fitted with a mixture of some TS features and some MA features.

| Feature                                                      | Source       |
|--------------------------------------------------------------|--------------|
| Activation energy (TSs only)                                 |              |
| Intermediate energy difference (intermediates only)          |              |
| Electronic Energy                                           | Goodvibes    |
| Gibbs Free Energy                                           | Goodvibes    |
| Enthalpy                                                    | Goodvibes    |
| Entropy                                                     | Goodvibes    |
| Quasiharmonic Entropy                                       | Goodvibes    |
| Zero-Point Energy                                           | Goodvibes    |
| Quasiharmonic Gibbs Free Energy                             | Goodvibes    |
| Mulliken and APT atomic charges for key atoms, summed and not-summed | CCLIB\textsuperscript{14} |
| Total Electrotopological State Index                        | RDKit\textsuperscript{15,16} |
| Total Accessible Surface Area                               | RDKit\textsuperscript{15,17} |
| Total Topological Polar Surface Area                        | RDKit\textsuperscript{15,18} |
| Total Partial Equalization of Orbital Electronegativities (Partial Charges) | RDKit\textsuperscript{15,19} |
| Molecular Chemical Potential                                | HSAB\textsuperscript{20} |
| Molecular Electrophilic Index                               | HSAB\textsuperscript{20} |
| Molecular Hardness                                          | HSAB\textsuperscript{20} |
| Molecular Softness                                          | HSAB\textsuperscript{20} |
3. Additional Figures

| Structure            | CAS No | No of Conformers | No of Conformers | Activation Energy ΔG° (kcal/mol) | Intermediate Energy Difference ΔG_int (kcal/mol) |
|----------------------|--------|------------------|------------------|---------------------------------|-----------------------------------------------|
| Ketones              |        |                  |                  |                                 |                                               |
| 1-pentene-3-one*     | 1629–58–9 | 3.1              | 6                | 10.37                           | 2.42                                        |
| 3-pentene-2-one      | 625–33–2  | 1.43             | 7                | 10.12                           | 3.12                                        |
| 2-cyclopentene-1-one | 930–50–3  | 1.41             | 3                | 12.71                           | 7.15                                        |
| 4-hexene-3-one       | 2407–21–4 | 1.38             | 10               | 13.06                           | 6.78                                        |
| 3-methyl-3-pentene-2-one | 505–62–8   | -0.11            | 7                | 14.39                           | 10.61                                       |
| 4-methyl-3-pentene-2-one | 141–79–7—6    | -0.63            | 6                | 15.78                           | 9.33                                        |
| 3-methyl-2-cyclopentene-1-one | 2758–18–1   | -1.13            | 3                | 15.99                           | 11.62                                       |
| Alddehydes           |         |                  |                  |                                 |                                               |
| methacrylic aldehyde | 78–85–3    | 2.31             | 8                | 10.05                           | 2.75                                        |
| 2-ethyl acrylon      | 922–63–4   | 1.77             | 11               | 10.81                           | 3.37                                        |
| trans-2-pentenyl     | 1576–87–0  | 1.45             | 8                | 11.01                           | 3.59                                        |
| 4-methyl-2-pentenyl  | 5362–56–1  | 1.63             | 14               | 11.69                           | 3.94                                        |
| trans-2,4-hexadien   | 142–83–6   | 0.83             | 11               | 13.23                           | 7.45                                        |
| 3-methyl-2-butenal   | 107–86–8   | 0.22             | 8                | 13.99                           | 7.14                                        |
| trans-2,3-methyl-2-butenal | 497–03–0     | -0.32            | 7                | 12.47                           | 6.33                                        |
| Esters               |         |                  |                  |                                 |                                               |
| methyl acrylate      | 96–33–3    | 1.06             | 8                | 11.30                           | 6.19                                        |
| n-propyl acrylate    | 955–49–0   | 1.01             | 20               | 11.70                           | 6.55                                        |
| iso-butyl acrylate   | 106–63–8   | 0.97             | 21               | 9.65                            | 6.38                                        |
| tert-butyl acrylate  | 1603–38–4  | 0.4              | 8                | 12.19                           | 7.77                                        |
| ethyl crotonate      | 623–70–1   | -0.79            | 12               | 14.44                           | 9.76                                        |
| methyl crotonate     | 623–43–8   | -0.79            | 8                | 14.14                           | 9.86                                        |
| methacrylaldehyde    | 80–62–6    | -1.14            | 6                | 14.02                           | 10.16                                       |
| ethyl methacrylate   | 97–83–2    | -1.24            | 12               | 14.07                           | 10.43                                       |
| methyl tiglate       | 6622–76–0  | -2.15            | 6                | 16.08                           | 13.28                                       |

Table S1. CAS No, kinetic glutathione chemoassay data, number of conformers, activation energies and intermediate energy differences for each structure included in this study. Compounds marked with an asterisk (*) have been truncated as described in the computational methods.

| Compound Name        | log(k_on) | No of TS Conformations | Barrier 1 (TS-1) | Barrier 2 (TS-2) |
|----------------------|-----------|------------------------|------------------|------------------|
| 1-pentene-3-one      | 3.1       | 11                     | 10.37            | 6.93             |
| 4-methyl-3-pentene-2-one | -0.68   | 11                     | 15.78            | 7.42             |
| methacrylaldehyde    | 2.31      | 8                      | 10.05            | 6.80             |
| 3-methyl-2-butenal   | 0.23      | 9                      | 13.99            | 8.06             |
| methyl acrylate      | 1.06      | 12                     | 11.30            | 5.65             |
| methyl tiglate       | -2.15     | 9                      | 16.08            | 4.21             |

Table S2. For six compounds, activation barriers were calculated for the protonation step (TS-2). The number of TS conformers and TS barriers (TS-1 and TS-2) can be seen in the table.

4. References

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1_methylacrolein_conf2_min

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -231.224444    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -231.159496    |
| Number of Imaginary Frequencies                                      | 0              |

Frequencies (Top 3 out of 27)

1. 162.8136 cm⁻¹
2. 186.7364 cm⁻¹
3. 267.3495 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C          | -1.488416 | -0.947821 | -0.000050 |
| H          | -1.295875 | -2.013946 | -0.000048 |
| H          | -2.522579 | -0.629191 | -0.000082 |
| C          | -0.483058 | -0.074945 | -0.000016 |
| C          | 0.886248  | -0.627889 | 0.000026  |
| H          | 0.952205  | -1.729573 | 0.000023  |
| O          | 1.885483  | 0.051408  | 0.000061  |
| C          | -0.626254 | 1.413151  | -0.000016 |
| H          | -0.137437 | 1.841181  | 0.875870  |
| H          | -0.137385 | 1.841186  | -0.875871 |
| H          | -1.673908 | 1.704105  | -0.000046 |
**1_methylacrolein_HEI_1**

| Datum                                                        | Value                  |
|--------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                        | -669.445937            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  | -669.346859            |
| Number of Imaginary Frequencies                              | 0                      |

**Frequencies (Top 3 out of 42)**

1. 53.5027 cm⁻¹  
2. 98.2001 cm⁻¹  
3. 157.6711 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C          | C          | O          | H          | C          | H          | H          | H          | S          | H          | H          | H          |
|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|   | -1.795566  | -0.587764  | -0.146618  | -1.701804  | 0.249566   | -1.778541  | 1.247960   | 0.581801   | 0.581801   | 0.581801   | 0.581801   | 0.581801   |
|   | -1.002628  | 0.501571   | 0.099758   | 0.155625   | 0.388712   | 0.314185   | 1.017382   | 0.099758   | 0.099758   | 0.099758   | 0.099758   | 0.099758   |
|   | 0.156625   | 0.388712   | 1.017382   | -1.701804  | -1.778541  | 0.314185   | 0.314185   | 0.099758   | 0.099758   | 0.099758   | 0.099758   | 0.099758   |
|   | 0.249566   | 1.247960   | 0.168744   | 0.249566   | 0.249566   | 1.247960   | 0.249566   | 1.247960   | 0.249566   | 0.249566   | 0.249566   | 0.249566   |
|   | 0.087078   | -0.581801  | 1.616724   | 0.087078   | -0.581801  | 1.616724   | 0.087078   | -0.581801  | 0.087078   | -0.581801  | 0.087078   | -0.581801  |
|   | 1.587141   | -1.130589  | -0.820198  | 0.249566   | 1.247960   | -0.820198  | 0.249566   | 1.247960   | 0.249566   | 1.247960   | -1.130589  | -0.820198  |
|   | 1.618040   | -2.026782  | -0.203154  | 1.587141   | -1.130589  | -0.203154  | 1.587141   | -1.130589  | 1.587141   | -1.130589  | -2.026782  | -0.203154  |
|   | 0.624220   | -1.072722  | -1.326297  | 1.618040   | -2.026782  | -1.326297  | 1.618040   | -2.026782  | 1.618040   | -2.026782  | -1.072722  | -1.326297  |
|   | 2.388800   | -1.168613  | -1.554203  | 0.624220   | -1.072722  | -1.326297  | 0.624220   | -1.072722  | 0.624220   | -1.072722  | -1.168613  | -1.554203  |
|   | 1.808656   | 0.351363   | 0.179546   | 2.388800   | -1.168613  | -1.554203  | 2.388800   | -1.168613  | 2.388800   | -1.168613  | 0.351363   | 0.179546   |
|   | -2.637992  | -0.380029  | -0.840503  | 1.808656   | 0.351363   | 0.179546   | -2.637992  | -0.380029  | -2.637992  | -0.380029  | -0.380029  | -0.840503  |
|   | -1.237374  | 1.824088   | -0.569068  | -2.637992  | -0.380029  | -0.840503  | -1.237374  | 1.824088   | -1.237374  | 1.824088   | -0.569068  | -0.840503  |
|   | -1.385469  | 2.637055   | 0.152362   | -1.237374  | 1.824088   | -0.569068  | -1.385469  | 2.637055   | -1.385469  | 2.637055   | 0.152362   | -0.569068  |
|   | -2.123927  | 1.784727   | -1.205592  | -1.385469  | 2.637055   | 0.152362   | -2.123927  | 1.784727   | -2.123927  | 1.784727   | -1.205592  | -1.205592  |
|   | -0.393569  | 2.126888   | -1.200522  | -2.123927  | 1.784727   | -1.205592  | -0.393569  | 2.126888   | -0.393569  | 2.126888   | -1.200522  | -1.200522  |

**1_methylacrolein_HEI_2**

| Datum                                                        | Value                  |
|--------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                        | -669.446447            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  | -669.348159            |
| Number of Imaginary Frequencies                              | 0                      |
Frequencies (Top 3 out of 42)

1. 37.9712 cm⁻¹
2. 80.5166 cm⁻¹
3. 110.1660 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -1.668595 | 0.665640 | 0.425978 |
| C | -0.860345 | -0.426995 | 0.249741 |
| C | 0.406965  | -0.541433 | 1.004051 |
| O | -2.772191 | 0.953715  | -0.151915 |
| H | 0.456060  | 0.190401  | 1.812304 |
| H | 0.564669  | -1.535271 | 1.433210 |
| C | 1.658696  | 1.368886  | -0.587140 |
| H | 0.705627  | 1.412255  | -1.111708 |
| H | 1.642734  | 2.071411  | 0.245489 |
| H | 2.464138  | 1.636058  | -1.267346 |
| S | 1.956372  | -0.306439 | -0.001182 |
| H | -1.296041 | 1.380926  | 1.190452 |
| C | -1.180339 | -1.491547 | -0.757491 |
| H | -2.206382 | -1.380245 | -1.107898 |
| H | -0.523495 | -1.452465 | -1.634956 |
| H | -1.070025 | -2.497080 | -0.336144 |

1_methylacrolein_HEI_3

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.442564 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.343355 |

Number of Imaginary Frequencies

0

Frequencies (Top 3 out of 42)

1. 62.3601 cm⁻¹
2. 82.7731 cm⁻¹
3. 144.6139 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
1_methylacrolein_HEI_4_reopt

| Datum | Value  |
|-------|--------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy       | -669.443215 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.344318 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 42)

1. 50.2597 cm⁻¹
2. 81.4307 cm⁻¹
3. 140.8306 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 2.235860 | 0.072582 | -0.151597 |
| C     | 0.964323 | 0.492579 | 0.134320  |
| C     | -0.027166| -0.461948| 0.692018  |
| O     | 2.756127 | -1.090943| -0.019166 |
| H     | 0.455038 | -1.419112| 0.884679  |
| H     | -0.484337| -0.114011| 1.624474  |
| C     | -2.656329| 0.387587 | 0.167788  |
| H     | -2.865360| 0.259328 | 1.228514  |
| H     | -2.284933| 1.393975 | -0.010604 |
| H     | -3.577123| 0.242388 | -0.393249 |
| S     | -1.473263| -0.856007| -0.392850 |
| H     | 2.892449 | 0.876486 | -0.547250 |
| C     | 0.516763 | 1.899130 | -0.131382 |
| H     | -0.243814| 1.955363 | -0.920206 |
| H     | 1.357471 | 2.519571 | -0.449445 |
| H     | 0.073107 | 2.370083 | 0.755144  |
1_methylacrolein_HEI_5

| Datum                                                      | Value                          |
|-------------------------------------------------------------|-------------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -669.444643                   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.345843                   |
| Number of Imaginary Frequencies                             |                               |
| Frequencies (Top 3 out of 42)                               |                               |
| 1. 64.5044 cm⁻¹                                            |                               |
| 2. 69.2061 cm⁻¹                                            |                               |
| 3. 133.8647 cm⁻¹                                           |                               |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C               | -2.088236 | -0.559327 | -0.117311 |
|-----------------|----------|----------|----------|
| C               | -1.173400| 0.409488 | 0.194917 |
| C               | 0.165717 | 0.022546 | 0.711318 |
| O               | -1.969358| -1.831206| -0.033272|
| H               | 0.532826 | 0.713664 | 1.475398 |
| H               | 0.144345 | -0.987481| 1.119428 |
| C               | 2.917060 | -0.282987| 0.340933 |
| H               | 3.072588 | 0.508170 | 1.072921 |
| H               | 2.843618 | -1.240922| 0.853491 |
| H               | 3.765749 | -0.308710| -0.338955|
| S               | 1.428250 | 0.034702 | -0.628735|
| H               | -3.059344| -1.63550 | -0.482730|
| C               | -1.454308| 1.871485 | 0.000777 |
| H               | -1.363486| 2.442057 | 0.933019 |
| H               | -2.467571| 2.022495 | -0.377883|
| H               | -0.766853| 2.341455 | -0.712555|
1_methylacrolein_HEI_6_reopt

| Datum                                                                 | Value               |
|-----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -669.443215         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -669.344319         |
| Number of Imaginary Frequencies                                       | 0                   |

**Frequencies (Top 3 out of 42)**

1. 50.1842 cm⁻¹  
2. 81.4468 cm⁻¹  
3. 140.8596 cm⁻¹  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

1_methylacrolein_HEI_7

| Datum                                                                 | Value               |
|-----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -669.444692         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -669.346248         |
| Number of Imaginary Frequencies                                       | 0                   |
**Frequencies (Top 3 out of 42)**

1. 59.2241 cm\(^{-1}\)
2. 72.6788 cm\(^{-1}\)
3. 118.4455 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 1.962181 | -0.818063 | 0.065785 |
|-------|----------|-----------|----------|
| C     | 1.029423 | 0.160290  | 0.288614 |
| C     | -0.344473| -0.205295 | 0.715228 |
| O     | 3.175515 | -0.703444 | -0.319545|
| H     | -0.40133 | -1.251513 | 1.020228 |
| H     | -0.710956| 0.416140  | 1.538988 |
| C     | -3.102648| -0.271184 | 0.271192 |
| H     | -3.109420| -1.275338 | 0.692517 |
| H     | -3.216720| 0.458093  | 1.071867 |
| H     | -3.936591| -0.171399 | -0.419736|
| S     | -1.575236| 0.044644  | -0.643474|
| H     | 1.588436 | -1.845949 | 0.262172 |
| C     | 1.340174 | 1.615847  | 0.087960 |
| H     | 2.413968 | 1.753878  | -0.039338|
| H     | 0.845355 | 2.043307  | -0.791747|
| H     | 1.018415 | 2.219349  | 0.944321 |

**1_methylacrolein_HEI_8**

| Datum                                                      | Value        |
|------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -669.438669  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.34      |

**Frequencies (Top 3 out of 42)**

1. 60.7119 cm\(^{-1}\)
2. 85.7641 cm\(^{-1}\)
3. 149.4392 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
1_methylacrolein_min

| Datum                                           | Value                  |
|------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -231.218956            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -231.154806 |
| Number of Imaginary Frequencies                 | 0                      |

Frequencies (Top 3 out of 27)

1. 88.3416 cm⁻¹
2. 158.9962 cm⁻¹
3. 288.8251 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.384897 | 1.454325 | -0.000007 |
|-------|----------|----------|-----------|
| H     | -0.564562| 1.973557 | -0.000008 |
| H     | 1.290019 | 2.047147 | -0.000010 |
| C     | 0.422966 | 0.125783 | -0.000001 |
| C     | -0.861391| -0.630657| 0.000003  |
| H     | -0.756462| -1.730282| 0.000008  |
| O     | -1.958598| -0.129084| 0.000002  |
| C     | 1.673998 | -0.698832| 0.000002  |
| H     | 1.708908 | -1.347060| 0.877592  |
### 1_methylacrolein_TS_1

**Datum** | **Value**
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.429165
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.332207
Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 42)

1. 160.4792 cm⁻¹
2. 66.9159 cm⁻¹
3. 73.3202 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C      | -1.779610 | -0.679458 | -0.278568 |
| C      | -1.142745 | 0.511158  | 0.232828  |
| C      | -0.335587 | 0.407860  | 1.319810  |
| O      | -1.681290 | -1.814503 | 0.177600  |
| H      | 0.066465  | 1.286246  | 1.802068  |
| H      | -0.289221 | -0.520547 | 1.868464  |
| C      | 1.539673  | -0.429006 | -1.267330 |
| H      | 1.770802  | -1.461114 | -1.532323 |
| H      | 0.449732  | -0.309333 | -1.323453 |
| H      | 1.980071  | 0.225185  | -2.020187 |
| S      | 2.111996  | -0.015641 | 0.395356  |
| H      | -2.421074 | -0.516818 | -1.166555 |
| C      | -1.277437 | 1.798046  | -0.533586 |
| H      | -1.474132 | 2.641808  | 0.128626  |
| H      | -2.090981 | 1.745551  | -1.258523 |
| H      | -0.358320 | 2.023702  | -1.083534 |

### 1_methylacrolein_TS_2

**Datum**

| Datum | Value |
--- | --- |

### 1-methylacrolein_TS_3_reopt

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.423398 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.327402 |

#### Frequencies (Top 3 out of 42)

1. -186.9039 cm⁻¹
2. 28.5678 cm⁻¹
3. 74.8581 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          | x    | y    | z    |
|----------|------|------|------|
| C        | -1.666722 | 0.586483 | 0.622399 |
| C        | -0.968121  | -0.583774 | 0.202601 |
| C        | 0.074482   | -1.030555 | 0.973662 |
| O        | -2.617990  | 1.115221  | 0.040742 |
| H        | 0.246239   | -0.581410 | 1.942369 |
| H        | 0.474728   | -2.023844 | 0.837044 |
| C        | 1.527322   | 1.340978  | -0.588757 |
| H        | 0.433621   | 1.277441  | -0.522964 |
| H        | 1.845892   | 2.224661  | -0.036460 |
| H        | 1.787185   | 1.479118  | -1.637941 |
| S        | 2.244000   | -0.173924 | 0.0880155 |
| H        | -1.308684  | 1.021860  | 1.575472 |
| C        | -1.329073  | -1.215272 | -1.109084 |
| H        | -2.409959  | -1.312964 | -1.218519 |
| H        | -0.978072  | -0.608100 | -1.949666 |
| H        | -0.878347  | -2.202912 | -1.202683 |

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### SI_aldehydes.md

#### Datum

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.433075 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.33653 |

#### Number of Imaginary Frequencies

1

#### Frequencies (Top 3 out of 42)

1. -186.9039 cm⁻¹
2. 28.5678 cm⁻¹
3. 74.8581 cm⁻¹
1. -226.3737 cm\(^{-1}\)
2. 25.6547 cm\(^{-1}\)
3. 72.8376 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

\[
\begin{array}{rrr}
C & 2.252621 & -0.229025 & -0.263867 \\
C & 1.144823 & 0.535661 & 0.230660 \\
C & 0.214566 & -0.085750 & 1.016507 \\
O & 2.442710 & -1.436200 & -0.112445 \\
H & 0.424853 & -1.074591 & 1.396367 \\
H & -0.527032 & 0.492131 & 1.551289 \\
C & -2.634899 & 0.641892 & -0.015815 \\
H & -2.939843 & 0.753491 & 1.025600 \\
H & -1.981917 & 1.479479 & -0.264946 \\
H & -3.528654 & 0.713975 & -0.634842 \\
S & -1.782338 & -0.944314 & -0.285101 \\
H & 3.002610 & 0.355232 & -0.832502 \\
C & 0.977870 & 1.952918 & -0.244533 \\
H & 0.408167 & 2.002628 & -1.177626 \\
H & 1.943291 & 2.426543 & -0.431737 \\
H & 0.444367 & 2.555558 & 0.491866 \\
\end{array}
\]

**1_methylacrolein_TS_4_reopt**

| Datum                                               | Value       |
|-----------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy               | -669.433075 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.336534 |

Number of Imaginary Frequencies

1

**Frequencies (Top 3 out of 42)**

1. -186.9448 cm\(^{-1}\)
2. 28.3226 cm\(^{-1}\)
3. 75.0938 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
1_methylacrolein_TS_5

| Datum                                                                 | Value      |
|----------------------------------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.423712 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.328152 |
| Number of Imaginary Frequencies                                      | 1          |
| **Frequencies** (Top 3 out of 42)                                    |            |
| 1. -202.4437 cm⁻¹                                                   |            |
| 2. 27.4233 cm⁻¹                                                     |            |
| 3. 58.9429 cm⁻¹                                                     |            |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C  | -2.127813 | -0.759451 | -0.155647 |
| C  | -1.372688 | 0.383551  | 0.268626  |
| C  | -0.135735 | 0.190073  | 0.816528  |
| O  | -1.767428 | -1.936111 | -0.119244 |
| H  | 0.389147  | 1.006887  | 1.292498  |
| H  | 0.169856  | -0.808242 | 1.095521  |
| C  | 2.895308  | -0.287622 | 0.620369  |
| H  | 2.521287  | 0.155655  | 1.546932  |
| H  | 2.924200  | -1.368780 | 0.757392  |
| H  | 3.916794  | 0.062267  | 0.475798  |
### 1_methylacrolein_TS_6_reopt

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.433075    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.336531    |
| Number of Imaginary Frequencies                                      | 1              |
| **Frequencies** (Top 3 out of 42)                                     |                |
| 1.                                                                 | -186.9112 cm⁻¹ |
| 2.                                                                 | 28.5351 cm⁻¹   |
| 3.                                                                 | 74.8778 cm⁻¹   |

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|        |             |             |             |
|--------|-------------|-------------|-------------|
| C      | -1.666826   | 0.586302    | -0.622487   |
| C      | -0.968104   | -0.583846   | -0.202533   |
| C      | 0.074418    | -1.030701   | -0.973643   |
| O      | -2.618052   | 1.115117    | -0.040849   |
| H      | 0.474774    | -2.023926   | -0.836885   |
| H      | 0.246091    | -0.581672   | -1.942421   |
| C      | 1.527154    | 1.340975    | 0.588777    |
| H      | 0.433469    | 1.277398    | 0.522795    |
| H      | 1.786837    | 1.478961    | 1.638027    |
| H      | 1.845772    | 2.224762    | 0.036673    |
| S      | 2.244013    | -0.173786   | -0.080269   |
| H      | -1.308912   | 1.021490    | -1.575693   |
| C      | -1.328759   | -1.215092   | 1.109350    |
| H      | -2.409665   | -1.311624   | 1.219550    |
| H      | -0.878999   | -2.203213   | 1.202546    |
| H      | -0.976467   | -0.608369   | 1.949723    |

### 1_methylacrolein_TS_7_reopt
| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.427905|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -669.332021|
| Number of Imaginary Frequencies                                       | 1           |
| **Frequencies** (Top 3 out of 42)                                     |             |
| 1. -223.8011 cm⁻¹                                                   |             |
| 2.  48.7662 cm⁻¹                                                    |             |
| 3.  64.3882 cm⁻¹                                                    |             |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C          | C          | C          | O          | H          | H          | H          | H          | C          | S          | H          | C          | H          | H          | H          |
|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|   | 1.990916   | -0.894101  | 0.126105   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | 1.179836   | 0.248374   | 0.358277   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | -0.091800  | 0.051568   | 0.847503   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | 0.315343   | -0.227880  | 0.508109   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | -2.750504  | 0.115789   | 1.465339   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | -4.042451  | 0.363620   | 0.293376   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | -3.456958  | -1.267260  | 0.629419   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | -1.901265  | -0.041172  | -0.793804  | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | 1.530770   | -1.857160  | 0.421305   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | 1.683063   | 1.600396   | -0.054859  | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | 2.704372   | 1.767234   | 0.291019   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | 1.698255   | 1.706942   | -1.144105  | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |
|   | 1.049030   | 2.390999   | 0.346249   | 3.131717   | -0.897468  | 0.126105   | 0.126105   | -0.897468  | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.894101  | 0.126105   | -0.897468  |

**1_methylacrolein_TS_8_reopt**

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.427926|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -669.331687|
| Number of Imaginary Frequencies                                       | 1           |
| **Frequencies** (Top 3 out of 42)                                     |             |
| 1.  -223.8011 cm⁻¹                                                  |             |
| 2.   48.7662 cm⁻¹                                                  |             |
| 3.   64.3882 cm⁻¹                                                  |             |
1.  -223.6741 cm⁻¹
2.    47.6865 cm⁻¹
3.    63.0025 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |          |          |
|----------|----------|----------|
| C        | 2.016968 | -0.852783| 0.207117 |
| C        | 1.171804 | 0.282539 | 0.332755 |
| C        | -0.093846| 0.094305 | 0.838226 |
| O        | 3.158522 | -0.866983| -0.265214|
| H        | -0.345896| -0.856214| 1.291119 |
| H        | -0.677926| 0.939016 | 1.176573 |
| C        | -3.138727| -0.032106| 0.530234 |
| H        | -3.423566| 1.012537 | 0.655673 |
| H        | -4.039509| -0.606065| 0.317367 |
| H        | -2.736312| -0.386606| 1.482907 |
| S        | -1.902846| -0.237735| -0.785168|
| H        | 1.584252 | -1.797243| 0.590533 |
| C        | 1.634424 | 1.604833 |-0.204276 |
| H        | 0.994945 | 2.413966 | 0.148313 |
| H        | 2.661122 | 1.818659 | 0.096333 |
| H        | 1.616509 | 1.620855 | -1.298753|

2_crotonaldehyde_conf2_min

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -231.22527 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -231.160531 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 27)

1.  126.4104 cm⁻¹
2.  201.8334 cm⁻¹
3.  215.7423 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### 2_crotonaldehyde_HEI-1

| Datum                                      | Value               |
|--------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -669.447041         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.347856         |
| Number of Imaginary Frequencies            | 0                   |
| **Frequencies (Top 3 out of 42)**          |                     |
| 1. 41.3776 cm⁻¹                            |                     |
| 2. 76.1837 cm⁻¹                            |                     |
| 3. 160.6684 cm⁻¹                           |                     |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -2.090259 | 0.058779 | 0.390104 |
| C | -0.892238 | 0.648011 | 0.700559 |
| C | 0.236079  | 0.750750 | -0.255128 |
| O | -2.455476 | -0.488250 | -0.703059 |
| H | -0.753258 | 1.053837 | 1.697348 |
| H | -0.122801 | 0.509511 | -1.256328 |
| C | 0.672105  | -2.011146 | 0.001769 |
| H | -0.228935 | -1.908131 | 0.605208 |
| H | 0.397324  | -2.253790 | -1.023247 |
| H | 1.298512  | -2.803968 | 0.404559 |
| S | 1.601811  | -0.472235 | 0.077744 |
| H | -2.831776 | 0.081216 | 1.215152 |
| C | 0.912631  | 2.117565 | -0.256241 |
| H | 1.264872  | 2.366161 | 0.746881 |
2_crotonaldehyde_HEI-2

| Datum                                                                 | Value                  |
|-----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.439061            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.340034            |
| Number of Imaginary Frequencies                                       | 0                      |

**Frequencies (Top 3 out of 42)**

1. 53.0826 cm⁻¹
2. 98.2506 cm⁻¹
3. 152.5675 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C        | 1.765393 | -0.257856 | -0.266316 |
|----------|----------|-----------|-----------|
| C        | 1.021599 | 0.517816  | 0.574869  |
| C        | -0.450360| 0.812291  | 0.482545  |
| O        | 3.028781 | -0.474621 | -0.243485 |
| H        | 1.533541 | 1.027615  | 1.389353  |
| H        | -0.883315| 0.797328  | 1.488030  |
| C        | -1.121975| -1.907521 | 0.444332  |
| H        | -0.091787| -2.228664 | 0.310611  |
| H        | -1.320843| -1.755163 | 1.504208  |
| H        | -1.797126| -2.669955 | 0.061648  |
| S        | -1.445114| -0.391823 | -0.471034 |
| H        | 1.185791 | -0.767503 | -1.060483 |
| C        | -0.759173| 2.182088  | -0.129621 |
| H        | -1.825952| 2.413884  | -0.098441 |
| H        | -0.420854| 2.213975  | -1.166906 |
| H        | -0.220777| 2.953719  | 0.421545  |

2_crotonaldehyde_HEI-3

| Datum | Value |
|-------|-------|
|       |       |
| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.443351 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.344361 |

Number of Imaginary Frequencies: 0

**Frequencies (Top 3 out of 42)**

1. 40.4011 cm⁻¹
2. 71.5523 cm⁻¹
3. 168.9786 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | -2.183815 | -0.133830 | -0.290819 |
| C       | -1.022022 | 0.179187  | 0.363074  |
| C       | 0.158007  | 0.755642  | -0.329338 |
| O       | -3.264728 | -0.623308 | 0.173558  |
| H       | -0.948705 | 0.007317  | 1.433961  |
| H       | -0.133537 | 1.079784  | -1.331124 |
| C       | 1.775477  | -1.220644 | 0.881305  |
| H       | 2.170601  | -0.493627 | 1.588379  |
| H       | 0.847424  | -1.639978 | 1.266017  |
| H       | 2.503542  | -2.018908 | 0.755892  |
| S       | 1.497659  | -0.485618 | -0.739588 |
| H       | -2.157390 | 0.087487  | -1.381189 |
| C       | 0.784587  | 1.929535  | 0.419192  |
| H       | 1.639989  | 2.342270  | -0.115038 |
| H       | 1.118421  | 1.616058  | 1.410081  |
| H       | 0.041540  | 2.716600  | 0.557477  |

**2_crotonaldehyde_HEI-4**

| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.442746 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.343168 |

Number of Imaginary Frequencies: 0

**Frequencies (Top 3 out of 42)**


1. 62.2852 cm⁻¹
2. 86.6997 cm⁻¹
3. 155.7593 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| C | -1.993369 | -0.092694 | 0.173908 |
| C | -1.002727 | 0.133431 | -0.743480 |
| C | 0.269698 | 0.860144 | -0.487598 |
| O | -3.090530 | -0.729015 | 0.012647 |
| H | -1.120607 | -0.291997 | -1.736947 |
| H | 0.509820 | 1.513435 | -1.330642 |
| C | 1.404346 | -1.330234 | 0.873840 |
| H | 1.680093 | -0.858000 | 1.814253 |
| H | 0.337109 | -1.557612 | 0.873194 |
| H | 1.968178 | -2.252977 | 0.759994 |
| S | 1.762202 | -0.272484 | -0.538667 |
| H | -1.818751 | 0.345119 | 1.175773 |
| C | 0.319469 | 1.692668 | 0.788282 |
| H | 1.259616 | 2.239122 | 0.848546 |
| H | 0.234427 | 1.068197 | 1.677345 |
| H | -0.505386 | 2.406692 | 0.806277 |

**2_crotonaldehyde_HEI-5**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.445342 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.346054 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 42)

1. 42.7298 cm⁻¹
2. 74.1069 cm⁻¹
3. 160.8299 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
2_crotonaldehyde_HEI-6

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -669.446501   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.347102   |
| Number of Imaginary Frequencies            | 0             |

Frequencies (Top 3 out of 42)

1. 61.4940 cm⁻¹  
2. 74.0728 cm⁻¹  
3. 157.8426 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 2.394361 | -0.166161 | -0.187353 |
|-----|---------|-----------|-----------|
| C   | 1.313484 | 0.605146  | -0.526904 |
| C   | 0.022249 | 0.554474  | 0.212180  |
| O   | 2.495779 | -1.020888 | 0.752971  |
| H   | 1.392822 | 1.280258  | -1.371718 |
| H   | 0.196898 | 1.49488  | 1.211077  |
| C   | -2.513248 | -0.719141 | 0.482288  |
| H   | -2.188154 | -0.827045 | 1.516625  |
| H   | -3.124688 | 0.175048  | 0.384435  |
| H   | -3.112469 | -1.586064 | 0.211551  |
2_crotonaldehyde_HEI-7

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -669.445    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.345987 |
| Number of Imaginary Frequencies                           | 0           |

Frequencies (Top 3 out of 42)

1. 66.3520 cm⁻¹
2. 77.1418 cm⁻¹
3. 158.6728 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     |          |          |          |
|-----|----------|----------|----------|
| C   | 2.289980 | -0.253060 | 0.371236 |
| C   | 1.258574 | 0.299781 | -0.339834 |
| C   | -0.097661 | 0.502814 | 0.238505 |
| O   | 3.486044 | -0.491564 | 0.004462 |
| H   | 1.409569 | 0.588152 | -1.377437 |
| H   | -0.058463 | 0.365086 | 1.322029 |
| C   | -2.787173 | -0.471063 | 0.400638 |
| H   | -2.642182 | -0.274620 | 1.462482 |
| H   | -3.278398 | 0.380898 | -0.063760 |
| H   | -3.423299 | -1.347040 | 0.291324 |
| S   | -1.201089 | -0.849157 | -0.382484 |
| H   | 2.020470 | -0.514385 | 1.418838 |
| C   | -0.696003 | 1.866863 | -0.082173 |
| H   | -1.698876 | 1.990436 | 0.326857 |
| H   | -0.745704 | 2.009625 | -1.163125 |
| H   | -0.060350 | 2.648848 | 0.336601 |

2_crotonaldehyde_HEI-8
| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.442516 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.342601 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 42)

1. 78.4562 cm⁻¹
2. 91.4444 cm⁻¹
3. 179.3331 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -1.944143 | -0.408179 | -0.529983 |
|-------|-----------|-----------|-----------|
| C     | -0.922407 | 0.328764  | -1.073463 |
| C     | 0.195260  | 0.995486  | -0.344503 |
| O     | -2.198091 | -0.706656 | 0.683348  |
| H     | -0.898210 | 0.397118  | -2.155403 |
| H     | 0.540079  | 1.852672  | -0.927569 |
| C     | 1.146566  | -1.511297 | 0.504344  |
| H     | 1.014858  | -1.353312 | 1.572760  |
| H     | 0.193085  | -1.789240 | 0.057283  |
| H     | 1.875517  | -2.303211 | 0.346975  |
| S     | 1.756246  | -0.027149 | -0.315251 |
| H     | -2.652996 | -0.788693 | -1.296675 |
| C     | -0.129194 | 1.475270  | 1.066646  |
| H     | -0.338334 | 0.634563  | 1.722575  |
| H     | 0.698372  | 2.057192  | 1.473021  |
| H     | -1.024071 | 2.100282  | 1.046005  |

**2_crotonaldehyde_min**

| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -231.221346 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -231.156905 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

1. 78.4562 cm⁻¹
2. 91.4444 cm⁻¹
3. 179.3331 cm⁻¹
1. 127.4799 cm⁻¹
2. 207.2556 cm⁻¹
3. 210.2038 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C          | H           | O           |
|---|------------|-------------|-------------|
| 1 | 0.833395   | -0.300960   | 0.000005    |
| 2 | 0.459425   | -1.320761   | 0.000064    |
| 3 | -0.062330  | 0.686072    | -0.000036   |
| 4 | 0.243512   | 1.725503    | -0.000095   |
| 5 | -1.509582  | 0.414698    | -0.000000   |
| 6 | -2.159499  | 1.305108    | -0.000036   |
| 7 | -2.006005  | -0.690078   | 0.000064    |
| 8 | 2.309102   | -0.118985   | -0.000026   |
| 9 | 2.747323   | -0.603514   | 0.874603    |
|10 | 2.747296   | -0.603598   | -0.874621   |
|11 | 2.586470   | 0.932936    | -0.000081   |

2_crotonaldehyde_TS-1-0

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -669.430976    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.333262 |
| Number of Imaginary Frequencies            | 1              |

Frequencies (Top 3 out of 42)

|   |   |
|---|---|
| 1 | -164.5178 cm⁻¹ |
| 2 | 72.4989 cm⁻¹   |
| 3 | 85.5952 cm⁻¹   |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C          |   |
|---|------------|---|
| 1 | -2.041327  | -0.543778 |
| 2 | -1.188109  | 0.536885 |
| 3 | -0.338169  | 1.141408 |
| 4 | -2.123236  | -1.036449 |
| 5 | -1.199129  | 0.824279 | 1.697810 |
### 2_crotonaldehyde_TS-2-1_reopt

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.428939 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -669.330865 |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 42)

1. -197.1535 cm⁻¹
2. 64.4987 cm⁻¹
3. 91.3577 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C         | -2.004658  | -0.225343 | 0.182474 |
|-----------|------------|-----------|----------|
| C         | -1.127216  | 0.319156  | -0.793124 |
| C         | -0.060881  | 1.135563  | -0.492229 |
| O         | -2.975071  | -0.956437 | -0.045429 |
| H         | -1.307723  | 0.036803  | -1.824450 |
| H         | 0.405180   | 1.658087  | -1.315076 |
| C         | 1.317780   | -1.405252 | 0.738126  |
| H         | 0.223793   | -1.343074 | 0.671748  |
| H         | 1.598239   | -2.438067 | 0.534562  |
| H         | 1.610215   | -1.168995 | 1.761417  |
| S         | 2.051365   | -0.269555 | -0.459212 |
| H         | -1.799569  | 0.061146  | 1.229105  |
| C         | 0.150331   | 1.748064  | 0.866344  |
| H         | 1.079334   | 2.309987  | 0.891878  |
| H         | 0.192597   | 0.990892  | 1.648411  |
| H         | -0.675479  | 2.424373  | 1.103692  |
2_crotonaldehyde_TS-3-1

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.432504            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.335085            |
| Number of Imaginary Frequencies                                      | 1                      |

**Frequencies** (Top 3 out of 42)

1. -183.7478 cm⁻¹  
2. 47.6205 cm⁻¹  
3. 88.0625 cm⁻¹  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C          | 2.025929 | -0.222633 | 0.322221 |
| C          | 1.102338 | 0.651269  | -0.315544|
| C          | -0.008035| 1.107314  | 0.348423 |
| O          | 3.071038 | -0.668685 | -0.155393|
| H          | 1.289700 | 0.935544  | -1.345990|
| H          | -0.077872| 0.876989  | 1.404549 |
| C          | -0.924515| -1.988573 | -0.121017|
| H          | -1.244815| -2.619976 | -0.949462|
| H          | 0.112390 | -1.690132 | -0.315834|
| H          | -0.938716| -2.587955 | 0.789302 |
| S          | -1.945054| -0.504805 | 0.018098 |
| H          | 1.752977 | -0.494863 | 1.361371 |
| C          | -0.774008| 2.308209  | -0.116104|
| H          | -1.771939| 2.341073  | 0.314930 |
| H          | -0.859452| 2.318991  | -1.201891|
| H          | -0.239963| 3.213163  | 0.188733 |

2_crotonaldehyde_TS-4-0

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.428939            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.330865            |
**Datum** | **Value**
--- | ---
Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 42)

1. -197.1970 cm⁻¹  
2. 64.4652 cm⁻¹  
3. 91.3721 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| C | -2.004616 | 0.225299 | 0.182401 |
| C | -1.127123 | 0.319075 | -0.793197 |
| C | -0.060777 | 1.135506 | -0.492346 |
| O | -2.975049 | -0.956399 | -0.045462 |
| H | -1.307589 | 0.036629 | -1.824505 |
| H | 0.405238 | 1.657958 | -1.315262 |
| C | 1.317773 | -1.405203 | 0.738348 |
| H | 1.610508 | -1.169044 | 1.761573 |
| H | 0.237778 | -1.342825 | 0.672239 |
| H | 1.598000 | -2.438056 | 0.534660 |
| S | 2.051252 | -0.269590 | -0.459125 |
| H | -1.799576 | 0.061303 | 1.229011 |
| C | 0.150342 | 1.748111 | 0.866200 |
| H | 1.079359 | 2.310005 | 0.891772 |
| H | 0.192528 | 0.991069 | 1.648313 |
| H | -0.675468 | 2.424457 | 1.103446 |

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**2_crotonaldehyde_TS-5-0**

| Datum | Value |
|---|---|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.430976 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.333263 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 42)

1. -164.3790 cm⁻¹  
2. 72.4706 cm⁻¹  
3. 85.5731 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | -2.041107 | -0.544644 | 0.258355 |
| C    | -1.188432 | 0.536460  | 0.652745 |
| C    | -0.338882 | 1.141403  | -0.227766 |
| O    | -2.122708 | -1.037238 | -0.866350 |
| H    | -1.199601 | 0.823825  | 1.697864 |
| H    | -0.451069 | 0.886082  | -1.272387 |
| C    | 1.141489  | -1.742593 | 0.580133 |
| H    | 1.799982  | -2.047051 | 1.393506 |
| H    | 0.181286  | -1.448987 | 1.023938 |
| H    | 0.962252  | -2.608793 | -0.057452 |
| S    | 1.820682  | -0.345293 | -0.341462 |
| H    | -2.679304 | -0.955360 | 1.062597 |
| C    | 0.366263  | 2.424046  | 0.081407 |
| H    | 0.649431  | 2.473468  | 1.132194 |
| H    | 1.257644  | 2.549119  | -0.528499 |
| H    | -0.305853 | 3.262259  | -0.126813 |

2_crotonaldehyde_TS-6-1

| Datum                                                                 | Value   |
|-----------------------------------------------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -669.426361 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.329209 |
| Number of Imaginary Frequencies                                      | 1       |

Frequencies (Top 3 out of 42)

1. -221.2025 cm\(^{-1}\)
2. 61.6153 cm\(^{-1}\)
3. 88.3603 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 2.484692 | -0.375707 | -0.130261 |
| C    | 1.574201 | 0.688233  | -0.393812 |
| C    | 0.366532 | 0.794523  | 0.249806 |
| O    | 2.313521 | -1.314873 | 0.650780 |
### 2_crotonaldehyde_TS-7-0

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.427889 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.330708 |

**Number of Imaginary Frequencies** 1

**Frequencies** (Top 3 out of 42)

1.  -231.3141 cm⁻¹
2.   58.7215 cm⁻¹
3.   84.2343 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 2.311382 | -0.431483 | 0.368312 |
|-------|----------|-----------|----------|
| C     | 1.457324 | 0.521032  | -0.237834|
| C     | 0.191318 | 0.747292  | 0.259643 |
| O     | 3.455051 | -0.735925 | 0.017068 |
| H     | 1.797248 | 1.029507  | -1.133824|
| H     | -0.03906 | 0.327393  | 1.232849 |
| C     | -2.767705| -0.440908 | 0.629090 |
| H     | -2.318232| 0.040674  | 1.502855 |
| H     | -3.480318| 0.259619  | 0.193091 |
| H     | -3.320446| -1.310792 | 0.982368 |
| S     | -1.473408| -0.915830 | -0.553753|
| H     | 1.875530 | -0.934892 | 1.254896 |
| C     | -0.577209| 1.975214  | -0.127140|
| H     | -1.631163| 1.899609  | 0.126603 |
### 2_crotonaldehyde_TS-8-0

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.426801 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.32931 |
| Number of Imaginary Frequencies | 1 |

#### Frequencies (Top 3 out of 42)

1. -164.8974 cm⁻¹
2. 33.7760 cm⁻¹
3. 68.1241 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | -1.851664 | -0.974747 | -0.193688 |
| C   | -1.016642 | -0.200989 | -1.058995 |
| C   | -0.383925 | 0.971942  | -0.735455 |
| O   | -2.163129 | -0.733047 | 0.973127  |
| H   | -0.822456 | -0.644212 | -2.028258 |
| H   | 0.145227  | 1.465105  | -1.539412 |
| C   | 1.704841  | -1.464870 | 0.135839  |
| H   | 1.757681  | -1.895387 | 1.135744  |
| H   | 0.701093  | -1.669579 | -0.261656 |
| H   | 2.424768  | -1.982315 | -0.497319 |
| S   | 1.979558  | 0.320527  | 0.158185  |
| H   | -2.248597 | -1.897088 | -0.660114 |
| C   | -0.745929 | 1.853330  | 0.422190  |
| H   | -0.848981 | 1.287024  | 1.341278  |
| H   | -0.001305 | 2.634436  | 0.557136  |
| H   | -1.710614 | 2.329954  | 0.217272  |

### 3_4-methyl-2-pentenal_1

| Datum | Value |
|-------|-------|

---
| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -309.842254 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.723854 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 45)**

1. 77.0282 cm⁻¹
2. 150.5143 cm⁻¹
3. 153.7262 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| C   | 2.289949| -0.359574| -0.058781|
| C   | 0.956989| 0.238206 | -0.017555|
| C   | -0.100594| -0.478274| -0.402997|
| C   | -1.530482| -0.041565| -0.406826|
| C   | -2.352749| -1.004162| 0.458880 |
| O   | 3.306627| 0.209048 | 0.272222 |
| C   | -1.731375| 1.401999 | 0.030064 |
| H   | 2.326229| -1.402002| -0.422480|
| H   | 0.881571| 1.260677 | 0.331574 |
| H   | 0.074726| -1.499360| -0.737199|
| H   | -1.881877| -0.151853| -1.438741|
| H   | -3.410907| -0.751846| 0.398378 |
| H   | -2.226264| -2.037124| 0.135264 |
| H   | -2.041898| -0.931186| 1.502257 |
| H   | -2.786740| 1.665976 | -0.027245|
| H   | -1.406055| 1.540235 | 1.063022 |
| H   | -1.172241| 2.094319 | -0.599316|

**3_4-methyl-2-pentenal_2**

| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -309.841991 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.724126 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 45)**
1. 55.6678 cm⁻¹
2. 144.8724 cm⁻¹
3. 153.5429 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -1.444070 | -1.873389 | 0.000000 |
| C    | -0.185809  | -1.130521 | 0.000000 |
| C    | -0.197408  |  0.202975 | -0.000000 |
| C    |  1.002775  |  1.090996 | -0.000000 |
| C    |  1.002775  |  1.963360 |  1.258037 |
| O    | -1.527196  | -3.081552 |  0.000000 |
| C    |  1.002775  |  1.963360 | -1.258037 |
| H    | -2.356094  | -1.250250 |  0.000000 |
| H    |  0.736229  | -1.700756 |  0.000000 |
| H    | -1.161407  |  0.711773 | -0.000000 |
| H    |  1.897473  |  0.465226 | -0.000000 |
| H    |  1.873570  |  2.618953 |  1.258648 |
| H    |  0.107866  |  2.587915 |  1.287333 |
| H    |  1.026132  |  1.355999 |  2.162160 |
| H    |  1.026132  |  1.355999 | -2.162160 |
| H    |  0.107866  |  2.587915 | -1.287333 |

### 3_4-methyl-2-pentenal_3_2

| Datum                                      | Value      |
|--------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -309.838276|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.720113|
| Number of Imaginary Frequencies            | 0          |

### Frequencies (Top 3 out of 45)

1. 71.4940 cm⁻¹
2. 119.9612 cm⁻¹
3. 170.1273 cm⁻¹
3_4-methyl-2-pentenal_4

| Datum                               | Value               |
|-------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -309.838039        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.720504        |
| Number of Imaginary Frequencies     | 0                   |

**Frequencies** (Top 3 out of 45)

1. 57.1896 cm⁻¹
2. 95.2675 cm⁻¹
3. 148.8433 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | 2.370651 | 0.368677 | 0.211938 |
|---------|----------|----------|----------|
| C       | 0.925911 | 0.648440 | 0.135694 |
| C       | 0.065838 | -0.266758| -0.312251|
| C       | -1.418363| -0.123808| -0.422682|
| C       | -2.093320| -1.235040| 0.391195 |
| O       | 2.892982 | -0.673097| -0.117128|
| C       | -1.938386| 1.247937 | -0.018953|
| H       | 2.992377 | 1.191238 | 0.602121 |
| H       | 0.604590 | 1.629659 | 0.460483 |
| H       | 0.472411 | -1.228514| -0.616147|
| H       | -1.664946| -0.299324| -1.475982|
| H       | -3.173357| -1.199640| 0.251552 |
| H       | -1.739331| -2.220376| 0.088576 |
| H       | -1.880728| -1.105947| 1.453661 |
| H       | -3.018400| 1.292977 | -0.154764|
| H       | -1.723607| 1.446969 | 1.032855 |
| H       | -1.880728| 1.292977 | -0.154764|
| H       | -1.486847| 2.041052 | -0.614974|
### 3_4-methyl-2-pentenal_5

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -309.842254   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.723854 |
| Number of Imaginary Frequencies            | 0             |

#### Frequencies (Top 3 out of 45)

1. 77.0283 cm\(^{-1}\)
2. 150.5142 cm\(^{-1}\)
3. 153.7262 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -2.289949 | -0.359574 | -0.058780 |
| C | -0.956990 | 0.238206  | -0.017557 |
| C | 0.100594  | -0.478275 | -0.402996 |
| C | 1.530481  | -0.041565 | -0.406826 |
| C | 1.731374  | 1.401999  | 0.030065  |
| O | -3.306628 | 0.209048  | 0.272222  |
| C | 2.352750  | -1.004162 | 0.458879  |
| H | -2.326229 | -1.402004 | -0.422476 |
| H | -0.881573 | 1.260678  | 0.331569  |
| H | -0.074726 | -1.499362 | -0.737195 |
| H | 1.881876  | -0.151852 | -1.438741 |
| H | 2.786740  | 1.665976  | -0.027243 |
| H | 1.172241  | 2.094319  | -0.599315 |
| H | 1.406054  | 1.540235  | 1.063023  |
| H | 3.410908  | -0.751845 | 0.398376  |
| H | 2.041900  | -0.931187 | 1.502256  |
| H | 2.226265  | -2.037123 | 0.135262  |
### 3_4-methyl-2-pentenal_6_2

| Datum                                           | Value             |
|-------------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -309.838276       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy       | -309.720113       |
| Number of Imaginary Frequencies                 | 0                 |
| **Frequencies** (Top 3 out of 45)               |                   |
| 1. 71.4940 cm⁻¹                                 |                   |
| 2. 119.9612 cm⁻¹                                |                   |
| 3. 170.1273 cm⁻¹                                |                   |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C      | 2.370651 | 0.368677 | 0.211938 |
|--------|----------|----------|----------|
| C      | 0.925911 | 0.648440 | 0.135694 |
| C      | 0.065838 | -0.266758| -0.312251|
| C      | -1.418363| -0.123808| -0.422682|
| C      | -2.093320| -1.235040| 0.391195 |
| O      | 2.892982 | -0.673097| -0.117128|
| C      | -1.938386| 1.247937 | -0.018953|
| H      | 2.992377 | 1.191238 | 0.602121 |
| H      | 0.604590 | 1.629659 | 0.460483 |
| H      | 0.472411 | -1.228514| -0.616147|
| H      | -1.664946| -0.299324| -1.475982|
| H      | -3.173357| -1.199640| 0.251552 |
| H      | -1.739331| -2.220376| 0.088575 |
| H      | -1.880728| -1.105947| 1.453661 |
| H      | -3.018400| 1.292977 | -0.154764|
| H      | -1.723607| 1.446969 | 1.032855 |
| H      | -1.486847| 2.041052 | -0.614974|

### 3_4methyl2pentenal_HEI_10_reopt

| Datum                                           | Value             |
|-------------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -748.056188       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy       | -747.90247        |
### Number of Imaginary Frequencies

| Datum                          | Value |
|-------------------------------|-------|
| Number of Imaginary Frequencies | 0     |

### Frequencies (Top 3 out of 60)

| Rank | Frequency (cm⁻¹) |
|------|------------------|
| 1.   | 39.5306          |
| 2.   | 97.7714          |
| 3.   | 125.2402         |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X             | Y             | Z             |
|------|---------------|---------------|---------------|
| C    | -2.176302     | -1.052080     | -0.320348     |
| C    | -0.916938     | -1.025317     | -0.867469     |
| C    | 0.114671      | 0.055473      | -0.846495     |
| O    | -2.826719     | -0.201864     | 0.372691      |
| H    | 0.342545      | 0.369682      | -1.871800     |
| C    | 1.472742      | -1.657695     | 1.045575      |
| H    | 1.542629      | -1.101139     | 1.976660      |
| H    | 2.203646      | -2.463272     | 1.048735      |
| H    | 0.471498      | -2.077006     | 0.944226      |
| S    | 1.800785      | -0.619712     | -0.392991     |
| H    | -2.701892     | -2.003975     | -0.552165     |
| H    | -0.639385     | -1.911912     | -1.428764     |
| C    | -0.249692     | 1.321523      | -0.058269     |
| H    | -1.281852     | 1.540795      | -0.337070     |
| C    | -0.216978     | 1.112305      | 1.450782      |
| H    | 0.814436      | 1.030129      | 1.800755      |
| H    | -0.675332     | 1.961800      | 1.960818      |
| H    | -0.765176     | 0.212445      | 1.725187      |
| C    | 0.627634      | 2.504431      | -0.454545     |
| H    | 1.675168      | 2.301459      | -0.222260     |
| H    | 0.552447      | 2.716241      | -1.522748     |
| H    | 0.331639      | 3.403207      | 0.089367      |

### 3_4methyl2pentenal_HEI_11

| Datum                                | Value        |
|--------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.056228  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903943  |
| Number of Imaginary Frequencies      | 0            |
**Frequencies** (Top 3 out of 60)

1. 39.9568 cm⁻¹  
2. 75.1045 cm⁻¹  
3. 94.4170 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        |   X         |   Y         |   Z         |
|--------|-------------|-------------|-------------|
| C      | -0.564340   | 1.878985   | 0.272468    |
| C      | -0.169342   | 1.029292   | -0.722716   |
| C      | 0.142327    | -0.429650  | -0.559314   |
| O      | -0.812737   | 3.132057   | 0.202199    |
| H      | 0.073135    | -0.901054  | -1.544109   |
| C      | -2.570680   | -1.065700  | -0.466530   |
| H      | -3.386254   | -1.582036  | 0.035113    |
| H      | -2.774135   | 0.002726   | -0.495090   |
| H      | -2.477103   | -1.446125  | -1.482974   |
| S      | -1.067145   | -1.375862  | 0.470545    |
| H      | -0.696276   | 1.397386   | 1.262619    |
| H      | -0.058315   | 1.432458   | -1.725971   |
| C      | 1.552208    | -0.781652  | -0.024096   |
| H      | 1.618250    | -1.874269  | 0.007575    |
| C      | 2.615912    | -0.273620  | -0.992731   |
| H      | 2.591834    | 0.816377   | -1.040427   |
| H      | 3.611231    | -0.579450  | -0.666764   |
| H      | 2.453227    | -0.660326  | -2.000454   |
| C      | 1.818477    | -0.246142  | 1.377838    |
| H      | 1.772826    | 0.843935   | 1.379727    |
| H      | 1.088723    | -0.614806  | 2.099791    |
| H      | 2.811717    | -0.546546  | 1.715129    |

**3_4methyl2pentenal_HEI_12_reopt**

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.060377|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.90724|
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 60)
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |          |          |          |
|----------|----------|----------|----------|
| C        | -2.576931| -0.797694| 0.024301 |
| C        | -1.279604| -1.083768| -0.311626|
| C        | -0.138492| -0.273106| 0.195880 |
| O        | -3.016196| 0.150039 | 0.756019 |
| H        | -0.450237| 0.216442 | 1.122357 |
| C        | 0.623046 | 2.496165 | 0.221492 |
| H        | 0.559148 | 3.435946 | -0.323634|
| H        | -0.097193| 2.516872 | 1.038950 |
| H        | 1.626250 | 2.388035 | 0.625101 |
| S        | 0.189909 | 1.174847 | -0.935450|
| H        | -3.325350| -1.498129| -0.399055|
| H        | -1.091182| -1.924842| -0.965487|
| C        | 1.128998 | -1.098617| 0.478383 |
| H        | 0.807072 | -1.863655| 1.193534 |
| C        | 1.677175 | -1.810545| -0.754745|
| H        | 1.966404 | -1.080834| -1.513677|
| H        | 2.563290 | -2.391001| -0.493241|
| H        | 0.950521 | -2.491738| -1.194943|
| C        | 2.235302 | -0.279754| 1.135499 |
| H        | 2.666656 | 0.423595 | 0.420500 |
| H        | 1.861477 | 0.287657 | 1.989846 |
| H        | 3.037200 | -0.932300| 1.483699 |

### 3_4methyl2pentenal_HEI_13

| Datum                                                                 | Value       |
|-----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -748.059015|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -747.905512|
| Number of Imaginary Frequencies                                       | 0           |

**Frequencies** (Top 3 out of 60)

1. 57.7081 cm⁻¹
2. 78.4632 cm⁻¹
3. 94.6954 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |          |          |
|----------|----------|----------|
| C        | 0.458998 | -2.233533| 0.007936 |
| C        | -0.051461| -1.248743| 0.812232 |
| C        | -0.070112| 0.211483 | 0.518015 |
| O        | 1.037198 | -2.143571| -1.124532|
| H        | -0.221508| 0.759520 | 1.454137 |
| C        | -2.866205| -0.059650| 0.407072 |
| H        | -3.803932| 0.178970 | -0.090220|
| H        | -2.732547| -1.138726| 0.436520 |
| H        | -2.894421| 0.330058 | 1.424283 |
| S        | -1.540866| 0.714952 | -0.532420|
| H        | 0.352309 | -3.252439| 0.437284 |
| H        | -0.534545| -1.570343| 1.727250 |
| C        | 1.184568 | 0.797679 | -0.156390|
| H        | 1.248838 | 0.376212 | -1.160394|
| C        | 1.124816 | 2.322225 | -0.248295|
| H        | 0.996120 | 2.756826 | 0.747237 |
| H        | 2.053435 | 2.714545 | -0.665568|
| H        | 0.303415 | 2.670175 | -0.872821|
| C        | 2.439884 | 0.382052 | 0.606010 |
| H        | 2.381457 | 0.709674 | 1.647927 |
| H        | 2.562181 | -0.698423| 0.589748 |
| H        | 3.322546 | 0.844215 | 0.160117 |

3_4methyl2pentenal_HEI_14

| Datum                                           | Value        |
|------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -748.063057  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy      | -747.910899  |
| (Quasiharmonic)                                 |              |
| Number of Imaginary Frequencies                 | 0            |

Frequencies (Top 3 out of 60)

1. 10.4434 cm-1
2. 44.9594 cm-1
3. 78.4348 cm-1

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### 3_4methyl2pentenal_HEI_1

| Datum                                           | Value              |
|------------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -748.062562        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.90903         |

**Number of Imaginary Frequencies**

0

**Frequencies (Top 3 out of 60)**

1. 52.3327 cm⁻¹  
2. 66.5114 cm⁻¹  
3. 82.2815 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C      | 2.096709 | -1.376211 | 0.281680 |
|--------|----------|-----------|----------|
| C      | 0.852486 | -0.976812 | 0.697296 |
| C      | -0.092419| -0.238842 | -0.178860|
| O      | 2.657521 | -1.219048 | -0.854043|
### 3_4methyl2pentenal_HEI_2_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.062571 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.909681 |

Number of Imaginary Frequencies

0

**Frequencies** (Top 3 out of 60)

1. 56.3983 cm⁻¹
2. 66.3749 cm⁻¹
3. 68.4523 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -1.718864 | -1.657512 | -0.289788 |
|-------|-----------|-----------|-----------|
| C     | -0.656342 | -0.957162 | -0.794185 |
| C     | 0.206238  | -0.067494 | 0.021222  |
| O     | -2.167165 | -1.688883 | 0.905788  |
| H     | 0.038603  | -0.271012 | 1.082339  |
| C     | -1.996212 | 1.678957  | 0.161661  |
| H     | -2.427513 | 2.629016  | -0.146706 |
| H     | -2.454840 | 0.863752  | -0.395000 |
| H     | -2.168317 | 1.534429  | 1.226440  |
| Datum | Value     |
|-------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy   | -748.06354 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910087 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 60)**

1. 57.7480 cm⁻¹
2. 70.2200 cm⁻¹
3. 89.2619 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 1.150831 | 1.907229 | 0.648074 |
|-------|----------|----------|----------|
| C     | -0.294913| 0.856481 | 0.852243 |
| C     | 0.144352 | -0.047676| -0.239081|
| O     | -1.683947| 2.313234 | -0.439019|
| H     | -0.241323| 0.345424 | -1.181885|
| C     | -2.343466| -1.307104| -0.219652|
| H     | -2.593625| -0.960293| -1.221027|
| H     | -2.932939| -2.190982| 0.013154 |
| H     | -2.558155| -0.520108| 0.502243 |
| S     | -0.602580| -1.749463| -0.106493|
| H     | -1.394538| 2.475719 | 1.569322 |
| H     | 0.037928 | 0.656681 | 1.864107 |
| C     | 1.666025 | -0.235577| -0.390686|
| H     | 1.823674 | -0.983316| -1.174606|
| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.055402   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.902079   |
| Number of Imaginary Frequencies            | 0             |

### Frequencies (Top 3 out of 60)

1. 56.8000 cm⁻¹
2. 88.2384 cm⁻¹
3. 114.1695 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Datum | Value         |
|-------|---------------|
| C     | -2.309675     |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |

| Datum | Value         |
|-------|---------------|
| C     | 2.309675      |
| H     | 2.174636      |
| H     | 3.379846      |
| H     | 1.863092      |
| C     | 2.337853      |
| H     | 2.254386      |
| H     | 1.888876      |
| H     | 3.398815      |
### 3_4methyl2pentenal_HEI_5_reopt

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.059736         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -747.906472         |
| Number of Imaginary Frequencies                                      | 0                   |

#### Frequencies (Top 3 out of 60)

1. 64.3784 cm⁻¹
2. 76.8199 cm⁻¹
3. 104.0134 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C           | -0.630212 | -0.328559 |
|-------------|-----------|-----------|
| C           | -0.386983 | 0.302577  |
| C           | -0.345090 | -0.432416 |
| O           | -0.695287 | 0.161970  |
| H           | -0.703680 | -1.450003 |
| C           | 2.300370  | 0.686245  |
| H           | 3.347333  | 0.516872  |
| H           | 1.957645  | 1.586281  |
| H           | 2.195218  | 0.812199  |
| S           | 1.397186  | -0.774395 |
| H           | -0.797966 | -1.424209 |
| H           | 1.957645  | 1.586281  |
| C           | -1.214546 | 0.173305  |
| H           | -2.192989 | 0.329158  |
| C           | -0.707492 | 1.523232  |
| H           | 0.241648  | 1.399425  |
| H           | -1.419710 | 1.965095  |
| H           | -0.557615 | 2.226767  |
| C           | -1.402336 | -0.784496 |
| H           | -0.453122 | -0.959263 |
| H           | -1.790839 | -1.748020 |
| H           | -2.103049 | -0.370934 |
3_4methyl2pentenal_HEI_6_reopt

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.056352|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -747.903411|

Number of Imaginary Frequencies

**Frequencies (Top 3 out of 60)**

1. 58.9854 cm⁻¹
2. 73.3153 cm⁻¹
3. 77.3794 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |       |       |       |
|---|-------|-------|-------|
| C | -1.930909 | -0.936274 | -0.368427 |
| C | -1.197327 | -0.241456 | 0.554169  |
| C | 0.260405  | 0.045724  | 0.452374  |
| O | -3.182817 | -1.187521 | -0.363422 |
| H | 0.668489  | 0.197456  | 1.456868  |
| C | -0.588412 | 2.736941  | 0.402507  |
| H | -0.457363 | 3.743817  | 0.011745  |
| H | -1.598636 | 2.392194  | 0.194108  |
| H | -0.425998 | 2.750990  | 1.479748  |
| S | 0.623609  | 1.683610  | -0.409816 |
| H | -1.350179 | -1.340232 | -1.222750 |
| H | -1.722986 | 0.189120  | 1.401408  |
| C | 1.136502  | -1.020972 | -0.232144 |
| H | 0.802826  | -1.130029 | -1.267587 |
| C | 2.615071  | -0.630754 | -0.249318 |
| H | 2.960962  | -0.418964 | 0.766116  |
| H | 3.216656  | -1.450372 | -0.644319 |
| H | 2.808909  | 0.249698  | -0.859638 |
| C | 0.987948  | -2.369576 | 0.471287  |
| H | -0.034831 | -2.735724 | 0.432252  |
| H | 1.643687  | -3.110127 | 0.011036  |
| H | 1.273595  | -2.277215 | 1.522767  |

3_4methyl2pentenal_HEI_7_reopt
### M06-2X/def2tzvpp-IEFPCM(water) Energy

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.059201 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.906398 |

### Number of Imaginary Frequencies

0

### Frequencies (Top 3 out of 60)

|   | Frequencies (cm⁻¹) |
|---|--------------------|
| 1 | 54.3414 cm⁻¹       |
| 2 | 67.3312 cm⁻¹       |
| 3 | 74.2457 cm⁻¹       |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -2.501080 | 0.010601 | -0.327930 |
| C | -1.303547 | -0.014386 | 0.331375 |
| C | 0.004059 | 0.120545 | -0.363650 |
| O | -3.684398 | -0.097006 | 0.138257 |
| H | -0.163030 | 0.451045 | -1.394836 |
| C | 1.227576 | -1.988613 | 1.044088 |
| H | 1.564389 | -3.022683 | 1.036781 |
| H | 2.016919 | -1.363610 | 1.459756 |
| H | 0.334415 | -1.911346 | 1.663124 |
| S | 0.846407 | -1.523410 | -0.653603 |
| H | -2.404178 | 0.150750 | -1.427802 |
| H | -1.293232 | -0.130264 | 1.412875 |
| C | 0.955638 | 1.128361 | 0.313551 |
| H | 1.071040 | 0.817594 | 1.357539 |
| C | 2.338037 | 1.200546 | -0.328031 |
| H | 2.247604 | 1.402318 | -1.398932 |
| H | 2.920147 | 2.008792 | 0.116989 |
| H | 2.894529 | 0.272538 | -0.211923 |
| C | 0.320793 | 2.519356 | 0.306291 |
| H | 0.166311 | 2.854691 | -0.723221 |
| H | -0.644432 | 2.521076 | 0.807817 |
| H | 0.973343 | 3.241242 | 0.799258 |

### 3_4methyl2pentenal_HEI_8_reopt

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.059773 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.906799 |
### Number of Imaginary Frequencies

| Datum | Value |
|-------|-------|
| 0     |       |

### Frequencies (Top 3 out of 60)

| Rank | Frequency   |
|------|-------------|
| 1    | 51.3662 cm⁻¹ |
| 2    | 60.7087 cm⁻¹ |
| 3    | 105.3849 cm⁻¹ |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -2.359251 | -0.081134 | -0.214321 |
| C    | -1.088021 | -0.009818 | 0.291299  |
| C    | 0.101520  | 0.155238  | -0.575811 |
| O    | -3.464251 | -0.222251 | 0.404049  |
| H    | -0.243360 | 0.323449  | -1.599541 |
| C    | 0.865473  | -2.272294 | 0.774049  |
| H    | 1.374370  | -3.20655  | 0.691669  |
| H    | 1.281654  | -1.718905 | 1.613619  |
| H    | -0.195918 | -2.439361 | 0.942529  |
| S    | 1.119125  | -1.413374 | -0.789401 |
| H    | -2.408321 | 0.005736  | -1.322661 |
| H    | -0.947091 | -0.094979 | 1.364379  |
| C    | 1.044873  | 1.322176  | -0.217251 |
| H    | 1.859103  | 1.307713  | -0.948091 |
| C    | 0.314267  | 2.655358  | -0.354421 |
| H    | -0.464323 | 2.744990  | 0.404189  |
| H    | 1.009409  | 3.487626  | -0.232621 |
| H    | -0.160783 | 2.747399  | -1.333131 |
| C    | 1.661853  | 1.191294  | 1.170469  |
| H    | 0.887163  | 1.169796  | 1.939379  |
| H    | 2.258610  | 0.282922  | 1.254859  |
| H    | 2.313215  | 2.041352  | 1.379339  |

### 3_4methyl2pentenal_HEI_9

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.059537 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.905485 |
| 0     | Number of Imaginary Frequencies |

Datum Value

0
Frequencies (Top 3 out of 60)

|   | Frequency (cm⁻¹) |
|---|-----------------|
| 1 | 45.0618         |
| 2 | 94.5538         |
| 3 | 123.8491        |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| C | -1.458115| 1.732865| 0.222941|
| C | -0.655907| 1.024827| 1.078796|
| C | 0.122914 | -0.218439| 0.789867|
| O | -1.775475| 1.511903|-0.993779|
| H | 0.223121 | -0.803675| 1.711456|
| C | 1.724336 | 1.146421|-1.058391|
| H | 1.514055 | 0.506549|-1.913923|
| H | 2.653949 | 1.683119| 1.234323|
| H | 0.907274 | 1.853872|-0.921504|
| S | 1.913118 | 0.181866| 0.450879|
| H | -1.903936| 2.632045| 0.699482|
| H | -0.515857| 1.450223| 2.066538|
| C | -0.466681| -1.158200|-0.276384|
| H | -0.498860| -0.614995|-1.221144|
| C | 0.355833 | -2.432185| 0.447424|
| H | 0.460748 | -2.950484| 0.510594|
| H | -0.139020| -3.113303|-1.141524|
| H | 1.355566 | -2.224949| 0.824797|
| C | -1.903134| -1.522091| 0.096365|
| H | -1.932035| -1.993351| 1.083456|
| H | -2.532778| -0.635830| 0.110016|
| H | -2.313791| -2.233486|-0.622785|

3_4methyl2pentenal_TS_10_reopt

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.040295   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -747.887866 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 60)
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -2.014532 | -1.353347 | -0.350691 |
| C    | -0.925625  | -0.876409  | -1.137470  |
| C    | -0.227747  | 0.302171   | -0.983804  |
| O    | -2.574692  | -0.810992  | 0.606082   |
| H    | 0.330735   | 0.641583   | -1.845301  |
| C    | 1.568307   | 0.302171   | -0.983804  |
| H    | 1.544695   | -1.411519  | 1.843329   |
| H    | 2.190743   | -2.608826  | 0.711222   |
| H    | 0.546798   | -1.991887  | 0.502147   |
| S    | 2.159217   | -0.391593  | -0.276506  |
| H    | -2.414200  | -2.324723  | -0.701973  |
| H    | -0.654269  | -1.518332  | -1.967568  |
| C    | -0.573181  | 1.377957   | 0.019783   |
| H    | -1.657911  | 1.509018   | -0.065959  |
| C    | -0.286075  | 1.012609   | 1.476607   |
| H    | 0.788141   | 1.043039   | 1.655343   |
| H    | -0.777916  | 1.728483   | 2.138505   |
| H    | -0.653861  | 0.017463   | 1.713445   |
| C    | 0.113385   | 2.690596   | -0.341518  |
| H    | 1.196763   | 2.559039   | -0.300013  |
| H    | -0.154452  | 3.020216   | -1.346424  |
| H    | -0.162382  | 3.479164   | 0.359963   |

### 3-4methyl2pentenal_TS_11_reopt

| Datum                                                      | Value     |
|------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -748.041224 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.889344 |
| Number of Imaginary Frequencies                            | 1         |

#### Frequencies (Top 3 out of 60)

1. -176.7543 cm⁻¹
2. 63.9120 cm⁻¹
3. 78.7026 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Datum                  | Value       |
|------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.041188 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.890445 |
| Number of Imaginary Frequencies | 1           |

Frequencies (Top 3 out of 60)

1. -182.4349 cm⁻¹
2. 33.4077 cm⁻¹
3. 83.6796 cm⁻¹
### 3_4methyl2pentenal_TS_13

| Datum                                                               | Value            |
|---------------------------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -748.044411      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)         | -747.892723      |
| Number of Imaginary Frequencies                                     | 1                |
| **Frequencies** (Top 3 out of 60)                                   |                  |
| 1. -145.8993 cm⁻¹                                                   |                  |
| 2.  59.7193 cm⁻¹                                                   |                  |
| 3.  69.5881 cm⁻¹                                                   |                  |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|      |      |      |
|------|------|------|
| C    | 0.243068 | -2.232001 | 0.080831 |
| C    | 0.090694 | -1.183936 | 1.043711 |
| C    | 0.378872 | 0.138864  | 0.839937 |
| O    | 0.659182 | -2.133854 | -1.072948 |
### 3_4methyl2pentenal_TS_14

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.042991 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.891822 |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 60)

1. -201.7196 cm⁻¹
2. 51.0479 cm⁻¹
3. 83.7100 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -2.689455 | -0.492755 | 0.382201 |
|-------|-----------|-----------|----------|
| C     | -1.514358 | 0.273697  | 0.623679 |
| C     | -0.476185 | 0.385210  | -0.277814|
| O     | -2.914549 | -1.215063 | -0.593936|
| H     | -0.679630 | -0.114208 | -1.255066|
| C     | 2.664176  | -1.291338 | -0.356551|
| H     | 3.009847  | -0.431374 | 0.220513 |
| H     | 3.355707  | -2.114799 | -0.175554|
| H     | 2.724693  | -1.033635 | -1.414652|
### 3_4methyl2pentenal_TS_1

| Datum                                                                 | Value             |
|-----------------------------------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.047486       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -747.895836       |
| Number of Imaginary Frequencies                                      | 1                 |
| **Frequencies** (Top 3 out of 60)                                    |                   |
| 1.  -144.4930 cm⁻¹                                                   |                   |
| 2.   56.5960 cm⁻¹                                                    |                   |
| 3.   84.1070 cm⁻¹                                                    |                   |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 2.048478 | -1.460567 | 0.154202 |
| C | 0.683161 | -1.280083 | 0.543047 |
| C | -0.244193 | -0.778657 | -0.326765 |
| O | 2.534883 | -1.215531 | -0.949883 |
| H | 0.067063 | -0.684697 | -1.359416 |
| C | 1.585179 | 1.825183 | 0.742146 |
| H | 2.485517 | 2.090775 | 0.187181 |
| H | 1.488928 | 2.507065 | 1.587059 |
| H | 1.730773 | 0.814889 | 1.146148 |
| S | 0.110800 | 1.844350 | -0.300185 |
| H | 2.710191 | -1.862972 | 0.943809 |
| H | 0.434952 | -1.504813 | 1.572340 |
| C | -1.732787 | -0.842393 | -0.103295 |
| H | -1.985164 | -1.888596 | -0.326174 |
3_4methyl2pentenal_TS_2

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.047304      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.896043     |
| Number of Imaginary Frequencies            | 1                |

**Frequencies** (Top 3 out of 60)

1. -142.7631 cm⁻¹  
2.  46.2474 cm⁻¹  
3.  77.1197 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|       |                  |                  |                  |
|-------|------------------|------------------|------------------|
| C     | 1.360982         | 2.017131         | -0.061959        |
| C     | 0.255378         | 1.289114         | -0.606591        |
| C     | -0.476666        | 0.417968         | 0.146385         |
| O     | 1.769388         | 1.965430         | 1.097843         |
| H     | -0.301620        | 0.420282         | 1.215696         |
| C     | 2.383804         | -1.155389        | -0.669015        |
| H     | 2.663875         | -1.758810        | -1.532385        |
| H     | 2.154016         | -0.145098        | -1.032612        |
| H     | 3.247443         | -1.081160        | -0.007624        |
| S     | 0.935355         | -1.829300        | 0.172357         |
| H     | 1.879641         | 2.684762         | -0.774761        |
| H     | 0.051162         | 1.415093         | -1.664082        |
| C     | -1.796744        | -0.145517        | -0.312531        |
| H     | -1.662674        | -0.562273        | -1.313771        |
| C     | -2.331930        | -1.226688        | 0.618379         |
| H     | -2.447282        | -0.826601        | 1.628911         |
| H     | -3.311383        | -1.569899        | 0.282967         |
| H     | -1.659576        | -2.081036        | 0.662705         |
| C     | -2.814659        | 1.001722         | -0.404954        |
3_4methyl2pentenal_TSI3

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.048293 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.896631 |

Number of Imaginary Frequencies

1

Frequencies (Top 3 out of 60)

1. -159.1055 cm⁻¹
2. 47.2820 cm⁻¹
3. 77.8179 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C | 0.151889 | 2.028077 | 0.457287 |
| C | 0.059284 | 1.130452 | 0.680192 |
| C | 0.472363 | 0.382469 | -0.333390 |
| O | -1.719280 | 2.240707 | -0.614316 |
| H | 0.159162 | 0.636351 | 1.337849 |
| C | -2.335243 | -1.175895 | 0.555595 |
| H | -3.283036 | -0.941630 | -0.070234 |
| H | -2.517701 | -1.936536 | 1.314666 |
| H | -1.990466 | -0.269219 | 1.070494 |
| S | -1.074830 | -1.697188 | -0.627267 |
| H | -1.501520 | 2.571159 | 1.355106 |
| H | 0.280380 | 1.020326 | 1.702113 |
| C | 1.790745 | 0.356442 | -0.235750 |
| H | 1.741261 | -1.186266 | -0.942747 |
| C | 2.910697 | 0.582636 | -0.680000 |
| H | 3.003046 | 1.421220 | 0.012290 |
| H | 3.861267 | 0.047550 | -0.698069 |
| H | 2.726165 | 0.983418 | 1.677362 |
| C | 2.060375 | -0.915743 | 1.152192 |
| H | 2.209959 | -0.112673 | 1.876212 |
| H | 1.229190 | -1.536260 | 1.488123 |
| H | 2.967226 | -1.521414 | 1.140830 |
3_4methyl2pentenal_TS_4_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.039783 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.888584 |

Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 60)

1. -200.8048 cm⁻¹
2. 41.0501 cm⁻¹
3. 71.9174 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    | x   | y   | z   |
|----|-----|-----|-----|
| C  | -2.400588 | -0.206089 | 0.115552 |
| C  | -1.258208 | -0.572065 | -0.642982 |
| C  | -0.102477 | 0.177295 | -0.723081 |
| O  | -3.442346 | -0.863692 | 0.213851 |
| H  | 0.579897 | -0.089109 | -1.520732 |
| C  | 1.451789 | -2.453270 | -0.330908 |
| H  | 2.135340 | -3.242099 | -0.019168 |
| H  | 0.432186 | -2.810258 | -0.177453 |
| H  | 1.593082 | -2.290381 | -1.401472 |
| S  | 1.746000 | -0.930605 | 0.611181 |
| H  | -2.350239 | 0.768593 | 0.631561 |
| H  | -1.317154 | -1.510461 | -1.182775 |
| C  | 0.027933 | 1.612439 | -0.239605 |
| H  | -0.891806 | 2.117719 | -0.550765 |
| C  | 0.149854 | 1.789789 | 1.276105 |
| H  | 1.157590 | 1.536262 | 1.603854 |
| H  | -0.046433 | 2.829670 | 1.543043 |
| H  | -0.546851 | 1.155481 | 1.821588 |
| C  | 1.195181 | 2.303614 | -0.939283 |
| H  | 1.071280 | 2.294555 | -2.022797 |
| H  | 1.280026 | 3.341560 | -0.615193 |
| H  | 2.124955 | 1.787396 | -0.694180 |

3_4methyl2pentenal_TS_5_reopt3
| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.048698    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -747.897228    |
| Number of Imaginary Frequencies                                      | 1              |

**Frequencies** (Top 3 out of 60)

1. -163.5265 cm⁻¹  
2. 50.0915 cm⁻¹  
3. 80.3001 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |          |          |          |
|---|----------|----------|----------|
| C | 2.265285 | -0.875265| -0.453713|
| C | 0.992204 | -1.015273| 0.158666 |
| C | -0.146087| -0.607190| -0.499832|
| O | 3.353788 | -1.232215| 0.006121 |
| H | -0.019639| -0.317182| -1.537116|
| C | 1.173885 | 2.234998 | 0.412764 |
| H | 1.698721 | 2.764726 | -0.382396|
| H | 1.226452 | 2.839195 | 1.318051 |
| H | 1.710080 | 1.299251 | 0.607153 |
| S | -0.534615| 1.855577 | -0.030686|
| H | 2.239650 | -0.403369| -1.456758|
| H | 0.954536 | -1.431814| 1.158388 |
| C | -1.523755| -1.129265| -0.165800|
| H | -1.511812| -2.151632| -0.568064|
| C | -1.801785| -1.228604| 1.329433 |
| H | -1.753126| -0.235291| 1.777045 |
| H | -2.798498| -1.637918| 1.498869 |
| H | -1.086410| -1.874052| 1.837747 |
| C | -2.648013| -0.390198| -0.884576|
| H | -2.827759| 0.582162 | -0.426632|
| H | -2.407891| -0.232191| -1.937114|
| H | -3.571163| -0.968613| -0.828812|

---

3_4methyl2pentenal_TS_6

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.044861    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -747.893366    |
Number of Imaginary Frequencies

1

Frequencies (Top 3 out of 60)

1. -149.5598 cm⁻¹
2. 42.6122 cm⁻¹
3. 74.2561 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |          |          |          |
|----------|----------|----------|----------|
| C        | 0.183317 | 2.116694 | -0.296001|
| C        | 0.188674 | 1.178224 | 0.770687 |
| C        | -0.403126| -0.063895| 0.696587 |
| O        | 0.694860 | 3.240162 | -0.277618|
| H        | -0.435588| -0.632171| 1.618949 |
| C        | 2.750220 | -0.531045| -0.113083|
| H        | 3.274943 | -0.545518| -1.067966|
| H        | 2.354267 | 0.480644 | 0.035724 |
| H        | 3.473576 | -0.730266| 0.677525 |
| S        | 1.377502 | -1.704664| -0.096783|
| H        | -0.333677| 1.792498 | -1.217778|
| H        | 0.747506 | 1.452429 | 1.658302 |
| C        | -1.495060| -0.444093| -0.283602|
| H        | -1.146166| -0.271035| -1.302873|
| C        | -1.894357| -1.909814| -0.144767|
| H        | -2.231247| -2.110439| 0.875555 |
| H        | -2.718133| -2.145646| -0.819376|
| H        | -1.063224| -2.575274| -0.368481|
| C        | -2.728728| 0.435418 | -0.033739|
| H        | -2.512639| 1.488895 | -0.204316|
| H        | -3.545789| 0.134493 | -0.691089|
| H        | -3.068392| 0.325786 | 0.998810 |

3_4methyl2pentenal_TS_7_reopt

|          |          |
|----------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.048605 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.897766 |

Number of Imaginary Frequencies

1
**Frequencies (Top 3 out of 60)**

1. -153.0426 cm⁻¹  
2. 37.1393 cm⁻¹  
3. 65.1461 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|    |    |    |    |
|----|----|----|----|
| C  | -1.839648 | -1.434292 | 0.431906 |
| C  | -0.680211  | -1.091526  | -0.314322 |
| C  | 0.349469   | -0.392604  | 0.265667  |
| O  | -2.807852  | -2.089036  | 0.038545  |
| H  | 0.299853   | -0.241007  | 1.339305  |
| C  | -1.910912  | 1.936210   | -0.284592 |
| H  | -2.508156  | 2.292112   | 0.554841  |
| H  | -2.220491  | 2.478274   | -1.177815 |
| H  | -2.145688  | 0.876951   | -0.443102 |
| S  | -0.139198  | 2.106548   | 0.016570  |
| H  | -1.831003  | -1.068460  | 1.478367  |
| H  | -0.634614  | -1.385004  | -1.358566 |
| C  | 1.739308   | -0.384521  | -0.324894 |
| H  | 1.661144   | -0.090256  | -1.374316 |
| C  | 2.693786   | 0.560407   | 0.395283  |
| H  | 2.730320   | 0.316406   | 1.460114  |
| H  | 3.703435   | 0.456736   | -0.003925 |
| H  | 2.388161   | 1.599391   | 0.293769  |
| C  | 2.300379   | -1.813684  | -0.268675 |
| H  | 2.346929   | -2.162156  | 0.765726  |
| H  | 1.676402   | -2.506734  | -0.830706 |
| H  | 3.310660   | -1.838682  | -0.679409 |

**3_4methyl2pentenal_TS_8_reopt2**

| Datum                                              | Value        |
|----------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy              | -748.049605  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.898555  |

Number of Imaginary Frequencies  

**Frequencies (Top 3 out of 60)**
| Datum                                            | Value              |
|--------------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy             | -748.044411        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.892722        |

**Number of Imaginary Frequencies**

1

**Frequencies (Top 3 out of 60)**

1. -145.9067 cm⁻¹
2. 29.0902 cm⁻¹
3. 75.6837 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -0.243050 | 2.232039 | 0.080805 |
| C | -0.090703 | 1.183978 | 1.043689 |
| C | -0.378813 | -0.138802 | 0.839926 |
| O | -0.659039 | 2.133869 | -1.073023 |
| H | -0.233057 | -0.796634 | 1.690127 |
| C | 2.810245 | 0.372958 | -0.127783 |
| H | 3.669967 | 0.323038 | 0.540725 |
| H | 2.163058 | 1.188976 | 0.219813 |
| S | 1.868500 | -1.168735 | -0.146960 |
| H | 0.064840 | 3.230627 | 0.445160 |
| H | 0.384092 | 1.475935 | 1.972563 |
| C | -1.305424 | -0.686982 | -0.217298 |
| H | -0.969706 | -0.336642 | -1.191276 |
| C | -1.340050 | -2.210733 | -0.199184 |
| H | -1.669213 | -2.570530 | 0.779284 |
| H | -2.042153 | -2.586677 | -0.944578 |
| H | -0.356955 | -2.630431 | -0.405905 |
| C | -2.717215 | -0.134880 | 0.027534 |
| H | -3.078341 | -0.433641 | 1.014287 |
| H | -2.724403 | 0.951881 | -0.030774 |
| H | -3.409693 | -0.530815 | -0.717258 |

4_3-methyl-2-butenal_1

| Datum | Value     |
|-------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -270.536544 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.445858 |

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 36)

1. 109.1233 cm⁻¹
2. 127.1964 cm⁻¹
3. 188.3092 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### 4_3-methyl-2-butenal_2

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFCM(water) Energy | -270.533343          |
| M06-2X/def2tzvpp-IEFCM(water) Free Energy (Quasiharmonic) | -270.442682          |

Number of Imaginary Frequencies: 0

**Frequencies (Top 3 out of 36)**

1. 45.7040 cm⁻¹
2. 158.7467 cm⁻¹
3. 206.6602 cm⁻¹

**M06-2X/def2tzvpp-IEFCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 1.638163 | -0.639888 | -0.005787 |
| C | 0.211152 | -0.949676 | -0.001293 |
| O | 2.131375 | 0.470672 | 0.010782 |
| C | -0.779466 | -0.040936 | -0.001606 |
| C | -2.209336 | -0.477601 | 0.004757 |
| H | -2.719828 | -0.075603 | -0.873426 |
| H | 2.299437 | -1.523464 | -0.025395 |
| H | -2.717105 | -0.057610 | 0.876109 |
| H | -2.312842 | -1.559805 | 0.016025 |
| C | -0.549501 | 1.441027 | -0.006843 |
| H | -0.036212 | -2.004258 | 0.000150 |
| H | -1.495564 | 1.976663 | -0.048626 |
4_3methyl2butenal_HEI_1_reopt

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -708.751636            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.62551             |
| Number of Imaginary Frequencies                                      | 0                      |

**Frequencies** (Top 3 out of 51)

1. 57.7972 cm⁻¹
2. 70.8871 cm⁻¹
3. 161.7503 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -2.177944 | -0.228024 | -0.221621 |
| C     | -0.997152 | -0.198924 | 0.470778  |
| C     | 0.189792  | 0.650022  | 0.160623  |
| O     | -3.212735 | -0.939879 | 0.012802  |
| C     | 1.701109  | -1.776240 | 0.265656  |
| H     | 2.055466  | -1.532833 | 1.265797  |
| H     | 0.748288  | -2.297848 | 0.330830  |
| H     | 2.431792  | -2.422583 | -0.216089 |
| S     | 1.537268  | -0.304429 | -0.756789 |
| H     | -2.239622 | 0.460554  | -1.085877 |
| H     | -0.900445 | -0.858684 | 1.330162  |
| C     | -0.092030 | 1.819352  | -0.780611 |
| H     | -0.452819 | 1.484318  | -1.751851 |
| H     | -0.847548 | 2.470934  | -0.338493 |
| H     | 0.816872  | 2.403083  | -0.938095 |
| C     | 0.813039  | 1.186546  | 1.450695  |
| H     | 1.712829  | 1.768182  | 1.246086  |
| H     | 0.088676  | 1.825538  | 1.960926  |
| H     | 1.071226  | 0.372852  | 2.129679  |

4_3methyl2butenal_HEI_2_reopt
| Datum                                                                 | Value         |
|---------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -708.753779   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -708.627524   |
| Number of Imaginary Frequencies                                     | 0             |

**Frequencies** (Top 3 out of 51)

1. 73.6207 cm⁻¹
2. 94.3094 cm⁻¹
3. 158.3724 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        | x       | y       | z       |
|--------|---------|---------|---------|
| C      | 2.085757| -0.159826| 0.144805|
| C      | 1.011266| 0.362886 | -0.523863|
| C      | -0.315730| 0.705144 | 0.057990 |
| O      | 3.229405| -0.481056| -0.327979|
| C      | -0.978167| -2.055117| 0.220675 |
| H      | 0.103343| -2.066181| 0.076035 |
| H      | -1.280913| -2.141606| 1.280479 |
| H      | -1.420667| -2.895625| -0.309074|
| S      | -1.633273| -0.536764| -0.486070|
| H      | 1.942036 | -0.307822| 1.232471 |
| H      | 1.102405 | 0.506246 | -1.599007|
| C      | -0.344196| 0.771528 | 1.582329 |
| H      | -0.101547| -0.186135| 2.040618 |
| H      | 0.385202 | 1.504369 | 1.933785 |
| H      | -1.335016| 1.071869 | 1.924416 |
| C      | -0.840140| 2.022711 | -0.516139|
| H      | -1.857444| 2.230648 | -0.177678|
| H      | -0.191980| 2.837737 | -0.189254|
| H      | -0.833032| 1.999214 | -1.606609|

**4_3methyl2butenal_HEI_3**

| Datum                                                                 | Value         |
|---------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -708.751636   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -708.625506   |
| Number of Imaginary Frequencies                                     | 0             |
**Frequencies (Top 3 out of 51)**

1. 58.0269 cm\(^{-1}\)
2. 70.8933 cm\(^{-1}\)
3. 161.9189 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| C | -2.178043 | -0.228208 | -0.221573 |
| C | -0.997237 | -0.199096 | 0.470796  |
| O | 0.189665  | 0.649932  | 0.160661  |
| C | -3.212787 | -0.940139 | 0.012814  |
| C | 1.702057  | -1.775626 | 0.265774  |
| H | 2.058137  | -1.531773 | 1.265187  |
| H | 0.749166  | -2.296899 | 0.332747  |
| H | 2.431730  | -2.422486 | -0.216807 |
| S | 1.537005  | -0.304306 | -0.757175 |
| H | -2.239775 | 0.460439  | -1.085777 |
| H | -0.900441 | -0.858909 | 1.330119  |
| C | -0.092315 | 1.819465  | -0.780272 |
| H | -0.453120 | 1.484634  | -1.751579 |
| H | -0.847889 | 2.470848  | -0.337958 |
| H | 0.816517  | 2.403327  | -0.937661 |
| C | 0.813048  | 1.186150  | 1.450784  |
| H | 1.712907  | 1.767712  | 1.246253  |
| H | 0.088789  | 1.825141  | 1.961162  |
| H | 1.071138  | 0.372272  | 2.129589  |

**4_3methyl2butenal_HEI_4**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.7526   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.626411 |

**Frequencies (Top 3 out of 51)**

1. 61.7198 cm\(^{-1}\)
2. 79.3981 cm\(^{-1}\)
3. 164.6308 cm\(^{-1}\)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|         | C        | C        | C        |
|---------|----------|----------|----------|
|         | 2.362695 | -0.192805| -0.253665|
|         | 1.251735 | -0.014626| 0.525857 |
|         | -0.091936| 0.465390 | 0.067663 |
|         | 3.516683 | -0.609385| 0.104009 |
|         | -2.855508| -0.446549| -0.173463|
|         | -3.215994| 0.137158 | 0.670610 |
|         | -2.919506| 0.145768 | -1.084321|
|         | -3.490394| -1.323532| -0.287454|
|         | -1.173888| -1.055653| 0.102442 |
|         | 2.241682 | 0.067603 | -1.321932|
|         | 1.324707 | -0.262403| 1.582903 |
|         | -0.185480| 1.044064 | -1.343379|
|         | 0.221710 | 0.315173 | -2.082170 |
|         | -1.109578| 1.375535 | -1.610960|
|         | 0.557908 | 1.910422 | -1.393351|
|         | -0.659918| 1.496667 | 1.042896 |
|         | -0.680391| 1.098063 | 2.057554 |
|         | -0.021218| 2.382486 | 1.033896 |
|         | -1.669724| 1.806406 | 0.768618 |

4_3methyl2butenal_HEI_5

| Datum                                           | Value       |
|------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -708.753445 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.626703 |
| Number of Imaginary Frequencies                 | 0           |

Frequencies (Top 3 out of 51)

1. 82.4592 cm⁻¹
2. 96.7297 cm⁻¹
3. 184.8644 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|         | C        | C        | C        |
|---------|----------|----------|----------|
|         | -2.055218| 0.188164 | -0.631575|
|         | -0.789274| 0.657291 | -0.881876|
|         | 0.383445 | 0.697560 | 0.042016 |
### 4_3methyl2butenal_HEI_6

| Datum                                                                 | Value            |
|-----------------------------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -708.753076      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -708.626992      |
| Number of Imaginary Frequencies                                       | 0                |

**Frequencies (Top 3 out of 51)**

1. 48.0186 cm⁻¹  
2. 92.4239 cm⁻¹  
3. 161.3385 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C           | 2.004689  | -0.660063  | 0.624645  |
|-------------|-----------|------------|-----------|
| C           | 0.873806  | 0.018288   | 1.006569  |
| C           | -0.099853 | 0.715667   | 0.114595  |
| O           | 2.486714  | -0.867633  | -0.535309 |
| C           | -1.822185 | -1.531727  | 0.426014  |
| H           | -1.006148 | -1.858437  | 1.069756  |
| H           | -2.576485 | -1.018054  | 1.019158  |
| H           | -2.276756 | -2.39169   | -0.047687 |
| S           | -1.161307 | -0.481836  | -0.877587 |
| H           | 2.567552  | -1.084158  | 1.483473  |
| H           | 0.641463  | 0.011520   | 2.066017  |
### 4_3methyl2butenal_HEI_7_reopt

| Datum                                                                 | Value                  |
|-----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -708.7526              |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.626411            |
| Number of Imaginary Frequencies                                       | 0                      |

#### Frequencies (Top 3 out of 51)

1. 61.7116 cm\(^{-1}\)
2. 79.3979 cm\(^{-1}\)
3. 164.6184 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 2.362704 | -0.192802 | 0.253633 |
|-------|----------|-----------|----------|
| C     | 1.251731 | -0.014609 | -0.525867|
| C     | -0.091943| 0.465374  | -0.067648|
| O     | 3.516704 | -0.609331 | -0.104071|
| C     | -2.855502| -0.446494 | 0.173359 |
| H     | -2.919511| 0.146005  | 1.084094 |
| H     | -3.215939| 0.137053  | -0.670841|
| H     | -3.490414| -1.323436 | 0.287520 |
| S     | -1.173885| -1.055679 | -0.102379|
| H     | 2.241696 | 0.067547  | 1.321917 |
| H     | 1.324701 | -0.262299 | -1.582936|
| C     | -0.659974| 1.496652  | -1.042852|
| H     | -0.680505| 1.098052  | -2.057510|
| H     | -1.669763| 1.806378  | -0.768498|
| H     | -0.021278| 2.382474  | -1.033876|
| C     | -0.185457| 1.044012  | 1.343404 |
| H     | -1.109513| 1.375599  | 1.611002 |
| H     | 0.558047 | 1.910279  | 1.393406 |
| H     | 0.221645 | 0.315060  | 2.082178 |
### 4_3methyl2butenal_HEI_8_reopt

| Datum                                                   | Value          |
|---------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -708.752908    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.626869    |
| Number of Imaginary Frequencies                         | 0              |

**Frequencies** (Top 3 out of 51)

1. 51.9651 cm⁻¹
2. 58.6345 cm⁻¹
3. 152.8767 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 2.354399 | -0.199083 | -0.382324 |
|-------|----------|-----------|-----------|
| C     | 1.294497 | 0.633089  | -0.644030 |
| C     | -0.038010| 0.632696  | 0.046419  |
| O     | 2.474304 | -1.139251 | 0.467820  |
| C     | -2.517317| -0.876759 | 0.261808  |
| H     | -2.355335| -1.139185 | 1.305049  |
| H     | -3.053819| 0.068167  | 0.206086  |
| H     | -3.128295| -1.650066 | 0.200760  |
| S     | -0.961827| -0.822356 | -0.66967  |
| H     | 3.233889 | 0.005645  | -1.029494 |
| H     | 1.414714 | 1.337842  | -1.459492 |
| C     | -0.802057| 1.910721  | -0.291870 |
| H     | -0.888236| 2.037678  | -1.371045 |
| H     | -1.803399| 1.909696  | 0.140690  |
| H     | -0.262878| 2.770353  | 0.113556  |
| C     | 0.065093 | 0.487284  | 1.563172  |
| H     | 0.602629 | -0.420217 | 1.823661  |
| H     | 0.617618 | 1.342104  | 1.961051  |
| H     | -0.921720| 0.482001  | 2.030048  |

### 4_3methyl2butenal_TS_1_reopt

| Datum                                                   | Value          |
|---------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -708.752908    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.626869    |
### Datum  Value

|                      |          |
|----------------------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.741325 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.616614 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 51)

1. -208.3234 cm⁻¹
2. 79.4082 cm⁻¹
3. 94.3472 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|         |          |          |          |
|---------|----------|----------|----------|
| C       | 2.091595 | -0.312211 | 0.135513 |
| C       | 1.111889 | 0.466904 | -0.527016 |
| C       | -0.021653 | 0.987881 | 0.071106 |
| O       | 3.118188 | -0.776402 | -0.380040 |
| C       | -0.971028 | -2.048610 | 0.231938 |
| H       | -1.146313 | -2.945413 | -0.361552 |
| H       | 0.101493 | -1.823010 | 0.177943 |
| H       | -1.219216 | -2.273275 | 1.269673 |
| S       | -1.898024 | -0.635394 | -0.399382 |
| H       | 1.923986 | -0.491021 | 1.211961 |
| H       | 1.271403 | 0.647537 | -1.585630 |
| C       | -0.195263 | 0.950653 | 1.569719 |
| H       | -0.055401 | -0.048159 | 1.977945 |
| H       | 0.539595 | 1.613560 | 2.037203 |
| H       | -1.190431 | 1.293469 | 1.841439 |
| C       | -0.712364 | 2.136297 | -0.613557 |
| H       | -1.751339 | 2.219963 | -0.30768 |
| H       | -0.199161 | 3.064620 | -0.340270 |
| H       | -0.670794 | 2.033772 | -1.696529 |

### 4_3methyl2butenal_TS_2_reopt

|                      |          |
|----------------------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.741325 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.616613 |
| Number of Imaginary Frequencies | 1 |
Frequencies (Top 3 out of 51)

1.  -208.3351 cm⁻¹
2.  79.3728 cm⁻¹
3.  94.3455 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 2.091663 | -0.312286 | 0.135415 |
| C | 1.111932 | 0.466829 | -0.527074 |
| C | -0.021599 | 0.987824 | 0.071105 |
| O | 3.118218 | -0.776514 | -0.380189 |
| C | -0.971242 | -2.048662 | 0.231754 |
| H | 0.101265 | 1.822867 | -1.269250 |
| H | -1.219822 | -2.273988 | 0.178376 |
| H | -1.146140 | -2.945127 | 0.362358 |
| S | -1.898152 | -0.635218 | -0.399596 |
| H | 1.924106 | -0.491063 | 1.211876 |
| H | 1.271402 | 0.647432 | -1.585700 |
| C | -0.195077 | 0.950664 | 1.569738 |
| H | -0.055212 | -0.048139 | 1.977989 |
| H | 0.539847 | 1.613568 | 2.037128 |
| H | -1.190209 | 1.293521 | 1.841538 |
| C | -0.712272 | 2.136283 | -0.613533 |
| H | -1.751226 | 2.220028 | -0.300696 |
| H | -0.198990 | 3.064573 | -0.340284 |
| H | -0.670764 | 2.033744 | -1.696507 |

4_3methyl2butenal_TS_3_reopt

| Datum | Value       |
|-------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy       | -708.73922 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasi-harmonic) | -708.61578 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 51)

1.  -210.6124 cm⁻¹
2.  15.7090 cm⁻¹
3.  75.1336 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C              | O              | S              | H              |
|---|----------------|----------------|----------------|----------------|
| x | -2.082746      | -3.060104      | 1.822939       | -1.963669      |
| y | -0.298087      | 0.214245       | -0.606791      | -0.057435      |
| z | -0.305528      | 0.978383       | 0.364790       | 0.521262       |

4_3methyl2butenal_TS_4_reopt

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.73642|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.613138|

Number of Imaginary Frequencies

1

Frequencies (Top 3 out of 51)

1. -235.2005 cm⁻¹
2. 54.8442 cm⁻¹
3. 67.8513 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C              | C              | C               |
|---|----------------|----------------|-----------------|
| x | 2.414797       | 1.426443       | 0.237243        |
| y | -0.399566      | 0.231917       | 0.756203        |
| z | 0.257266       | -0.529194      | -0.041389       |
4_3methyl2butenal_TS_5_reopt

| Datum                                         | Value       |
|-----------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy         | -708.738578 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.614633 |

Number of Imaginary Frequencies
1

**Frequencies** (Top 3 out of 51)

1. -183.9125 cm⁻¹
2. 15.1941 cm⁻¹
3. 80.8369 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |      |      |      |
|---|------|------|------|
| C | -1.926815 | -0.844339 | -0.513329 |
| C | -1.020163 | 0.169400 | -0.932439 |
| C | -0.269408 | 1.004050 | -0.126553 |
| O | -2.236090 | -1.180910 | 0.634706 |
| C | 1.350938 | -1.910937 | -0.296308 |
| H | 1.183029 | -2.633469 | 0.502791 |
| H | 0.403641 | -1.779481 | -0.835200 |
| H | 2.073488 | -2.333670 | -0.994178 |
| S | 1.887617 | -0.307479 | 0.334513 |
| H | -2.400093 | -1.385497 | -1.356236 |
| H | -0.866025 | 0.226371 | -2.004484 |
### 4_3methyl2butenal_TS_6_reopt

| Datum | Value            |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.738577 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.614637 |

Number of Imaginary Frequencies
1

**Frequencies** (Top 3 out of 51)

1. -184.0066 cm⁻¹
2. 15.0399 cm⁻¹
3. 80.8497 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          |                   |                   |
|----------|-------------------|-------------------|
| C        | -0.610177         | 1.229303          | 1.321957  |
| H        | -0.852743         | 0.304986          | 1.831539  |
| H        | 0.210299          | 1.730396          | 1.832316  |
| H        | -1.489074         | 1.883234          | 1.368299  |
| C        | 0.422147          | 2.171688          | -0.779098 |
| H        | 0.748183          | 1.932921          | -1.789560 |
| H        | -0.284267         | 3.007283          | -0.833893 |
| H        | 1.281281          | 2.498893          | -0.196626 |
| C        | -1.927107         | -0.843703         | -0.513374 |
| C        | -1.020134         | 0.169745          | -0.932451 |
| C        | -0.269047         | 1.004064          | -0.126532 |
| O        | -2.236455         | -1.180218         | 0.636457  |
| C        | 1.350319          | -1.911366         | -0.296184 |
| H        | 0.403252          | -1.779689         | -0.835421 |
| H        | 2.072964          | -2.334563         | -0.993676 |
| H        | 1.181867          | -2.633579         | 0.503090  |
| S        | 1.887396          | -0.387909         | 0.334374  |
| H        | -2.400595         | -1.384663         | -1.356290 |
| H        | -0.866022         | 0.226740          | -2.004499 |
| C        | -0.609659         | 1.229292          | 1.322017  |
| H        | -0.852255         | 0.304973          | 1.831578  |
| H        | 0.210917          | 1.730279          | 1.832324  |
| H        | -1.488507         | 1.883275          | 1.368483  |
| C        | 0.422928          | 2.171492          | -0.778998 |
| H        | 0.748818          | 1.932702          | -1.789497 |
| H        | -0.283158         | 3.007375          | -0.833666 |
| H        | 1.282222          | 2.498297          | -0.196539 |
## 4_3methyl2butenal_TS_7_reopt

| Datum                                      | Value    |
|--------------------------------------------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.736359 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.612899 |
| Number of Imaginary Frequencies            | 1        |

**Frequencies (Top 3 out of 51)**

1. -234.3194 cm⁻¹
2. 56.3730 cm⁻¹
3. 70.7858 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 2.379981 | -0.443584 | 0.298332 |
| C   | 1.448510 | 0.263359  | -0.493328 |
| C   | 0.239670 | 0.768542  | -0.833496 |
| O   | 3.459222 | -0.912547 | -0.091423 |
| C   | -2.987843| -0.510669 | 0.320556  |
| H   | -2.976073| -0.571307 | 1.409372  |
| H   | -3.187469| 0.527297  | 0.044497  |
| H   | -3.822499| -1.111923 | -0.041278 |
| S   | -1.413399| -1.074476 | -0.394456 |
| H   | 2.113402 | -0.576327 | 1.361197  |
| H   | 1.682318 | 0.362942  | -1.548630 |
| C   | -0.461305| 1.776399  | -0.903905 |
| H   | -0.331282| 1.548580  | -1.959868 |
| H   | -1.524126| 1.835636  | -0.677598 |
| H   | -0.022401| 2.761421  | -0.709287 |
| C   | -0.053240| 0.933458  | 1.435381  |
| H   | -1.117498| 1.102395  | 1.590677  |
| H   | 0.484796 | 1.813279  | 1.803699  |
| H   | 0.246809 | 0.074976  | 2.028659  |

## 4_3methyl2butenal_TS_8_reopt

| Datum                                      | Value    |
|--------------------------------------------|----------|
### 5_trans-2-methyl-2-butenal_1

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -270.538087 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.447305 |
| Number of Imaginary Frequencies | 0 |
**Frequencies** (Top 3 out of 36)

1. 108.7589 cm⁻¹
2. 122.1360 cm⁻¹
3. 131.1117 cm⁻¹

**5_trans-2-methyl-2-butenal_2**

| Datum  | Value               |
|--------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy  | -270.532018          |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.442103 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

1. 89.6715 cm⁻¹
2. 106.4637 cm⁻¹
3. 123.8075 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 1.312579  | -0.734221 | 0.000069  |
| C    | 0.062951  | 0.040129  | -0.000018 |
| O    | 2.418535  | -0.241163 | 0.000094  |
| C    | -1.069661 | -0.673486 | -0.000004 |
| C    | -2.470035 | -0.169541 | -0.000047 |
| H    | 1.189450  | -1.831499 | 0.000115  |
| H    | -0.965311 | -1.755549 | 0.000062  |
| C    | 0.198028  | 1.530427  | -0.000085 |
| H    | -3.000560 | -0.550929 | 0.874504  |
| H    | -2.533251 | 0.914581  | -0.000286 |
| H    | -3.000664 | -0.551334 | -0.874356 |
| H    | -0.764555 | 2.032662  | -0.000412 |
| H    | 0.761448  | 1.855832  | 0.875341  |
| H    | 0.761987  | 1.855698  | -0.875211 |
### 5_trans2methyl2butenal_HEI_1_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.75467 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.628993 |

#### Frequencies (Top 3 out of 51)

1. 49.7297 cm⁻¹
2. 78.5463 cm⁻¹
3. 137.5390 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 1.553772 | 0.082458 | 0.000067 |
|-------|----------|----------|----------|
| C     | 0.091055 | 0.335848 | -0.000016 |
| O     | 2.082802 | -1.004616 | 0.000135 |
| C     | -0.725378 | -0.721320 | -0.000029 |
| C     | -2.214258 | -0.728253 | -0.000082 |
| H     | 2.179440 | 0.993649 | 0.000063 |
| H     | -0.246130 | -1.695813 | 0.000016 |
| C     | -0.305178 | 1.783055 | -0.000057 |
| H     | -2.582505 | -1.268902 | 0.874134 |
| H     | -2.648686 | 0.267239 | -0.000231 |
| H     | -2.582452 | -1.269155 | -0.874163 |
| H     | -1.382445 | 1.917659 | -0.000488 |
| H     | 0.099788 | 2.290694 | 0.877460 |
| H     | 0.100505 | 2.290829 | -0.877164 |
| Datum                                      | Value            |
|--------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.755606      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.630275     |
| Number of Imaginary Frequencies            | 0                |

**Frequencies (Top 3 out of 51)**

1. 38.4957 cm⁻¹  
2. 77.8926 cm⁻¹  
3. 133.7383 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C           | -1.774222 | -0.511772 | -0.618394 |
|-------------|-----------|-----------|-----------|
| C           | -0.887792 | 0.332741  | 0.006332  |
| C           | 0.440680  | 0.586473  | -0.604037 |
| O           | -2.948217 | -0.860627 | -0.241155 |
| C           | 1.294382  | -1.991993 | 0.096364  |
| H           | 0.299594  | -2.100277 | 0.524749  |
| H           | 1.267726  | -2.285251 | -0.952587 |
| H           | 1.995657  | -2.630564 | 0.629004  |
| S           | 1.850526  | -0.289962 | 0.268825  |
| H           | -1.398882 | -0.936362 | -1.566192 |
| C           | 0.856378  | 2.054748  | -0.637922 |
| H           | 0.926672  | 2.461099  | 0.372271  |
| H           | 1.823184  | 2.187280  | -1.125031 |
| H           | 0.108930  | 2.634578  | -1.181286 |
| H           | 0.458059  | 0.179784  | -1.617678 |
| C           | -1.202669 | 0.966826  | 1.330503  |
| H           | -2.114482 | 0.531950  | 1.739099  |
| H           | -1.354397 | 2.050313  | 1.266012  |
| H           | -0.395209 | 0.809719  | 2.054604  |
### 5_trans2methyl2butenal_HEI_3

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.753544 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.627407 |

#### Frequencies (Top 3 out of 51)

1. 61.1096 cm⁻¹
2. 78.9349 cm⁻¹
3. 138.7183 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          |          |          |          |
|----------|----------|----------|----------|
| C        | 2.134114 | -0.724772| 0.012877 |
| C        | 1.244096 | 0.312284 | -0.070909|
| C        | -0.116269| 0.165993 | 0.530429 |
| O        | 1.985120 | -1.872337| 0.561244 |
| C        | -2.835710| -0.563495| 0.076362 |
| H        | -2.687770| -1.141873| 0.987893 |
| H        | -3.272566| 0.401139 | 0.324549 |
| H        | -3.520890| -1.103671| -0.573744|
| S        | -1.268695| -0.387593| -0.808042|
| H        | 3.115885 | -0.515533| -0.462081|
| C        | -0.643843| 1.423093 | 1.209495 |
| H        | -0.766049| 2.235003 | 0.491522 |
| H        | -1.604641| 1.249330 | 1.693689 |
| H        | 0.064581 | 1.748740 | 1.974464 |
| H        | -0.091515| -0.659610| 1.242900 |
| C        | 1.577864 | 1.584400 | -0.798099|
| H        | 0.871766 | 1.801529 | -1.608872|
| H        | 1.575849 | 2.467047 | -0.148436|
| H        | 2.572001 | 1.513062 | -1.244088|

### 5_trans2methyl2butenal_HEI_4

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.752508 |
### Datum

|                       | Value                    |
|-----------------------|--------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.62562 |
| Number of Imaginary Frequencies | 0                        |

#### Frequencies (Top 3 out of 51)

1. 61.6042 cm⁻¹
2. 79.1990 cm⁻¹
3. 117.2525 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -1.781358 | 0.456369  | 0.452595  |
| C | -0.876732 | -0.013469 | -0.461942 |
| C | 0.432137  | 0.646806  | -0.727101 |
| O | -2.906596 | -0.059182 | 0.792638  |
| C | 1.357067  | -0.856653 | 1.471620  |
| H | 1.219701  | 0.033573  | 2.083290  |
| H | 0.424894  | -1.417736 | 1.440567  |
| H | 2.142601  | -1.469410 | 1.908870  |
| S | 1.877813  | -0.426175 | -0.196521 |
| H | -1.506426 | 1.405342  | 0.947070  |
| C | 0.630468  | 2.046913  | -0.159417 |
| H | 0.644716  | 2.040007  | 0.930625  |
| H | 1.575867  | 2.461225  | -0.506107 |
| H | -0.177997 | 2.706915  | -0.478436 |
| H | 0.615808  | 0.683543  | -1.806741 |
| C | -1.123142 | -1.310021 | -1.177521 |
| H | -2.180678 | -1.568771 | -1.137480 |
| H | -0.561834 | -2.145890 | -0.739241 |
| H | -0.819537 | -1.256221 | -2.228584 |

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### 5_trans2methyl2butenal_HEI.5

|                       | Value                    |
|-----------------------|--------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.748893 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.62345 |
| Number of Imaginary Frequencies | 0                        |

#### Frequencies (Top 3 out of 51)

1. 61.6042 cm⁻¹
2. 79.1990 cm⁻¹
3. 117.2525 cm⁻¹
1.  54.5171 cm⁻¹
2.  69.8699 cm⁻¹
3.  99.2142 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 1.637405 | 0.250749 | -0.753187 |
| C | 0.891074 | 0.033912 | 0.372258 |
| C | -0.439433 | 0.691751 | 0.575118 |
| O | 2.772639 | -0.247855 | -1.080102 |
| C | -1.558638 | -1.772329 | -0.226209 |
| H | -0.540973 | -2.024726 | -0.520272 |
| H | -1.723307 | -2.063836 | 0.810209 |
| H | -2.264076 | -2.302601 | -0.862190 |
| S | -1.830701 | -0.009285 | -0.457280 |
| H | 1.179003 | 0.953610 | -1.477832 |
| C | -0.494953 | 2.198555 | 0.329992 |
| H | -0.220973 | 2.441615 | -0.695755 |
| H | -1.495112 | 2.595015 | 0.516792 |
| H | 0.205877 | 2.701690 | 0.996486 |
| H | -0.755354 | 0.507734 | 1.604591 |
| C | 1.348121 | -0.924734 | 1.437965 |
| H | 2.344582 | -1.296278 | 1.200403 |
| H | 0.686042 | -1.792862 | 1.541901 |
| H | 1.392949 | -0.455379 | 2.427343 |

**5_trans2methyl2butenal_HEI_6_reopt**

| Datum                                                                 | Value          |
|-----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -708.750557    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -708.624244    |
| Number of Imaginary Frequencies                                       | 0              |

**Frequencies (Top 3 out of 51)**

1.  67.5161 cm⁻¹
2.  83.0977 cm⁻¹
3.  130.5373 cm⁻¹
**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atomic Symbol | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------------|--------------|--------------|--------------|
| C             | -2.196706    | 0.327898     | -0.469861    |
| C             | -1.024092    | 0.011249     | 0.162884     |
| C             | 0.196647     | 0.827939     | -0.089269    |
| O             | -3.333608    | -0.258707    | -0.406329    |
| C             | 2.499878     | -0.878875    | 0.242599     |
| H             | 3.053201     | -1.51579     | 0.832626     |
| H             | 1.874132     | -1.480864    | 0.897586     |
| H             | 3.208205     | -1.530831    | -0.264737    |
| S             | 1.521251     | -0.079149    | -1.048076    |
| H             | -2.130345    | 1.228072     | -1.117855    |
| C             | 0.815477     | 1.469664     | 1.151191     |
| H             | 1.080423     | 0.723099     | 1.899654     |
| H             | 1.714945     | 2.037101     | 0.907540     |
| H             | 0.086483     | 2.145022     | 1.600899     |
| H             | -0.063244    | 1.623931     | -0.791061    |
| C             | -0.922641    | -1.201984    | 1.041717     |
| H             | -1.921395    | -1.575252    | 1.267462     |
| H             | -0.416440    | -0.999458    | 1.990963     |
| H             | -0.368500    | -2.018541    | 0.561207     |

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**5_trans2methyl2butenal_HEI_7_reopt**

| Datum                                                      | Value     |
|------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -708.75341|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.628124|
| Number of Imaginary Frequencies                           | 0         |

**Frequencies (Top 3 out of 51)**

1. 51.6769 cm⁻¹
2. 57.0751 cm⁻¹
3. 123.8825 cm⁻¹

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**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atomic Symbol | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------------|--------------|--------------|--------------|
| C             | -2.027540    | -0.677132    | -0.576330    |
| C             | -1.114180    | 0.175088     | -0.015000    |
| C             | 0.277390     | 0.232479     | -0.553080    |
5_trans2methyl2butenal_TS_1_reopt

Datum | Value
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.741157
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.617051

Number of Imaginary Frequencies

Frequencies (Top 3 out of 51)

1. -175.5889 cm⁻¹
2. 65.7512 cm⁻¹
3. 83.2168 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | -1.694488 | -1.053723 | -0.181189 |
| C   | -1.151531 | 0.221389  | 0.175749  |
| C   | -0.304855 | 0.847739  | -0.704733 |
| O   | -1.509672 | -1.674754 | -1.231438 |
| C   | 1.508555  | -1.420185 | 0.875834  |
| H   | 0.422187  | -1.361265 | 1.025743  |
| H   | 1.732088  | -2.398185 | 0.449306  |
| H   | 1.980204  | -1.355258 | 1.856371  |
| S   | 2.028354  | -0.071550 | -0.203928 |
| H   | -2.352611 | -1.505440 | 0.587545  |
| C   | 0.072996  | 2.291358  | -0.578868 |
| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.743966 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.62048 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 51)

1. -192.0929 cm⁻¹
2. 35.8207 cm⁻¹
3. 89.8274 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.302908 | 2.558297 | 0.451069 |
|-------|----------|----------|----------|
| H     | 0.933356 | 2.532830 | -1.199176|
| H     | -0.767312| 2.913108 | -0.906522|
| H     | -0.235153| 0.414915 | -1.693015|
| C     | -1.419583| 0.777082 | 1.546712 |
| H     | -0.491033| 0.881056 | 2.118013 |
| H     | -1.886144| 1.764090 | 1.514308 |
| H     | -2.081337| 0.117207 | 2.109668 |

| Datum | Value       |
|-------|-------------|
| C     | -1.748642  | -0.581553 | -0.696017 |
| C     | -0.986565  | 0.421397  | -0.036054 |
| C     | 0.131712   | 0.911033  | -0.681325 |
| O     | -2.786421  | -1.120900 | -0.291930 |
| C     | 1.252896   | -1.941056 | 0.329144  |
| H     | 0.173078   | -1.749393 | 0.310392  |
| H     | 1.477682   | -2.688419 | -0.431553 |
| H     | 1.496576   | -2.360762 | 1.304726  |
| S     | 2.118577   | -0.385200 | 0.038950  |
| H     | -1.349378  | -0.873400 | -1.687297 |
| C     | 0.732139   | 2.241667  | -0.336659 |
| H     | 0.828724   | 2.367425  | 0.740173  |
| H     | 1.713845   | 2.364606  | -0.789343 |
| H     | 0.080024   | 3.038133  | -0.710105 |
| H     | 0.278897   | 0.582805  | -1.703368 |
| C     | -1.367263  | 0.866531  | 1.345718  |
| H     | -2.244350  | 0.318339  | 1.685434  |
| H     | -1.594892  | 1.933991  | 1.392018  |
| H     | -0.551729  | 0.682424  | 2.052326  |
### 5_trans2methyl2butenal_TS_3

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.735535 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.61188 |
| Number of Imaginary Frequencies | 1 |

**Frequencies (Top 3 out of 51)**

1. -227.2017 cm⁻¹
2. 58.2972 cm⁻¹
3. 91.5900 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C           | 2.052977 | -1.048834 | 0.057882 |
| C           | 1.426713 | 0.229584  | 0.014287 |
| C           | 0.185144 | 0.387618  | 0.596879 |
| O           | 1.605236 | -2.088321 | 0.556909 |
| C           | -2.894495| -0.386823 | 0.407078 |
| H           | -2.401418| -0.506307 | 1.376208 |
| H           | -3.484031| 0.529389  | 0.444165 |
| H           | -3.578678| -1.225252 | 0.280797 |
| S           | -1.657160| -0.343433 | -0.922422|
| H           | 3.056040 | -1.085955 | -0.411937|
| C           | -0.371455| 1.748829  | 0.886093 |
| H           | -0.297986| 2.401078  | 0.017477 |
| H           | -1.410782| 1.702945  | 1.201856 |
| H           | 0.211091 | 2.206458  | 1.693654 |
| H           | -0.154246| -0.421123 | 1.232240 |
| C           | 2.089537 | 1.347719  | -0.742545|
| H           | 1.498441 | 1.653766  | -1.612303|
| H           | 2.234124 | 2.240317  | -0.129235|
| H           | 3.069605 | 1.037622  | -1.107493|

### 5_trans2methyl2butenal_TS_4

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.735535 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.61188 |
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -1.737901 | 0.254599 | 0.703929 |
| C    | -1.009257  | 0.124744 | -0.505812 |
| C    | 0.112019   | 0.895936 | -0.758796 |
| O    | -2.733113  | -0.415269 | 1.023959 |
| C    | 1.525329   | -0.908701 | 1.346019 |
| H    | 2.023265   | -0.309790 | 2.108348 |
| H    | 0.445649   | -0.717752 | 1.410195 |
| H    | 1.686073   | -1.960895 | 1.577672 |
| S    | 2.092472   | -0.501718 | -0.317114 |
| H    | -1.397138  | 1.044234 | 1.394638 |
| C    | 0.518383   | 2.077742 | 0.082723 |
| H    | 0.665116   | 1.800462 | 1.125964 |
| H    | 1.449868   | 2.499808 | -0.284303 |
| H    | -0.251911  | 2.852821 | 0.048685 |
| H    | 0.448710   | 0.930409 | -1.786922 |
| C    | -1.424103  | -0.954080 | -1.464280 |
| H    | -2.502980  | -0.953637 | -1.627475 |
| H    | -1.162123  | -1.945971 | -1.081286 |
| H    | -0.926004  | -0.831483 | -2.426061 |

### 5_trans2methyl2butenal_TS_5_reopt

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.74078 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.616444 |
| Number of Imaginary Frequencies | 1 |
**Frequencies** (Top 3 out of 51)

1. \(-212.7943\) cm\(^{-1}\)
2. \(57.5735\) cm\(^{-1}\)
3. \(91.6194\) cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|         | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 1.737903| 0.254355| -0.703985|
| C       | 1.009235| 0.124966| 0.505798 |
| C       | -0.112040| 0.896269| 0.758464 |
| O       | 2.733113 | -0.415650| -1.023743 |
| C       | -1.525164| -0.909456| -1.345618 |
| H       | -0.445466| -0.718597| -1.409749 |
| H       | -1.685927| -1.961774| -1.576694 |
| H       | -2.022968| -0.310959| -2.108359 |
| S       | -2.092503| -0.501498| 0.317210  |
| H       | 1.397168 | 1.043733| -1.394997 |
| C       | -0.518374| 2.077756 | -0.083515 |
| H       | -0.665107| 1.800070| -1.126647 |
| H       | -1.449859| 2.499975| 0.283337  |
| H       | 0.251924 | 2.852844| -0.049775 |
| H       | -0.448765| 0.931131| 1.786566  |
| C       | 1.424004 | -0.953553| 1.464640  |
| H       | 2.502871 | -0.953063| 1.627910  |
| H       | 1.162049 | -1.945564| 1.081939  |
| H       | 0.925836 | -0.830645| 2.426344  |

**5_trans2methyl2butenal_TS_6_reopt**

| Datum | Value         |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy          | -708.737389 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.614079 |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 51)

1. \(-245.0999\) cm\(^{-1}\)
2. \(27.2601\) cm\(^{-1}\)
3. \(83.4120\) cm\(^{-1}\)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -2.180592 | -0.658954 | -0.387013 |
| C | -1.201631 | 0.309540  | -0.072426 |
| C | -0.074102 | 0.376043  | -0.882087 |
| O |  2.855281 | -0.055067 |  0.774371 |
| C |  3.289270 |  0.677063 |  0.093156 |
| H |  2.385326 |  0.484039 |  1.597251 |
| H |  3.667978 | -0.653783 |  1.185777 |
| S |  1.662137 | -1.128573 | -0.081330 |
| H | -1.957627 | -1.247693 | -1.299039 |
| C |  0.777934 |  1.609572 | -0.931812 |
| H |  1.085817 |  1.927789 |  0.063633 |
| H |  1.668954 |  1.458154 | -1.536478 |
| H |  0.193052 |  2.425382 | -1.368936 |
| H | -0.111473 | -0.198770 | -1.800164 |
| C | -1.324810 |  1.139001 |  1.172093 |
| H | -2.282927 |  0.949801 |  1.653282 |
| H | -1.251729 |  2.209838 |  0.968919 |
| H | -0.532797 |  0.894856 |  1.888724 |

5_trans2methyl2butenal_TS_7_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.738142 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.61449 |
| Number of Imaginary Frequencies | 2 |

**Frequencies** (Top 3 out of 51)

1. -231.7576 cm⁻¹
2. -11.7553 cm⁻¹
3. 66.1223 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -2.116060 | -0.727250 | -0.549130 |
| C | -1.262524 |  0.297543 | -0.073546 |
| C | -0.056736 |  0.484771 | -0.731428 |
6_2ethylacrolein_1

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -270.531295      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.439235      |

Number of Imaginary Frequencies
0

Frequencies (Top 3 out of 36)

1. 95.3467 cm⁻¹
2. 170.7274 cm⁻¹
3. 207.4475 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 1.310085 | -0.452009 | -0.129494 |
| O   | 1.149757 | -1.627067 | 0.102718  |
| C   | 0.290050 | 0.588786  | 0.117403  |
| C   | 0.638347 | 1.846849  | -0.147302 |
| C   | -1.050992| 0.154693  | 0.628937  |
| C   | -1.895121| -0.494931 | -0.469810 |
| H   | 2.265584 | -0.085257 | -0.543169 |
| H   | -0.040331| 2.673703  | 0.018235  |
| H   | 1.621695 | 2.081105  | -0.537450 |
| H   | -0.903122| -0.560239 | 1.440170  |
| H   | -1.573829| 1.018200  | 1.039448  |
### 6_2ethylacrolein_2

| Datum                                                                 | Value                  |
|-----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -270.531295            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -270.439235            |
| Number of Imaginary Frequencies                                       | 0                      |

**Frequencies (Top 3 out of 36)**

1. 95.3453 cm⁻¹  
2. 170.7257 cm⁻¹  
3. 207.4476 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C           | -1.310088 | -0.452001 | -0.129495 |
|-------------|-----------|-----------|-----------|
| O           | -1.149770 | -1.627060 | 0.102718  |
| C           | -0.290046 | 0.588787  | 0.117404  |
| C           | -0.638334 | 1.846852  | -0.147302 |
| C           | 1.050993  | 0.154684  | 0.628938  |
| C           | 1.895119  | -0.494939 | -0.469811 |
| H           | -2.265583 | -0.085241 | -0.543173 |
| H           | 0.040347  | 2.673702  | 0.018238  |
| H           | -1.621681 | 2.081113  | -0.537451 |
| H           | 1.573834  | 1.018188  | 1.039453  |
| H           | 0.903117  | -0.560251 | 1.440168  |
| H           | 2.852433  | -0.828794 | -0.071675 |
| H           | 1.382084  | -1.358144 | -0.892087 |
| H           | 2.087740  | 0.215607  | -1.273627 |

### 6_2ethylacrolein_3

| Datum                                                                 | Value                  |
|-----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -270.532199            |
### Datum Values

| Datum                                                      | Value                     |
|------------------------------------------------------------|---------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.440101               |

**Number of Imaginary Frequencies** 0

### Frequencies (Top 3 out of 36)

1. 94.6321 cm⁻¹  
2. 171.2586 cm⁻¹  
3. 215.7651 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|        | x       | y       | z       |
|--------|---------|---------|---------|
| C      | 1.590656| 0.175891| -0.000000|
| O      | 2.097329| -0.920862| 0.000002|
| C      | 0.131847| 0.412032| -0.000007|
| C      | -0.267919| 1.682388| 0.000002|
| C      | -0.755735| -0.796686| -0.000002|
| C      | -2.244360| -0.490955| 0.000002|
| H      | 2.216190| 1.084892| 0.000004|
| H      | -1.312391| 1.962621| 0.000004|
| H      | 0.458243| 2.486371| 0.000001|
| H      | -0.493861| -1.407551| -0.867749|
| H      | -0.493855| -1.407542| 0.867750|
| H      | -2.529538| 0.083239| 0.882147|
| H      | -2.529536| 0.083260| -0.882131|
| H      | -2.820809| -1.414415| -0.000010|

### 6_2ethylacrolein_4

| Datum                                                      | Value                     |
|------------------------------------------------------------|---------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -270.526283               |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.434897               |

**Number of Imaginary Frequencies** 0

### Frequencies (Top 3 out of 36)

1. 68.4703 cm⁻¹  
2. 124.2051 cm⁻¹  
3. 210.5525 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     |    X      |    Y      |    Z      |
|-----|-----------|-----------|-----------|
| C   |  1.027084 | -0.745879 |  0.216094 |
| O   |  2.167950 | -0.756447 | -0.177122 |
| C   | -1.307818 |  0.186805 |  0.570835 |
| C   | -2.060129 | -0.618122 | -0.490717 |
| H   | -0.011331 |  2.495876 | -0.245796 |
| H   |  1.647133 |  1.702382 | -0.500829 |
| H   | -1.325064 | -0.359357 |  1.517818 |
| H   | -1.807014 |  1.140026 |  0.741241 |
| H   | -3.080110 | -0.824678 | -0.169759 |
| H   | -2.097941 | -0.066494 | -1.429908 |
| H   | -1.569559 | -1.573666 | -0.683197 |

6_2ethylacrolein_5

| Datum | Value     |
|-------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -270.526283 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.434897 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 36)

1. 68.4702 cm⁻¹
2. 124.2054 cm⁻¹
3. 210.5523 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     |    X      |    Y      |    Z      |
|-----|-----------|-----------|-----------|
| C   | -1.027084 | -0.745879 |  0.216094 |
| O   | -2.167951 | -0.756447 | -0.177122 |
| C   | -1.18368 |  0.434282 |  0.171922 |
| C   | -0.607802 |  1.608760 | -0.213605 |
| C   |  1.307818 |  0.186801 |  0.570837 |
| C   |  2.060130 | -0.618120 | -0.490719 |
| H   | -0.588452 | -1.657596 |  0.660231 |
6_2ethylacrolein_6

Datum | Value
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -270.527037
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -270.435495
Number of Imaginary Frequencies | 0

Frequencies (Top 3 out of 36)

1. 73.1261 cm⁻¹
2. 112.3255 cm⁻¹
3. 232.7511 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

Datum | Value
--- | ---
C | -1.419323 -0.616328 0.000000
O | -2.504471 -0.088817 0.000000
C | -0.115308 0.106272 -0.000000
C | -0.122566 1.435613 -0.000000
C | 1.105552 -0.770304 -0.000000
C | 2.427074 -0.021733 0.000000
H | -1.341727 -1.718465 -0.000000
H | 0.788940 2.017154 -0.000000
H | -1.063328 1.970431 0.000000
H | 1.051039 -1.432506 0.869684
H | 1.051039 -1.432505 -0.869685
H | 3.261081 -0.721128 0.000000
H | 2.518073 0.613222 -0.881867
H | 2.518072 0.613221 0.881868

6_2ethylacrolein_HEI_10_reopt
### Datum | Value
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.746647
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.62038
Number of Imaginary Frequencies | 0

**Frequencies (Top 3 out of 51)**

1. 42.3216 cm⁻¹
2. 62.2812 cm⁻¹
3. 88.3811 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |  C           |  O           |  C           |  C           |  C           |  H           |  H           |  H           |  S           |
|---|---|---|---|---|---|---|---|---|---|
|   | 1.245352 | -1.370579 | -0.224901 | 2.355402 | -1.522765 | -0.846384 | 0.771041 | -0.279661 | 0.450207 |
|  O | 2.355402 | -1.522765 | -0.846384 | 0.771041 | -0.279661 | 0.450207 | 1.605645 | 0.964483 | 0.610315 |
|  C | -0.557408 | -0.331083 | 1.46137  | 1.605645 | 0.964483 | 0.610315 | 1.145558 | 2.176480 | -0.204059 |
|  C | 1.145558 | 2.176480 | -0.204059 | 0.548922 | -2.236546 | -0.223974 | -0.720487 | 0.588273 | 1.712314 |
|  H | 0.548922 | -2.236546 | -0.223974 | -0.720487 | 0.588273 | 1.712314 | -0.645030 | -1.156035 | 1.858595 |
|  H | 1.639905 | 1.261217 | 1.666238 | 2.630564 | 0.717977 | 0.326262 | 1.791366 | 3.041198 | -0.035921 |
|  H | 2.630564 | 0.717977 | 0.326262 | 1.791366 | 3.041198 | -0.035921 | 1.153412 | 1.947523 | -1.271208 |
|  H | 1.153412 | 1.947523 | -1.271208 | 0.127611 | 2.465482 | 0.063724 | 0.127611 | 2.465482 | 0.063724 |
|  H | 0.127611 | 2.465482 | 0.063724 | 0.127611 | 2.465482 | 0.063724 | 0.127611 | 2.465482 | 0.063724 |
|  C | -1.954456 | 0.801144 | -1.016816 | -2.101609 | 1.746911 | -0.497779 | -2.101609 | 1.746911 | -0.497779 |
|  H | -2.101609 | 1.746911 | -0.497779 | -2.101609 | 1.746911 | -0.497779 | -0.979060 | 0.797520 | -1.500881 |
|  H | -0.979060 | 0.797520 | -1.500881 | -2.732648 | 0.680227 | -1.767228 | -2.732648 | 0.680227 | -1.767228 |
|  H | -2.732648 | 0.680227 | -1.767228 | -2.732648 | 0.680227 | -1.767228 | -2.068160 | -0.589771 | 0.117227 |

### 6_2ethylacrolein_HEI_11_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.74867 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.622145 |
| Number of Imaginary Frequencies | 0 |
**Frequencies (Top 3 out of 51)**

1. 66.0674 cm⁻¹
2. 71.2197 cm⁻¹
3. 135.5803 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |  C  |  O  |  C  |  C  |  C  |  C  |  H  |  H  |  H  |  H  |  H  |  C  |  H  |  H  |  H  |  S  |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C | -2.220021 | -0.244154 | -0.037067 | 0.050472 | -0.628685 | -0.078893 | -0.418759 | -0.514184 | -1.893701 | 0.514184 | -0.806808 | 1.685120 | 0.217207 | -0.472595 | 2.647731 |
| O | -2.672552 | -1.411048 | -0.305459 | 0.130061 | 0.386757 | 0.657970 | 0.582511 | -0.662919 | -1.068898 | 1.644030 | 0.908182 | 1.397349 | -0.447068 | -1.441761 | -1.072225 |
| C | -0.971236 | 0.130061 | 0.386757 | -0.912178 | 1.584254 | 2.293390 | 0.607624 | 0.605417 | 0.988469 | 1.685120 | 1.397349 | 1.397349 | -0.447068 | -1.441761 | -1.072225 |
| C | 0.050472 | -0.912178 | 0.657970 | 0.582511 | 2.293390 | -0.662919 | 0.607624 | 0.605417 | 0.988469 | 1.685120 | 1.397349 | 1.397349 | -0.447068 | -1.441761 | -1.072225 |
| C | -0.628685 | 1.584254 | 0.582511 | 2.293390 | -0.662919 | -1.068898 | 1.644030 | 0.908182 | 1.397349 | 1.397349 | 1.397349 | -0.447068 | -1.441761 | -1.072225 |
| C | -0.078893 | 2.293390 | -0.662919 | -1.068898 | 1.644030 | 0.908182 | 1.397349 | 1.397349 | 1.397349 | 1.397349 | 1.397349 | -0.447068 | -1.441761 | -1.072225 |
| C | -0.628685 | 1.584254 | 0.582511 | 2.293390 | -0.662919 | -1.068898 | 1.644030 | 0.908182 | 1.397349 | 1.397349 | 1.397349 | -0.447068 | -1.441761 | -1.072225 |
| H | -2.926331 | 0.607624 | -0.146712 | -0.418759 | 0.514184 | -0.806808 | 1.685120 | 0.217207 | 3.322908 | -0.447068 | -1.441761 | -1.072225 |
| H | -0.418759 | -0.806808 | 1.685120 | 0.514184 | -0.806808 | 1.685120 | 0.217207 | 3.322908 | -0.447068 | -1.441761 | -1.072225 |
| H | 0.514184 | -0.806808 | 1.685120 | 0.217207 | 3.322908 | -0.447068 | -1.441761 | -1.072225 |
| H | -0.418759 | 0.514184 | -0.806808 | 1.685120 | 0.217207 | 3.322908 | -0.447068 | -1.441761 | -1.072225 |
| H | -0.843259 | 2.316994 | -1.441761 | 0.843259 | -2.316994 | -1.441761 | -1.072225 |
| H | 0.782784 | 1.765529 | -1.072225 | -0.782784 | 1.765529 | -1.072225 |
| C | 2.647731 | 0.100686 | 0.315483 | 2.647731 | 0.100686 | 0.315483 |
| H | 2.253956 | 1.115095 | 0.340262 | 2.253956 | 1.115095 | 0.340262 |
| H | 2.853590 | -0.232938 | 1.331383 | 2.853590 | -0.232938 | 1.331383 |
| H | 3.575890 | 0.094465 | -0.253402 | 3.575890 | 0.094465 | -0.253402 |
| S | 1.499845 | -1.032999 | -0.492387 | 1.499845 | -1.032999 | -0.492387 |

**6_2ethylacrolein_HE1_1_reopt**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.751352 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.624592 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 51)**

1. 58.1745 cm⁻¹
2. 66.7213 cm⁻¹
3. 92.2488 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -1.048424 | 1.364741 | -0.025295 |
| O | -0.392727 | 2.455703 | -0.197420 |
| C | -0.708911 | 0.093848 | -0.407164 |
| C | 0.568339  | -0.137604 | -1.129254 |
| C | -1.537110 | -1.134650 | -0.128642 |
| C | -2.849506 | -0.917888 | 0.615232  |
| H | -2.022344 | 1.452219  | 0.489984  |
| H | 0.969347  | 0.797130  | -1.517471 |
| H | 0.458483  | -0.844300 | -1.956833 |
| H | -1.758737 | -1.647699 | -1.075107 |
| H | -0.935260 | -1.854805 | 0.441474  |
| H | -3.367492 | -1.866461 | 0.760014  |
| H | -2.681124 | -0.474212 | 1.597634  |
| H | -3.515806 | -0.252349 | 0.064276  |
| C | 2.087252  | 0.363716  | 1.144394  |
| H | 2.580273  | 1.245851  | 0.740265  |
| H | 1.097408  | 0.636766  | 1.507906  |
| H | 2.681924  | -0.042773 | 1.959300  |
| S | 1.910332  | -0.911748 | -0.115482 |

6_2ethylacrolein_HEI_2

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.753478 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.627384 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 51)**

1. 25.3831 cm⁻¹
2. 69.2392 cm⁻¹
3. 87.5653 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 0.961022  | -1.708862 | 0.182958 |
| O | 0.378202  | -2.710489 | -0.360735 |
| C | 0.785315  | -0.368017 | -0.043610 |
6_2ethylacrolein_HEI_3_reopt

| Datum                                      | Value             |
|--------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.751683       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.625381 |

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 51)

1. 45.9582 cm⁻¹
2. 75.4815 cm⁻¹
3. 88.5131 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
6_2ethylacrolein_HEI_4_reopt

| Datum                                    | Value             |
|------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -708.74784        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.621306      |
| Number of Imaginary Frequencies          | 0                 |

**Frequencies** (Top 3 out of 51)

1. 51.6127 cm⁻¹
2. 68.7305 cm⁻¹
3. 118.6205 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -1.849233 | -0.926036 | -0.085076 |
| O | -1.904784 | -2.210069 | -0.063489 |
| C | -0.797545 | -0.110617 | 0.237936  |
| C | 0.480087  | -0.719532 | 0.691553  |
| C | -0.814638 | 1.391600  | 0.126053  |
| C | -2.153494 | 2.035889  | -0.215089 |
| H | -2.769542 | -0.399081 | -0.395915 |
| H | 0.345052  | -1.789500 | 0.837718  |
| H | 0.853239  | -0.287147 | 1.625774  |
| H | -0.083897 | 1.712106  | -0.629744 |
| H | -0.448826 | 1.827577  | 1.066927  |
| H | -2.059587 | 3.122010  | -0.237401 |
| H | -2.514665 | 1.712787  | -1.192171 |
| H | -2.917449 | 1.777728  | 0.519997  |
| C | 2.723322  | 0.908900  | 0.175597  |
| H | 2.067870  | 1.775078  | 0.120144  |
| H | 3.030937  | 0.750328  | 1.207930  |
| H | 3.607770  | 1.091576  | -0.431183 |
| S | 1.912307  | -0.568384 | -0.473125 |
6_2ethylacrolein_HEI_5_reopt

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -708.750409         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -708.623966         |
| Number of Imaginary Frequencies                                      | 0                   |

**Frequencies (Top 3 out of 51)**

1. 46.3403 cm⁻¹
2. 80.1312 cm⁻¹
3. 116.1938 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |                  |                  |                  |
|-----|------------------|------------------|------------------|
| C   | -2.215912        | -0.343211        | -0.244514        |
| O   | -2.705190        | -1.460907        | 0.145725         |
| C   | -0.964011        | 0.176131         | -0.039470        |
| C   | 0.037560         | -0.610846        | 0.727721         |
| C   | -0.556457        | 1.498818         | -0.623847        |
| C   | -0.104946        | 2.538175         | 0.406531         |
| H   | -2.884962        | 0.321742         | -0.831064        |
| H   | -0.443070        | -1.499281        | 1.134113         |
| H   | 0.492022         | -0.064528        | 1.559238         |
| H   | -1.393384        | 1.904497         | -1.190840        |
| H   | 0.255866         | 1.366159         | -1.351898        |
| H   | 0.744844         | 2.176024         | 0.988449         |
| H   | -0.913031        | 2.758752         | 1.106201         |
| H   | 0.198974         | 3.471815         | -0.070535        |
| C   | 2.660082         | 0.102124         | -0.027024        |
| H   | 3.603153         | -0.214945        | -0.467411        |
| H   | 2.322068         | 1.008275         | -0.524449        |
| H   | 2.816906         | 0.304721         | 1.031500         |
| S   | 1.481890         | -1.250820        | -0.234093        |

6_2ethylacrolein_HEI_6

| Datum | Value |
|-------|-------|
|       |       |
|       |       |
|       |       |
|       |       |
### SI_aldehydes

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.75369 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.627786 |
| Number of Imaginary Frequencies | 0 |

#### Frequencies (Top 3 out of 51)

1. 49.5605 cm⁻¹
2. 70.7235 cm⁻¹
3. 84.1861 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C    | 0.970522  | -1.454678  | -0.383340  |
| O    | 1.917653  | -2.121459  | 0.158777   |
| C    | 0.636559  | -0.136657  | -0.209937  |
| C    | -0.503172 | 0.446218   | -0.954705  |
| C    | 1.399353  | 0.755015   | 0.728642   |
| C    | 2.423736  | 1.651121   | 0.023732   |
| H    | 0.317834  | -1.99522    | -1.102512  |
| H    | -0.818469 | -0.200839   | -1.775242  |
| H    | -0.286460 | 1.433168    | -1.372339  |
| H    | 0.700965  | 1.391370    | 1.284024   |
| H    | 1.916528  | 0.136785    | 1.465321   |
| H    | 2.930841  | 2.320137    | 0.722363   |
| H    | 3.180365  | 1.043095    | -0.474761  |
| H    | 1.941458  | 2.268139    | -0.737154  |
| C    | -2.441452 | -0.925644   | 0.487206   |
| H    | -2.732104 | -1.492046   | -0.396942  |
| H    | -1.577591 | -1.398988   | 0.951600   |
| H    | -3.270286 | -0.907391   | 1.191032   |
| S    | -2.034848 | 0.772576    | 0.051551   |

---

### 6_2ethylacrolein_HEI_7

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.750136 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.624003 |
| Number of Imaginary Frequencies | 0 |
**Frequencies (Top 3 out of 51)**

1. 50.9865 cm⁻¹  
2. 69.6115 cm⁻¹  
3. 73.6690 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  | C         | O         | C         | C         | C         | C         | H         | H         | H         | H         | H         | H         | C         | H         | H         | H         | S         | C         |
|---|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|  | -1.464276 | 1.279920  | -0.074037 |           |           |           | -2.521902 |           |           |           |           |           |           | 3.280926  |           |           |           | 1.717436  |
|  | -0.971776 | 2.465505  | -0.094588 |           |           |           | -1.422228 | 1.150819  |           |           |           |           |           |           |           |           |           |           |
|  | -0.847106 | 0.113045  | 0.288201  |           |           |           | -0.900219 | -1.923123 |           |           |           |           |           |           |           |           |           |
|  | 0.573458  | 0.150470  | 0.731692  |           |           |           | -3.590311 | -0.700166 |           |           |           |           |           |           |           |           |           |
|  | -1.492798 | -1.249952 | 0.260854  |           |           |           | -3.039428 | -0.930840 |           |           |           |           |           |           |           |           |           |
|  | -2.940476 | -1.304010 | -0.212341 |           |           |           | -3.109222 | -2.329316 |           |           |           |           |           |           |           |           |           |
|  |           |           |           | 3.280926  | -0.335666 | 0.263175  |           |           |           |           |           |           |           |           |           |           |           |
|  |           |           |           | 3.248188  | -1.083382 | 1.054295  |           |           |           |           |           |           |           |           |           |           |           |
|  |           |           |           | 3.496122  | 0.639927  | 0.696435  |           |           |           |           |           |           |           |           |           |           |           |
|  |           |           |           | 4.071602  | -0.594980 | -0.437331 |           |           |           |           |           |           |           |           |           |           |           |
|  |           |           |           | 1.717436  | -0.299494 | -0.638024 |           |           |           |           |           |           |           |           |           |           |           |

**6_2ethylacrolein_HEI_8**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.749671   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.623237 |
| Number of Imaginary Frequencies            | 0             |

**Frequencies (Top 3 out of 51)**

1. 47.3676 cm⁻¹  
2. 52.0017 cm⁻¹  
3. 99.9024 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C   | O   | S   |
|---|-----|-----|-----|
| C | 1.217199 | 1.433479 | -0.029129 |
| O | 2.243474 | 1.740017 | 0.668611 |
| C | 0.617806 | 0.212308 | -0.188691 |
| C | -0.561702 | 0.070345 | -1.082501 |
| C | 1.184742 | -1.024085 | 0.459530 |
| C | 2.199333 | -1.759030 | -0.424472 |
| H | 0.725873 | 2.255752 | -0.594172 |
| H | -0.598305 | -0.918623 | -1.544566 |
| H | -0.564925 | 0.809472 | -1.885119 |
| H | 1.671531 | -0.747866 | 1.398421 |
| H | 0.384342 | -1.723954 | 0.715979 |
| H | 2.577331 | -2.665946 | 0.053151 |
| H | 1.743274 | -2.045595 | -1.374528 |
| H | 3.048674 | -1.111322 | -0.646203 |
| C | -2.119568 | -0.690820 | 1.149315 |
| H | -2.034641 | -1.744772 | 0.888450 |
| H | -1.257200 | -0.389640 | 1.742187 |
| H | -3.026283 | -0.539592 | 1.730869 |
| S | -2.240270 | 0.340548 | -0.321104 |

6_2ethylacrolein_HEI_9

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.752205 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.626445 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 51)

1. 40.6516 cm⁻¹
2. 59.5642 cm⁻¹
3. 86.1327 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C   | O   | S   |
|---|-----|-----|-----|
| C | -1.532784 | -1.453451 | -0.120118 |
| O | -1.072975 | -2.571914 | 0.296833 |
| C | -0.977808 | -0.203845 | -0.027941 |
### 6_2ethylacrolein_TS_10_reopt

| Datum                                                      | Value        |
|------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -708.741213  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -708.615924  |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 51)

1.  -186.4154 cm\(^{-1}\)
2.   73.8370 cm\(^{-1}\)
3.   87.3594 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|    |    |    |
|----|----|----|
| C  | -1.449309 | -1.253680 | 0.077139 |
| O  | -2.471866 | -1.134509 | 0.758117 |
| C  | -0.841640 | -0.238981 | -0.721185 |
| C  | -0.278777 | -0.566970 | -1.443195 |
| C  | -1.397671 | 1.157270  | -0.679422 |
| C  | -1.015825 | 1.897813  | 0.605399  |
| H  | -0.942956 | -2.238036 | 0.036001  |
| H  | 0.628633  | 0.069487  | -2.245846 |
| H  | 0.588039  | -1.601716 | -1.499103 |
| H  | -1.031952 | 1.715714  | -1.543718 |
| H  | -2.486853 | 1.119406  | -0.758163 |
### 6_2ethylacrolein_TS_11_reopt

| Datum | Value                     |
|-------|---------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.731764 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.607797 |

#### Number of Imaginary Frequencies

1

#### Frequencies (Top 3 out of 51)

1. -223.3808 cm⁻¹
2. 48.4183 cm⁻¹
3. 71.2113 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -2.183047  | -0.588327  | -0.144863 |
|-------|------------|------------|-----------|
| O     | -2.283946  | -1.788981  | -0.403557 |
| C     | -1.101111  | 0.061854   | 0.532222  |
| C     | -0.080371  | -0.698254  | 1.038534  |
| C     | -1.071581  | 1.567651   | 0.541095  |
| C     | -0.613525  | 2.156605   | -0.796020 |
| H     | -3.008549  | 0.086729   | -0.448636 |
| H     | -0.201606  | -1.770407  | 1.087266  |
| H     | 0.639022   | -0.262666  | 1.718847  |
| H     | -2.064995  | 1.960271   | 0.778121  |
| H     | -0.404304  | 1.908863   | 1.336295  |
| H     | -0.561616  | 3.245809   | -0.758198 |
| H     | -1.307296  | 1.879196   | -1.592118 |
| H     | 0.369004   | 1.767214   | -1.065641 |
| H     | -0.404304  | 1.908863   | 1.336295  |
| H     | 2.692794   | 0.507339   | 0.276668  |
| H     | 1.976213   | 1.322444   | 0.399065  |
| H     | 3.093625   | 0.263116   | 1.261155  |
| H     | 3.514201   | 0.872711   | -0.338819 |
| S     | 1.898057   | -0.937665  | -0.489669 |
### 6_2ethylacrolein_TS_1

| Datum                                                                 | Value                      |
|-----------------------------------------------------------------------|----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -708.734214                |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.609492                |
| Number of Imaginary Frequencies                                        | 1                          |

**Frequencies** (Top 3 out of 51)

1.  -149.1867 cm⁻¹
2.   40.6311 cm⁻¹
3.   65.9663 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -1.194081 | 1.264713 | 0.402080 |
| O | -0.669064 | 2.365219 | 0.557307 |
| C | -0.819758 | 0.282644 | -0.590168 |
| C | 0.199740  | 0.586178 | -1.432623 |
| C | -1.420101 | -1.107079 | -0.612481 |
| C | -2.536253 | -1.382005 | 0.388983  |
| H | -2.029800 | 0.988997  | 1.066096  |
| H | 0.614932  | 1.582285  | -1.445436 |
| H | 0.457786  | -0.067488 | -2.252772 |
| H | -1.788235 | -1.320943 | -1.619071 |
| H | -0.605928 | -1.819863 | -0.436418 |
| H | -2.895884 | -2.404081 | 0.275863  |
| H | -2.190923 | -1.264270 | 1.417321  |
| H | -3.384816 | -0.712174 | 0.242598  |
| C | 1.546063  | -0.676067 | 1.328346  |
| H | 1.977225  | -0.117082 | 2.159056  |
| H | 0.492521  | -0.376572 | 1.243146  |
| H | 1.564005  | -1.736402 | 1.582334  |
| S | 2.405498  | -0.342779 | -0.224749 |
### M06-2X/def2tzvpp-IEFPCM(water) Energy

| Datum                              | Value   |
|-----------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.736714 |

### M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)

| Datum                              | Value   |
|-----------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.612756 |

### Number of Imaginary Frequencies

| Datum                              | Value   |
|-----------------------------------|---------|
| Number of Imaginary Frequencies | 1       |

### Frequencies (Top 3 out of 51)

1. -150.0792 cm⁻¹  
2. 30.6711 cm⁻¹  
3. 52.3600 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Datum                              | Value   |
|-----------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates |         |

### 6_2ethylacrolein_TS_3_reopt

| Datum                              | Value   |
|-----------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.736628 |

### M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)

| Datum                              | Value   |
|-----------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.611779 |

### Number of Imaginary Frequencies

| Datum                              | Value   |
|-----------------------------------|---------|
| Number of Imaginary Frequencies | 1       |
Frequencies (Top 3 out of 51)

1. -176.8316 cm\(^{-1}\)
2. 40.4011 cm\(^{-1}\)
3. 68.1290 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C          | O          | H          |
|---|------------|------------|------------|
|   | -1.490241  | 1.193859   | -0.397538  |
|   | -1.030703  | 2.328063   | -0.522331  |
|   | -1.067505  | 0.185430   | 0.537395   |
|   | -0.067422  | 0.476728   | 1.418813   |
|   | -1.712168  | -1.176374  | 0.464839   |
|   | -1.183260  | -2.089731  | -0.601743  |
|   | -2.334827  | 0.891211   | -1.049021  |
|   | 0.158490   | -0.190167  | 2.237861   |
|   | 0.279399   | 1.494694   | 1.508145   |
|   | -1.627654  | -1.659425  | 1.440388   |
|   | -2.782425  | -1.065068  | 0.268094   |
|   | -1.237442  | -1.663573  | -1.597515  |
|   | -1.569426  | -3.075966  | -0.590039  |
|   | -0.031910  | -2.207122  | -0.433364  |
|   | 1.649235   | -0.069669  | -1.296844  |
|   | 0.558269   | 0.035616   | -1.307398  |
|   | 2.074409   | 0.775894   | -1.837815  |
|   | 1.894380   | -0.983989  | -1.837471  |
|   | 2.225783   | -0.131129  | 0.414203   |

6_2ethylacrolein_TS_4_reopt2

| Datum                                           | Value        |
|------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -708.736714  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.612755  |
| Number of Imaginary Frequencies                 | 1            |

Frequencies (Top 3 out of 51)

1. -150.0580 cm\(^{-1}\)
2. 30.6804 cm\(^{-1}\)
3. 52.3396 cm\(^{-1}\)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       |           |           |           |
|-------|-----------|-----------|-----------|
| C     | -0.869534 | 1.627624  | 0.277545  |
| O     | -0.273218 | 2.561783  | -0.249946 |
| C     | -0.879016 | 0.253615  | -0.163704 |
| C     | -1.160204 | -0.087778 | -1.265334 |
| C     | -1.594983 | -0.780497 | 0.666312  |
| C     | -2.811260 | -1.388935 | -0.031588 |
| H     | -1.471327 | 1.826293  | 1.185978  |
| H     | 0.276331  | 0.681974  | -1.83485  |
| H     | -0.222901 | -1.079234 | -1.68847  |
| H     | -1.908241 | -0.331136 | 1.612307  |
| H     | -0.891083 | -1.578529 | 0.923716  |
| H     | -3.285080 | -2.152069 | 0.586809  |
| H     | -3.552159 | -0.619562 | -0.252794 |
| H     | -2.520416 | -1.851848 | -0.975463 |
| C     | 1.974348  | -0.152556 | 1.253448  |
| H     | 0.946499  | 0.225691  | 1.338967  |
| H     | 2.096261  | -0.941122 | 1.996235  |
| H     | 2.647717  | 0.665992  | 1.508368  |
| S     | 2.257127  | -0.760597 | -0.423268 |

6_2ethylacrolein_TS_5_reopt3

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.735787 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.610591 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 51)

1. -157.9454 cm\(^{-1}\)
2.  46.8608 cm\(^{-1}\)
3.  80.2895 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       |           |           |           |
|-------|-----------|-----------|-----------|
| C     | 1.423551  | -1.346452 | 0.381686  |
| O     | 0.926702  | -2.456874 | 0.210889  |
| C     | 1.143237  | -0.150281 | -0.374351 |
6_2ethylacrolein_TS_6

| Datum                                           | Value      |
|------------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -708.73997 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy     | -708.61589 |
| (Quasiharmonic)                                 |            |
| Number of Imaginary Frequencies                 | 1          |
| Frequencies (Top 3 out of 51)                   |            |
| 1.    -178.2163 cm⁻¹                             |            |
| 2.      32.0492 cm⁻¹                             |            |
| 3.      44.5987 cm⁻¹                             |            |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       |       |       |
|-------|-------|-------|
| C     | 1.018062 | -1.325609 | -0.578804 |
| O     | 1.862150 | -1.977163 | 0.042585  |
| C     | 0.689256 | 0.046752  | -0.374476 |
| C     | -0.259873 | 0.615751  | -1.187179 |
| C     | 1.360450 | 0.808547  | 0.734234  |
| C     | 2.718526 | 1.382477  | 0.325540  |
| H     | 0.450684 | -1.819387 | -1.392047 |
| H     | -0.620089 | 0.067853  | -2.047177 |
| H     | -0.368614 | 1.689093  | -1.236038 |
| H     | 0.703008 | 1.618929  | 1.057756  |
| H     | 1.497840 | 0.145234  | 1.591688  |
| Datum                                           | Value          |
|------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -708.731083    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.608764    |

Number of Imaginary Frequencies 1

**Frequencies** (Top 3 out of 51)

1. -186.6098 cm⁻¹
2. 11.1587 cm⁻¹
3. 25.0467 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
### 6_2ethylacrolein_TS_8_reopt

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -708.73997             |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.615915            |
| Number of Imaginary Frequencies                                      | 1                      |

**Frequencies** (Top 3 out of 51)

1. -178.2804 cm⁻¹  
2. 30.7166 cm⁻¹  
3. 44.2395 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C          | O          | C          | C          | C          | C          | H          | H          | H          | H          | H          | H          | H          | C          | H          | H          | H          | H          | S          |
|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|   | -1.018215  | 1.325444   | 0.579034   | -1.862352  | 1.976824   | -0.042483  | -0.689091  | -0.046838  | 0.374768   | 0.260171   | -0.615596  | 1.187524   | -1.359951  | -0.808745  | -0.734069  | -2.718238  | -1.382492  | -0.325816  |
|   | -1.359951  | -0.808745  | -0.734069  | 0.260171   | -0.615596  | 1.187524   | -1.359951  | -0.808745  | -0.734069  | 0.260171   | -0.615596  | 1.187524   | -1.359951  | -0.808745  | -0.734069  | -2.718238  | -1.382492  | -0.325816  |
|   | -2.718238  | -1.382492  | -0.325816  | 0.260171   | -0.615596  | 1.187524   | -1.359951  | -0.808745  | -0.734069  | 0.260171   | -0.615596  | 1.187524   | -1.359951  | -0.808745  | -0.734069  | -2.718238  | -1.382492  | -0.325816  |
|   | -0.451039  | 1.819362   | 1.392335   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   |
|   | -0.451039  | 1.819362   | 1.392335   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   |
|   | -0.451039  | 1.819362   | 1.392335   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   |
|   | -0.451039  | 1.819362   | 1.392335   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   |
|   | -0.451039  | 1.819362   | 1.392335   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   | 0.620122   | -0.067618  | 2.047583   | 0.369124   | -1.688915  | 1.236431   |

### 6_2ethylacrolein_TS_9_reopt

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -708.73997             |
### 7_transtrans24hexadienal_1

| Datum                                 | Value       |
|---------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -308.624168 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -308.528847 |
| Number of Imaginary Frequencies       | 0           |
**Frequencies (Top 3 out of 39)**

1. 72.3362 cm⁻¹  
2. 113.1949 cm⁻¹  
3. 170.0887 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -2.584532 | 0.333031 | 0.000000 |
| C | -1.321014 | -0.388965 | -0.000001 |
| C | -0.162188 | 0.287487 | -0.000001 |
| C | 1.150431 | -0.318567 | -0.000001 |
| C | 2.272680 | 0.406504 | 0.000001 |
| C | 3.650815 | -0.156300 | 0.000000 |
| O | -3.678052 | -0.192196 | 0.000001 |
| H | -2.495133 | 1.433941 | -0.000001 |
| H | -1.355495 | -1.472178 | -0.000002 |
| H | -0.197126 | 1.374428 | 0.000000 |
| H | 1.202933 | -1.402736 | 0.000003 |
| H | 2.186407 | 1.489703 | 0.000001 |
| H | 4.203838 | 0.189899 | 0.875302 |
| H | 3.638004 | -1.244521 | 0.000003 |
| H | 4.203836 | 0.189895 | -0.875304 |

**7_transtans24hexadienal_2**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -308.620617 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -308.525656 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 39)**

1. 101.1821 cm⁻¹  
2. 114.2937 cm⁻¹  
3. 115.8993 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
### 7_transtrans24hexadienal_3

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -308.624168 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -308.52885 |
| Number of Imaginary Frequencies | 0 |

#### Frequencies (Top 3 out of 39)

1. 72.6298 cm⁻¹
2. 113.5176 cm⁻¹
3. 170.2949 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -2.585041 | 0.332858 | -0.000023 |
| C | -1.321064 | -0.388932 | -0.000032 |
| C | -0.162102 | 0.287405 | -0.000026 |
| C | 1.150675 | -0.318539 | 0.000040 |
| C | 2.272891 | 0.406634 | 0.000111 |
| C | 3.651262 | -0.156348 | -0.000051 |
| O | -3.678600 | -0.192126 | 0.000021 |
| H | -2.495643 | 1.433933 | -0.000055 |
| H | -1.355131 | -1.472160 | -0.000016 |
| H | -0.196723 | 1.374408 | -0.000032 |
| H | 1.203140 | -1.402713 | 0.000076 |
### 7_transtrans24hexadienal_4

| Datum                                           | Value              |
|-------------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -308.619041        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy       | -308.524236        |
| Number of Imaginary Frequencies                  | 0                  |

#### Frequencies (Top 3 out of 39)

1. 80.3627 cm⁻¹
2. 109.3520 cm⁻¹
3. 126.9007 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | 2.515296  | 0.144962  | 0.054983 |
|--------|-----------|-----------|----------|
| C      | 1.093624  | -0.135462 | -0.092545|
| C      | 0.206325  | 0.863086  | 0.023087 |
| C      | -1.244259 | 0.760170  | -0.071492|
| C      | -1.936734 | -0.369079 | 0.091531 |
| C      | -3.420029 | -0.471501 | -0.002214|
| O      | 3.392329  | -0.689582 | -0.018618|
| H      | 2.767419  | 1.203677  | 0.244091 |
| H      | 0.805564  | -1.158298 | -0.303608|
| H      | 0.601262  | 1.860860  | 0.194916 |
| H      | -1.781086 | 1.684128  | -0.256808|
| H      | -1.402919 | -1.285673 | 0.325052 |
| H      | -3.838493 | -0.847123 | 0.933418 |
| H      | -3.873357 | 0.491514  | -0.229621|
| H      | -3.702364 | -1.185483 | -0.778594|

### 7_transtrans24hexadienal_5

| Datum | Value |
|-------|-------|
|       |       |
### 7_transtrans24hexadienal_6

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -308.615228 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -308.520463 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

1. 80.3624 cm⁻¹
2. 109.3520 cm⁻¹
3. 126.9007 cm⁻¹
1. 60.2935 cm⁻¹
2. 122.1685 cm⁻¹
3. 142.7241 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  |  |  |
|---|---|---|
| C | 2.521383 | -0.551417 | -0.034368 |
| C | 1.057877 | -0.560962 | -0.149314 |
| C | 0.347171 | 0.570313 | -0.047899 |
| C | -1.102818 | 0.693588 | -0.121398 |
| C | -1.962842 | -0.297959 | 0.121274 |
| C | -3.445427 | -0.167978 | 0.048315 |
| O | 3.195863 | 0.435791 | 0.168690 |
| H | 3.010949 | -1.532134 | -0.149941 |
| H | 0.588639 | -1.518479 | -0.336583 |
| H | 0.906269 | 1.490811 | 0.089805 |
| H | -1.490810 | 1.678721 | -0.357706 |
| H | -1.576067 | -1.270986 | 0.410136 |
| H | -3.900572 | -0.411395 | 1.010188 |
| H | -3.744345 | 0.838714 | -0.238004 |
| H | -3.853037 | -0.875089 | -0.677071 |

**7_transtrans24hexadienal_7**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -308.615228 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -308.520463 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 39)**

1. 60.2935 cm⁻¹
2. 122.1685 cm⁻¹
3. 142.7241 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.838593 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.710027 |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 54)**

1. 53.8882 cm⁻¹  
2. 67.3390 cm⁻¹  
3. 86.3989 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | -2.661727 | 0.648249 | 0.394123 |
| C   | -1.563496 | 0.476372 | -0.406208 |
| C   | -0.261901 | -0.015595 | 0.123886 |
| C   | 0.914936  | 0.761886 | -0.372604 |
| C   | 1.890249  | 1.240818 | 0.391251 |
| C   | 3.060186  | 2.030346 | -0.107731 |
| O   | -3.826843 | 1.055068 | 0.083744 |
| H   | -2.480545 | 0.397696 | 1.462765 |
| H   | -1.627047 | 0.690432 | -1.469682 |
| H   | -0.272886 | -0.012608 | 1.216553 |
| H   | 0.944638  | 0.926494 | -1.448176 |
### 7_transtrans24hexadienal_HEI_11

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -746.834771            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -746.705423            |
| Number of Imaginary Frequencies                                      | 0                      |

#### Frequencies (Top 3 out of 54)

1. 54.7698 cm\(^{-1}\)
2. 80.6596 cm\(^{-1}\)
3. 101.7824 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -2.419515 | 0.279058 | -0.154526 |
|-------|-----------|----------|-----------|
| C     | -1.630488 | -0.616069| 0.518829  |
| C     | -0.147789 | -0.483979| 0.687278  |
| C     | 0.350520  | 0.936350 | 0.657240  |
| C     | 1.142039  | 1.513876 | -0.236700 |
| C     | 1.570673  | 2.947917 | -0.184666 |
| O     | -3.675632 | 0.221186 | -0.36875  |
| H     | -1.881968 | 1.163466 | -0.548954 |
| H     | -2.084986 | -1.516286| 0.922162  |
| H     | 0.136541  | -0.895884| 1.661935  |
| H     | -0.014715 | 1.534778 | 1.490231  |
| H     | 1.503534  | 0.925760 | -1.074984 |
| H     | 2.658696  | 3.032624 | -0.149213 |
| H     | 1.158444  | 3.452536 | 0.688704  |
| H     | 1.243500  | 3.485776 | -1.076952 |
| C     | 2.376697  | -1.643655| 0.134304  |
| H     | 2.878043  | -0.686297| 0.009695  |
| H     | 2.922209  | -2.409772| -0.412609 |
### 7_transttrans24hexadienal_HEI_1

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.83439|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.704981|
| Number of Imaginary Frequencies            | 0         |

**Frequencies (Top 3 out of 54)**

1. 63.1028 cm⁻¹  
2. 68.0144 cm⁻¹  
3. 105.7739 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | -2.592552 | -0.840803 | -0.194326 | C          | -1.339762 | -0.571266 | 0.289806  | C          | -0.207294 | -0.177683 | -0.595824 | C          | 1.038180  | -0.977701 | -0.295623 | C          | 2.262126  | -0.547563 | -0.015966 | C          | 3.420018  | -1.443753 | 0.300036  | O          | -3.644172 | -1.177172 | 0.438802  | H          | -2.674124 | -0.750022 | -1.300620 | H          | -1.150412 | -0.635361 | 1.357188  | H          | -0.499048 | -0.380563 | -1.631443 | H          | 0.854861  | -2.050973 | -0.288136 | H          | 2.457565  | 0.520319  | -0.015252 | H          | 3.131415  | -2.493578 | 0.257868  | H          | 4.241076  | -1.284438 | -0.401828 | H          | 3.815279  | -1.236406 | 1.296606  | C          | 0.180737  | 2.041108  | 1.094003  | H          | 1.000032  | 1.516681  | 1.582656  | H          | 0.339164  | 3.113582  | 1.182425  | H          | -0.760123 | 1.774433  | 1.571331  | S          | 0.114311  | 1.651854  | -0.663365 |

### 7_transttrans24hexadienal_HEI_2
| Datum                                           | Value       |
|------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -746.83069  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.701697 |

Number of Imaginary Frequencies

0

**Frequencies** (Top 3 out of 54)

1. 52.3705 cm⁻¹
2. 68.3430 cm⁻¹
3. 98.6020 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -2.284946 | -0.992051 | -0.084089 |
| C     | -0.925440 | -1.134967 | -0.075881 |
| C     | 0.095426  | -0.151950 | -0.585724 |
| C     | 1.378557  | -0.255239 | 0.186335  |
| C     | 2.552665  | -0.582880 | -0.340169 |
| C     | 3.831546  | -0.708111 | 0.427704  |
| O     | -3.171731 | -1.831842 | 0.294457  |
| H     | -2.647455 | -0.015615 | -0.460999 |
| H     | -0.510459 | -2.065438 | 0.304371  |
| H     | 0.341341  | -0.305281 | -1.643828 |
| H     | 1.304498  | -0.077404 | 1.257232  |
| H     | 2.606338  | -0.777303 | -1.408929 |
| H     | 4.586333  | -0.017440 | 0.046235  |
| H     | 3.676874  | -0.496985 | 1.485318  |
| H     | 4.248778  | -1.712670 | 0.334800  |
| C     | -0.945667 | 1.903361  | 1.074909  |
| H     | -0.117690 | 1.727483  | 1.758451  |
| H     | -1.234888 | 2.950476  | 1.136465  |
| H     | -1.789152 | 1.275182  | 1.349780  |
| S     | -0.456470 | 1.606297  | -0.633316 |

**7_transtrans24hexadienal_HEI_3**

| Datum                                           | Value       |
|------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -746.836456 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.707235 |

Number of Imaginary Frequencies

0
**Frequencies (Top 3 out of 54)**

1. 51.6442 cm⁻¹  
2. 58.2323 cm⁻¹  
3. 79.4054 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| C | 2.317603 | 1.105414 | -0.225537 |
| C | 1.114427 | 0.612300 | 0.206406 |
| C | 0.182437 | -0.091684 | -0.703507 |
| C | -1.261860 | 0.327860 | -0.668525 |
| C | -1.804989 | 1.198022 | 0.175232 |
| C | -3.256335 | 1.566374 | 0.192875 |
| O | 3.224056 | 1.706836 | 0.435643 |
| H | 2.502858 | 0.952559 | -1.312008 |
| H | 0.847312 | 0.708640 | 1.254099 |
| H | 0.546935 | -0.005478 | -1.731047 |
| H | -1.904252 | -0.164177 | -1.395191 |
| H | -1.166721 | 1.691838 | 0.901045 |
| H | -3.809586 | 1.031125 | -0.578321 |
| H | -3.706999 | 1.336239 | 1.160531 |
| H | -3.390751 | 2.637921 | 0.031895 |
| C | -0.231284 | -2.068517 | 1.250162 |
| H | -1.165706 | -1.546502 | 1.453560 |
| H | -0.346619 | -3.120586 | 1.500358 |
| H | 0.565364 | -1.640450 | 1.855537 |
| S | 0.179732 | -1.964652 | -0.499265 |

**7_transtrans24hexadienal_HEI_4**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -746.837695 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.707671 |

Number of Imaginary Frequencies - 0

**Frequencies (Top 3 out of 54)**

1. 70.7266 cm⁻¹  
2. 76.5618 cm⁻¹  
3. 101.7503 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C     -2.056974   -1.570763    0.415619
C     -0.841663   -1.015681    0.724878
C     -0.051198   -0.209273   -0.246755
C      1.380423   -0.660703   -0.318995
C      2.475187    0.002013    0.035996
C      3.861899   -0.559898   -0.035914
O     -2.706225   -1.518983   -0.679863
H     -2.513459   -2.144237    1.248225
H     -0.435631   -1.155317    1.720177
H     -0.507538   -0.338215   -1.231328
H      1.488026   -1.682919   -0.676649
H      2.389650    1.018881    0.407988
H      4.497578    0.046167   -0.684469
H      4.333910   -0.567811    0.948589
H      3.853436   -1.579549   -0.420107
C     -1.899332    1.844675   -0.049753
H     -2.400972    1.128298    0.598723
H     -2.125273    2.858473    0.273176
H     -2.239330    1.707761   -1.074491
S     -0.118790    1.617382    0.073663

7_trans-trans24hexadienal_HEI_5

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -746.837712 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.709319 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 54)

1. 51.2689 cm⁻¹  
2. 59.7400 cm⁻¹  
3. 84.2701 cm⁻¹
7_tristrans24hexadienal_HEI_6

| Datum                                                      | Value                        |
|------------------------------------------------------------|------------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -746.837339                  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -746.708011                  |
| Number of Imaginary Frequencies                            | 0                            |

**Frequencies** (Top 3 out of 54)

1. 51.6892 cm⁻¹
2. 57.9151 cm⁻¹
3. 90.7455 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Datum | Value |
|-------|-------|
| C     | 2.134965 1.529574 0.512917 |
| C     | 1.036877 0.780228 0.849445 |
| C     | 0.116268 0.224402 -0.173899 |
| C     | -1.306655 0.172626 0.285591 |
| C     | -2.334774 0.717974 -0.354059 |
| C     | -3.755116 0.678186 0.117171 |
### 7_transtrans24hexadienal_HEI_7

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -746.837944         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -746.708558         |
| Number of Imaginary Frequencies                                      | 0                   |
| **Frequencies** (Top 3 out of 54)                                    |                     |
| 1. 62.6222 cm⁻¹                                                      |                     |
| 2. 73.8669 cm⁻¹                                                      |                     |
| 3. 96.0449 cm⁻¹                                                      |                     |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -2.641964 | 1.120193 | -0.215126 |
|-------|-----------|----------|-----------|
| C     | -1.312772 | 1.034534 | -0.542518 |
| C     | -0.355573 | 0.173846 | 0.217206  |
| C     | 0.961715  | 0.868560 | 0.432636  |
| C     | 2.123658  | 0.630351 | -0.162669 |
| C     | 3.371706  | 1.426384 | 0.065207  |
| O     | -3.268648 | 0.528042 | 0.721295  |
| H     | -3.224783 | 1.806644 | -0.862172 |
| H     | -0.934007 | 1.604558 | -1.381839 |
| H     | -0.802432 | -0.045830| 1.190596  |
| H     | 0.899816  | 1.695377 | 1.138585  |
| H     | 2.190848  | -0.192130| -0.868956 |
| H     | 3.205211  | 2.223724 | 0.789038  |
### 7 Transtrans24hexadienal_HEI_8

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.838725 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.708962 |
| Number of Imaginary Frequencies  | 0 |

**Frequencies (Top 3 out of 54)**

1. 55.3335 cm⁻¹  
2. 77.6082 cm⁻¹  
3. 88.6896 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| C | 1.368395 | 1.945961 | 0.356852 |
| C | 0.408388 | 1.014695 | 0.659504 |
| C | 0.003308 | -0.044915 | -0.289635 |
| C | -1.470154 | -0.300331 | -0.448434 |
| C | -2.446500 | 0.371737 | 0.150054 |
| C | -3.905318 | 0.093745 | -0.038176 |
| O | 2.030226 | 2.091576 | -0.723179 |
| H | 1.574821 | 2.664330 | 1.176371 |
| H | -0.035855 | 1.026234 | 1.647899 |
| H | 0.433554 | 0.179246 | -1.268962 |
| H | -1.733937 | -1.115898 | -1.119252 |
| H | -2.185356 | 1.189016 | 0.814856 |
| H | -4.065296 | -0.737266 | -0.724458 |
| H | -4.382556 | -0.149002 | 0.913409 |
| H | -4.422444 | 0.970586 | -0.433033 |
| C | 2.472190 | -1.322691 | 0.034133 |
| H | 2.666860 | -0.426394 | 0.621313 |
| H | 3.031206 | -2.161303 | 0.443322 |
| H | 2.775325 | -1.154374 | -0.997589 |
| S | 0.720012 | -1.722937 | 0.135360 |
### 7_transtans24hexadienal_HEI_9

| Datum                                                                 | Value                   |
|-----------------------------------------------------------------------|-------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -746.834781             |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -746.705081             |
| Number of Imaginary Frequencies                                       | 0                       |

**Frequencies (Top 3 out of 54)**

1. 54.1778 cm⁻¹  
2. 64.6646 cm⁻¹  
3. 91.7277 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 1.113208  | 2.038350  | -0.298211 |
|-----|-----------|-----------|-----------|
| C   | 0.935294  | 0.965688  | -1.135520 |
| C   | 0.114992  | -0.251934 | -0.869776 |
| C   | -1.077870 | -0.045851 | 0.012770  |
| C   | -2.327663 | -0.296006 | -0.361776 |
| C   | -3.535143 | -0.090416 | 0.500255  |
| O   | 0.651387  | 2.263158  | 0.867923  |
| H   | 1.765732  | 2.822048  | -0.738240 |
| H   | 1.475802  | 0.982123  | -2.074930 |
| H   | -0.229019 | -0.678890 | -1.814589 |
| H   | -0.873753 | 0.357844  | 0.997814  |
| H   | -2.508087 | -0.674718 | -1.365729 |
| H   | -3.254750 | 0.292420  | 1.481163  |
| H   | -4.230978 | 0.616052  | 0.042826  |
| H   | -4.083311 | -1.024525 | 0.640664  |
| C   | 1.874740  | -0.911843 | 1.242245  |
| H   | 1.144447  | -0.756088 | 2.033554  |
| H   | 2.658163  | -1.575653 | 1.601509  |
| H   | 2.304603  | 0.044418  | 0.949042  |
| S   | 1.127169  | -1.684890 | -0.202274 |

### 7_transtans24hexadienal_TS_10
### Datum

| M06-2X/def2tzvpp-IEFPCM(water) Energy | -746.825243 |
|-------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.698111 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 54)

1. -203.8656 cm⁻¹
2. 40.4172 cm⁻¹
3. 72.0519 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | -2.868991 | 0.439742 | 0.367412 |
|------|-----------|----------|----------|
| C    | -1.679587 | 0.704300 | -0.342267|
| C    | -0.440809 | 0.455889 | 0.235211 |
| C    | 0.785249  | 1.022528 | -0.314120|
| C    | 1.870389  | 1.293662 | 0.411918 |
| C    | 3.122511  | 1.909817 | -0.123267|
| O    | -4.030918 | 0.603325 | -0.029309|
| H    | -2.709658 | 0.052532 | 1.394303 |
| H    | -1.745515 | 1.055144 | -1.366411|
| H    | -0.421297 | 0.238133 | 1.296823 |
| H    | 0.776554  | 1.253234 | -1.376110|
| H    | 1.854435  | 1.059408 | 1.473317 |
| H    | 3.981012  | 1.255795 | 0.043535 |
| H    | 3.039971  | 2.104077 | -1.191859|
| H    | 3.342945  | 2.851567 | 0.383286 |
| C    | 1.826338  | -2.164916| 0.249756 |
| H    | 1.878921  | -2.663580| 1.216997 |
| H    | 2.369720  | -2.767332| -0.478188|
| H    | 2.338511  | -1.201165| 0.334681 |
| S    | 0.115697  | -1.876910| -0.275235|

**7_transtrans24hexadienal_TS_11_reopt**

| Datum                  | Value          |
|------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -746.814263 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.687558 |
| Number of Imaginary Frequencies | 1 |
**Frequencies** (Top 3 out of 54)

1. -230.6307 cm⁻¹
2. 27.7112 cm⁻¹
3. 57.3747 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |        |        |        |
|---|--------|--------|--------|
| C | -2.519707 | -0.065623 | -0.156748 |
| C | -1.597327 | -0.863380 | 0.565494 |
| C | -0.314116 | -0.470606 | 0.906789 |
| C | 0.148306  | 0.932817  | 0.824661 |
| C | 0.421333  | 1.621606  | -0.275457 |
| C | 0.858106  | 3.050959  | -0.297370 |
| O | -3.653363 | -0.419610 | -0.507410 |
| H | -2.188220 | 0.957739  | -0.395018 |
| H | -1.923690 | -1.862800 | 0.831786 |
| H | 0.177795  | -1.045275 | 1.681825 |
| H | 0.269956  | 1.419182  | 1.791192 |
| H | 0.354115  | 1.106759  | -1.229548 |
| H | 1.838315  | 3.150982  | -0.768232 |
| H | 0.913781  | 3.463850  | 0.709287 |
| H | 0.165946  | 3.660188  | -0.882324 |
| C | 2.795874  | -0.786964 | 0.138083 |
| H | 2.968752  | 0.166556  | -0.361631 |
| H | 3.694548  | -1.396206 | 0.043717 |
| H | 2.640302  | -0.579477 | 1.199825 |
| S | 1.347531  | -1.637342 | -0.549645 |

**7_transtrans24hexadienal_TS_1_reopt**

| Datum                                    | Value          |
|------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -746.828331    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.700822 |
| Number of Imaginary Frequencies          | 1              |

**Frequencies** (Top 3 out of 54)

1. -173.5738 cm⁻¹
2. 54.0718 cm⁻¹
3. 71.3456 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X           | Y           | Z           |
|---|-------------|-------------|-------------|
| C | -2.150344   | -1.386974   | -0.334630   |
| C | -0.957939   | -1.106072   | 0.376111    |
| C | 0.116237    | -0.499272   | -0.249838   |
| C | 1.464534    | -0.565887   | 0.316514    |
| C | 2.577962    | -0.522687   | -0.412059   |
| C | 3.963496    | -0.625864   | 0.138210    |
| O | -3.158357   | -1.956786   | 0.097985    |
| H | -2.135316   | -1.062662   | -1.394747   |
| H | -0.906636   | -1.366709   | 1.427970    |
| H | 0.066810    | -0.389356   | -1.326577   |
| H | 1.529209    | -0.687463   | 1.394634    |
| H | 2.486457    | -0.398353   | -1.488364   |
| H | 3.949011    | -0.751162   | 1.220215    |
| H | 4.498886    | -1.470835   | -0.300289   |
| H | 4.544026    | 0.268591    | -0.097717   |
| C | -1.856073   | 2.047895    | 0.120888    |
| H | -2.161728   | 2.677640    | 0.955753    |
| H | -2.328986   | 2.423195    | -0.786307   |
| H | -2.237518   | 1.036378    | 0.311189    |
| S | -0.061488   | 1.958012    | -0.026926   |

7_trtrans24hexadienal_TS_2_reopt

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.828331    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.700823 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 54)

1. -173.5988 cm⁻¹
2. 53.8751 cm⁻¹
3. 71.3407 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
7_transtrans24hexadienal_TS_3

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -746.826415 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.698285 |
| Number of Imaginary Frequencies                            | 1           |

**Frequencies** (Top 3 out of 54)

1. -207.2817 cm⁻¹  
2. 50.4696 cm⁻¹  
3. 70.6866 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | 2.475052 | 0.940885 | -0.237570 |
| C    | 1.100289 | 0.882224 | 0.074546  |
| C    | 0.285586 | 0.323135 | -0.828037 |
| C    | -1.249384| 0.508653 | -0.753750 |
| C    | -1.901911| 1.139816 | 0.223116  |
| C    | -3.387966| 1.297863 | 0.275633  |
### 7_transtrans24hexadienal_TS_4_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -746.825805 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.697552 |
| Number of Imaginary Frequencies | 1 |

#### Frequencies (Top 3 out of 54)

1. -150.2527 cm⁻¹
2. 48.7696 cm⁻¹
3. 74.9158 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| O     | 3.385956 | 1.389493 | 0.470846 |
|-------|----------|----------|----------|
| H     | 2.733477 | 0.539235 | -1.238568|
| H     | 0.782395 | 1.225164 | 1.051360 |
| H     | 0.589396 | 0.120561 | -1.820049|
| H     | -1.819369| 0.081376 | -1.571525|
| H     | -1.340620| 1.575450 | 1.043488 |
| H     | -3.863253| 0.848948 | -0.595848|
| H     | -3.799493| 0.827179 | 1.171346 |
| H     | -3.670095| 2.351847 | 0.319058 |
| C     | -0.042790| -1.784347| 1.306599 |
| H     | -0.867001| -1.106068| 1.546521 |
| H     | -0.192307| -2.714940| 1.851846 |
| H     | 0.885372 | -1.325645| 1.650816 |
| S     | 0.017537 | -2.086777| -0.471152|

| C     | -1.661197| -1.866867| 0.301472 |
|-------|----------|----------|----------|
| C     | -0.390260| -1.244894| 0.469398 |
| C     | 0.160655 | -0.468976| -0.523238|
| C     | 1.554302 | -0.007530| -0.535536|
| C     | 2.524376 | -0.466967| 0.253922 |
| C     | 3.941371 | 0.007369 | 0.213673 |
| O     | -2.383791| -1.806334| -0.697389|
| H     | -2.012185| -2.455811| 1.169134 |
| H     | 0.087502 | -1.345636| 1.435693 |
| H     | -0.335052| -0.495884| -1.483538|
| H     | 1.796545 | 0.747155 | -1.276935|
| H     | 2.292940 | -1.241395| 0.978746 |
| H     | 4.237748 | 0.428707 | 1.176835 |
### 7_transtrans24hexadienal_TS_5

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -746.828331    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -746.700822    |

**Number of Imaginary Frequencies**

1

**Frequencies (Top 3 out of 54)**

1. -173.6150 cm⁻¹
2. 54.0252 cm⁻¹
3. 71.3459 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C           | -2.150567 | 1.386799 | 0.334653 |
|-------------|-----------|----------|----------|
| C           | -0.958235 | 1.105840 | -0.376143|
| C           | 0.116066  | 0.499240 | 0.249844 |
| C           | 1.464365  | 0.566017 | -0.316530|
| C           | 2.577818  | 0.522896 | 0.412012 |
| C           | 3.963331  | 0.626177 | -0.138290|
| O           | -3.158691 | 1.956437 | -0.097958|
| H           | -2.135380 | 1.062745 | 1.394849 |
| H           | -0.907083 | 1.366208 | -1.428075|
| H           | 0.066700  | 0.389650 | 1.326616 |
| H           | 1.528999  | 0.687588 | -1.394651|
| H           | 2.486350  | 0.398538 | 1.488317 |
| H           | 3.948816  | 0.751585 | -1.220822|
| H           | 4.497908  | 1.471117 | 0.300284 |
| H           | 4.543892  | -0.268286| 0.097531 |
| C           | -1.855589 | -2.048185| -0.121126|
| H           | -2.237270 | -1.036649| -0.318864|
| H           | -2.160814 | -2.677462| -0.956499|
| H           | -2.328619 | -2.424228| 0.785696 |
| S           | -0.061069 | -1.957812| 0.027139 |
### 7_transtrans24hexadienal_TS_6_reopt

| Datum                                                                 | Value         |
|-----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -746.82759    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -746.699552   |
| Number of Imaginary Frequencies                                       | 1             |

#### Frequencies (Top 3 out of 54)

1. -167.2593 cm\(^{-1}\)
2. 64.6068 cm\(^{-1}\)
3. 74.1039 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C  |          |          |          |
|----|----------|----------|----------|
|    | -2.028910| -1.679916| 0.227778 |
| C  | -0.790071| -1.209275| 0.751429 |
| C  | 0.165365 | -0.634750| -0.055301|
| C  | 1.529590 | -0.400378| 0.407849 |
| C  | 2.585558 | -0.343083| -0.402499|
| C  | 3.996757 | -0.144384| 0.045612 |
| O  | -2.392180| -1.633141| -0.951075|
| H  | -2.710640| -2.131494| 0.971941 |
| H  | -0.637837| -1.277582| 1.821877 |
| H  | 0.029171 | -0.720579| -1.125058|
| H  | 1.669366 | -0.304001| 1.481629 |
| H  | 2.420611 | -0.440314| -1.472713|
| H  | 4.630162 | -0.975012| -0.272199|
| H  | 4.421493 | 0.759609 | -0.396323|
| H  | 4.057842 | -0.059106| 1.129829 |
| C  | -2.110846| 1.720503 | 0.430572 |
| H  | -2.220180| 0.733268 | 0.900731 |
| H  | -2.262618| 2.472710 | 1.204207 |
| H  | -2.900530| 1.824136 | -0.313990|
| S  | -0.465254| 1.833200 | -0.297124|

### 7_transtrans24hexadienal_TS_7_reopt
| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.825058    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.697095    |
| Number of Imaginary Frequencies            | 1              |

**Frequencies (Top 3 out of 54)**

1. -185.3946 cm⁻¹  
2. 33.1332 cm⁻¹  
3. 63.9940 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | 2.420591 | -1.222613 | -0.527066 |
|---|----------|-----------|-----------|
| C | 1.004908 | -1.080234 | -0.522322 |
| C | 0.338607 | -0.581216 | 0.577002  |
| C | -1.116672| -0.608409 | 0.740975  |
| C | -1.996686| -0.998643 | -0.182135 |
| C | -3.478345| -0.993217 | 0.014623  |
| O | 3.196512 | -0.921640 | 0.385320  |
| H | 2.843931 | -1.650276 | -1.454825 |
| H | 0.481334 | -1.345666 | -1.430603 |
| H | 0.915384 | -0.485798 | 1.486055  |
| H | -1.487314| -0.264069 | 1.700556  |
| H | -1.640372| -1.337529 | -1.149824 |
| H | -3.741416| -0.666072 | 1.019914  |
| H | -3.963470| -0.325861 | -0.701639 |
| H | -3.901305| -1.986649 | -0.148357 |
| C | -0.386559| 1.900258  | -1.129173 |
| H | -1.471754| 1.809687  | -1.073183 |
| H | -0.143706| 2.796237  | -1.699118 |
| H | 0.000136 | 1.035176  | -1.677950 |
| S | 0.363837 | 1.956149  | 0.513437  |

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.825805    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.697552    |
| Number of Imaginary Frequencies            | 1              |
**Frequencies (Top 3 out of 54)**

1. -150.2141 cm⁻¹
2. 48.8089 cm⁻¹
3. 74.9406 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          |         |         |         |
|----------|---------|---------|---------|
| C        | 1.661036| 1.866910| 0.301515|
| C        | 0.390071| 1.244918| 0.469412|
| C        | -0.160790| 0.469067| -0.523296|
| C        | -1.554355| 0.007353| -0.535458|
| C        | -2.524532| 0.466962| 0.253778|
| C        | -3.941430| -0.007685| 0.213738|
| O        | 2.383552| 1.806481| -0.697393|
| H        | 2.012082| 2.455747| 1.169224|
| H        | -0.087620| 1.345456| 1.435763|
| H        | 0.334947| 0.496156| -1.483574|
| H        | -1.796457| -0.747686| -1.276541|
| H        | -2.293244| 1.241742| 0.978273|
| H        | -4.081246| -0.769921| -0.551830|
| H        | -4.237586| -0.429017| 1.176973|
| H        | -4.626230| 0.817993| 0.010177|
| C        | 2.037274| -1.495016| 0.914483|
| H        | 1.859565| -0.472912| 1.275361|
| H        | 1.938443| -2.169053| 1.764764|
| H        | 3.062707| -1.546208| 0.548605|
| S        | 0.837661| -1.874325| -0.377068|

**7_transtans24hexadienal_TS_9**

| Datum                                           | Value    |
|-------------------------------------------------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -746.823513 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.695729 |
| Number of Imaginary Frequencies                 | 1        |

**Frequencies (Top 3 out of 54)**

1. -173.9639 cm⁻¹
2. 49.2037 cm⁻¹
3. 69.7490 cm⁻¹
## M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atoms | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-------|--------------|--------------|--------------|
| C     | 1.168410     | 2.114141     | -0.035225    |
| C     | 0.842226     | 1.167849     | -1.051076    |
| C     | -0.133566    | 0.195636     | -0.974358    |
| C     | -1.291105    | 0.238773     | -0.082351    |
| C     | -2.447697    | -0.350830    | -0.385883    |
| C     | -3.674494    | -0.305844    | 0.466276     |
| O     | 0.682391     | 2.210206     | 1.094739     |
| H     | 1.965905     | 2.825265     | -0.323370    |
| H     | 1.486111     | 1.182553     | -1.921444    |
| H     | -0.276829    | -0.415036    | -1.857550    |
| H     | -1.189243    | 0.809857     | 0.831390     |
| H     | -2.517078    | -0.916146    | -1.312464    |
| H     | -3.506053    | 0.283550     | 1.366730     |
| H     | -4.516702    | 0.126884     | -0.077540    |
| H     | -3.978747    | -1.311705    | 0.764494     |
| C     | 2.634981     | -1.125787    | 0.307193     |
| H     | 3.001808     | -1.101083    | 1.333133     |
| H     | 3.348988     | -1.681803    | -0.300458    |
| H     | 2.611789     | -0.091455    | -0.063291    |
| S     | 0.969900     | -1.812260    | 0.208437     |
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### _1_methylacrylate_1

| Datum                                                  | Value        |
|--------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -306.469104  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -306.399991  |
| Number of Imaginary Frequencies                        | 0            |

**Frequencies** (Top 3 out of 30)

1. 80.7656 cm⁻¹
2. 160.2674 cm⁻¹
3. 195.0324 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C  | -2.476962 | -0.006325 | 0.000003 |
| C  | -1.316811 | -0.645028 | -0.000009|
| C  | -0.040162 | 0.110489  | 0.000002 |
| O  | 1.009225  | -0.713357 | -0.000013|
| O  | 0.061530  | 1.312988  | 0.000021 |
| C  | 2.294302  | -0.087679 | -0.000003|
| H  | 3.018354  | -0.894679 | -0.000013|
| H  | 2.411071  | 0.529802  | -0.887953|
| H  | 2.411069  | 0.529779  | 0.887962 |
| H  | -2.508004 | 1.075665  | 0.000020 |
| H  | -3.415308 | -0.542627 | -0.000005|
| H  | -1.245427 | -1.723726 | -0.000026|
**1_methylacrylate_2**

| Datum                                                                 | Value          |
|-----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -306.468483    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -306.399337    |
| Number of Imaginary Frequencies                                        | 0              |

**Frequencies (Top 3 out of 30)**

1. 82.5695 cm⁻¹  
2. 172.8395 cm⁻¹  
3. 185.6286 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | -2.153096 | -0.765729 | -0.000031 |
|------------|-----------|-----------|-----------|
| C          | -1.489811 | 0.381469  | 0.000010  |
| C          | -0.011465 | 0.477417  | 0.000017  |
| O          | 0.601820  | -0.705129 | -0.000023 |
| O          | 0.581920  | 1.529935  | 0.000056  |
| C          | 2.030018  | -0.665791 | -0.000021 |
| C          | 2.391924  | -0.151988 | -0.887941 |
| H          | 2.391922  | -0.152050 | 0.887937  |
| H          | 2.355729  | -1.699935 | -0.000056 |
| H          | -1.635042 | -1.714906 | -0.000061 |
| H          | -3.234218 | -0.781858 | -0.000034 |
| H          | -1.994120 | 1.338091  | 0.000041  |

**1_methylacrylate_3**

| Datum                                                                 | Value          |
|-----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -306.460181    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -306.390271    |
| Number of Imaginary Frequencies                                        | 1              |

**Frequencies (Top 3 out of 30)**

1. 82.5695 cm⁻¹  
2. 172.8395 cm⁻¹  
3. 185.6286 cm⁻¹
1. -25.4437 cm⁻¹
2. 139.1780 cm⁻¹
3. 252.3368 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |          |          |
|----------|----------|----------|
| C        | -2.137839| -0.758454| 0.003226 |
| C        | -0.812182| -0.766893| -0.001633|
| C        | -0.069244| 0.523731 | -0.001633|
| O        | 1.268172 | 0.493218 | -0.00117 |
| O        | -0.614944| 1.599487 | -0.000532|
| C        | 1.992738 | -0.738761| 0.002456 |
| H        | 1.768593 | -1.320110| 0.894567 |
| H        | 1.777397 | -1.318609| -0.892799|
| H        | 3.040571 | -0.458560| 0.007825 |
| H        | -2.683613| 0.175710 | 0.012298 |
| H        | -2.702684| -1.680033| 0.001086 |
| H        | -0.266941| -1.697777| -0.013564|

1_methylacrylate_HEI_1_reopt

| Datum                              | Value        |
|------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.684095  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.581103  |
| Number of Imaginary Frequencies    | 0            |

**Frequencies** (Top 3 out of 45)

1. 44.7959 cm⁻¹
2. 78.8121 cm⁻¹
3. 105.7983 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |          |          |
|----------|----------|----------|
| C        | 1.039376 | -0.873494| -0.849006|
| C        | -0.053655| -1.334729| 0.026657 |
| C        | -1.250960| -0.668336| 0.203676 |
| O        | -1.389293| 0.476726 | -0.589112|
### 1_methylacrylate_HEI_2

| Datum                                         | Value            |
|-----------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy         | -744.685464      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.58318      |
| Number of Imaginary Frequencies               | 0                |

**Frequencies (Top 3 out of 45)**

1. 35.6100 cm⁻¹  
2. 66.9105 cm⁻¹  
3. 96.9908 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|       |       |       |       |
|-------|-------|-------|-------|
|       | -2.207128 | -0.967962 | 0.955479 |
|       | -2.590799 | 1.197238  | -0.425108 |
|       | -2.717249 | 1.541066  | 0.602354  |
|       | -2.524926 | 2.057134  | -1.088864 |
|       | -3.462200 | 0.598783  | -0.694062 |
|       | 0.681832  | -0.199077 | -1.624318 |
|       | 1.571211  | -1.693333 | -1.334424 |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
|       | 0.106630  | -2.208264 | 0.645092  |
| S     | 2.444521  | 0.031742  | -0.004941 |
|       | 1.521067  | 1.398293  | 0.715839  |
|       | 0.660345  | 1.000728  | 1.252822  |
|       | 2.174599  | 1.922115  | 1.409775  |
1_methylacrylate_HEI_3_reopt

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -744.683474            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -744.581113            |
| Number of Imaginary Frequencies                                      | 0                      |
| **Frequencies** (Top 3 out of 45)                                    |                        |
| 1. 37.4404 cm⁻¹                                                      |                        |
| 2. 70.8745 cm⁻¹                                                      |                        |
| 3. 95.7013 cm⁻¹                                                      |                        |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C          | 0.870181 | -0.062729 | 1.100380 |
|------------|----------|-----------|----------|
| C          | -0.073867| 0.952819  | 0.597169 |
| C          | -1.323229| 0.658925  | 0.084216 |
| O          | -1.631625| -0.704953 | 0.108011 |
| O          | -2.185868| 1.439827  | -0.376770|
| C          | -2.919188| -1.052653 | -0.353261|
| H          | -3.065648| -0.762338 | -1.394091|
| H          | -2.994396| -2.134560 | -0.264930|
| H          | -3.701999| -0.584864 | 0.245213 |
| H          | 0.364154 | -0.930059 | 1.521466 |
| H          | 1.537472 | 0.341393  | 1.862801 |
| H          | 0.233533 | 1.988643  | 0.560670 |
| S          | 2.021638 | -0.842733 | -0.153542|
| C          | 2.885084 | 0.645792  | -0.683176|
| H          | 3.463142 | 1.070169  | 0.137134 |
| H          | 3.558804 | 0.381932  | -1.495059|
| H          | 2.164790 | 1.381489  | -1.038426|

1_methylacrylate_HEI_4
| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.684881 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.58279 |

Number of Imaginary Frequencies  

Frequencies (Top 3 out of 45)

1. 42.6312 cm\(^{-1}\)  
2. 60.9345 cm\(^{-1}\)  
3. 84.9518 cm\(^{-1}\)  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

```
C   -1.069403   -0.593244   0.945556
C    0.118795    0.271835   0.846925
C    1.254007   -0.164245   0.193318
O    2.284055    0.783685   0.173644
O    1.466365  -1.268158  -0.355042
C    3.484180    0.374073  -0.444844
H    4.169608    1.216043  -0.371461
H    3.921456  -0.491980    0.054284
H    3.332428    0.122023  -1.495249
H   -1.658537   -0.394318   1.841585
H   -0.800055  -1.649549    0.941577
H    0.090020    1.278173   1.238579
S   -2.305348   -0.490927  -0.457398
C   -2.736445    1.250802  -0.305730
H   -1.837088    1.860517  -0.381043
H   -3.413748    1.508555  -1.116610
H   -3.228685    1.445820   0.646539
```
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          | C             | C             | C             | O             | O             | C             | H             | H             | H             | H             | H             | S             | C             | H             | H             | H             |
|----------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| X        | 0.963611      | -0.521287     | 1.088712      | -0.380973     | -0.643781     | 0.486384      | -1.188192     | 0.467002      | 0.328898      | -0.232664     | -0.948820     | 1.646463      | 0.705407      | -2.451551     | -0.936559     | -1.323449     | -3.867052     | -0.808802     | -1.100277     |
| Y        | -0.521287     | 1.088712      | -0.380973     | -0.643781     | 0.486384      | -1.188192     | 0.467002      | 0.328898      | -0.232664     | -0.948820     | 1.646463      | 0.705407      | -2.451551     | -0.936559     | -1.323449     | -3.867052     | -0.808802     | -1.100277     |
| Z        | 1.088712      | -0.380973     | -0.643781     | 0.486384      | -1.188192     | 0.467002      | 0.328898      | -0.232664     | -0.948820     | 1.646463      | 0.705407      | -2.451551     | -0.936559     | -1.323449     | -3.867052     | -0.808802     | -1.100277     |

### 1_methylacrylate_HEI_6

| Datum                                           | Value          |
|-------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -744.684949    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.583013    |
| Number of Imaginary Frequencies                 | 0              |

#### Frequencies (Top 3 out of 45)

1. 51.5583 cm⁻¹
2. 61.2358 cm⁻¹
3. 82.4448 cm⁻¹
1_methylacrylate_HEI_7

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.683508     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.581474     |
| Number of Imaginary Frequencies | 0               |

**Frequencies (Top 3 out of 45)**

1. 48.7548 cm⁻¹
2. 64.8197 cm⁻¹
3. 85.4350 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | -1.021142 | -0.417776 | 0.772622 |
| C   | 0.321814  | -0.894089 | 0.381916 |
| C   | 1.363296  | -0.004678 | 0.215682 |
| O   | 2.559517  | -0.619784 | -0.173657|
| O   | 1.370984  | 1.236494  | 0.374876 |
| C   | 3.662595  | 0.241396  | -0.352009|
| H   | 3.471004  | 0.988986  | -1.123024|
| H   | 4.496231  | -0.387480 | -0.658053|
| H   | 3.922612  | 0.762143  | 0.570590 |
| H   | -1.569600 | -1.140581 | 1.378967 |
| H   | -0.963208 | 0.522797  | 1.321166 |
| H   | 0.481691  | -1.941019 | 0.167721 |
| S   | -2.103778 | -0.084279 | -0.694445|
| C   | -3.625796 | 0.416747  | 0.139063 |
| H   | -3.458165 | 1.308749  | 0.740991 |
| H   | -4.374866 | 0.636792  | -0.618350|
| H   | -3.993858 | -0.385210 | 0.777715 |
**1_methylacrylate_HEI_8**

| Datum                                                                 | Value               |
|-----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -744.684708         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -744.581017         |
| Number of Imaginary Frequencies                                       | 0                   |
| **Frequencies** (Top 3 out of 45)                                     |                     |
| 1. 60.2485 cm⁻¹                                                      |                     |
| 2. 71.4733 cm⁻¹                                                      |                     |
| 3. 96.9943 cm⁻¹                                                      |                     |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.922844 | -0.523615 | 0.981867 |
|-------|-----------|-----------|----------|
| C     | 0.363955  | 0.121206  | 0.646300 |
| C     | 1.329903  | -0.595326 | -0.031157|
| O     | 2.542716  | 0.014978  | -0.354943|
| O     | 1.269876  | -1.788973 | -0.410400|
| C     | 2.752074  | 1.360163  | 0.003917 |
| H     | 2.018344  | 2.018919  | -0.466206|
| H     | 3.746859  | 1.628096  | -0.345786|
| H     | 2.703771  | 1.498873  | 1.086760 |
| H     | -0.810887 | -1.600485 | 1.104075 |
| H     | -1.363698 | -0.118762 | 1.893799 |
| H     | 0.501107  | 1.158091  | 0.903746 |
| S     | -2.270783 | -0.391644 | -0.296323|
| C     | -2.442643 | 1.400772  | -0.319850|
| H     | -1.488078 | 1.861774  | -0.569715|
| H     | -3.176992 | 1.663676  | -1.077667|
| H     | -2.781310 | 1.767990  | 0.648431 |
# 1_methylacrylate_TS_1_reopt

| Datum | Value            |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.675795     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.573834 |

Number of Imaginary Frequencies: 1

## Frequencies (Top 3 out of 45)

1. -197.5075 cm\(^{-1}\)
2. 35.7684 cm\(^{-1}\)
3. 60.6869 cm\(^{-1}\)

## M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -0.776248 | 1.271174 | -0.836549 |
|-------|-----------|----------|-----------|
| C     | 0.164355  | 1.395509 | 0.163366  |
| C     | 1.317395  | 0.557329 | 0.278639  |
| O     | 1.404303  | -0.396441| -0.690245 |
| O     | 2.188432  | 0.641199 | 1.139168  |
| C     | 2.542559  | -1.242180| -0.625403 |
| H     | 2.563783  | -1.794655| 0.313075  |
| H     | 2.453953  | -1.931584| -1.459894 |
| H     | 3.462587  | -0.666120| -0.714813 |
| H     | -0.525578 | 0.715886 | -1.726490 |
| H     | -1.498474 | 2.061713 | -0.974142 |
| H     | 0.031771  | 2.103838 | 0.969435  |
| S     | -2.515794 | -0.280045| -0.293589 |
| C     | -1.671733 | -1.046191| 1.102137  |
| H     | -0.793602 | -0.436112| 1.351884  |
| H     | -2.311515 | -1.089243| 1.982434  |
| H     | -1.330063 | -2.054922| 0.871404  |

# 1_methylacrylate_TS_2

| Datum | Value            |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.676976     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.575035 |
**Datum** | **Value**
---|---
Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 45)

1. -183.1926 cm⁻¹
2. 36.8285 cm⁻¹
3. 62.1603 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.973655  | -1.522416 | -0.111344 |
|-------|-----------|-----------|-----------|
| C     | -0.156295 | -1.014446 | -0.709225 |
| C     | -1.174331 | -0.392904 | 0.081279  |
| O     | -2.219571 | 0.056454  | -0.671535 |
| O     | -1.180453 | -0.247386 | 1.297699  |
| C     | -3.271470 | 0.687298  | 0.043345  |
| H     | -4.006305 | 0.984214  | -0.699139 |
| H     | -3.722572 | 0.001433  | 0.759242  |
| H     | -2.907516 | 1.563864  | 0.577846  |
| H     | 1.645114  | -2.143533 | -0.683997 |
| H     | 0.953082  | -1.710428 | 0.951282  |
| H     | -0.269405 | -0.986731 | -1.783498 |
| S     | 2.681662  | 0.148159  | 0.191234  |
| C     | 1.673852  | 1.559343  | -0.297695 |
| H     | 1.470615  | 2.225757  | 0.540164  |
| H     | 2.145515  | 2.135342  | -1.092758 |
| H     | 0.712609  | 1.185738  | -0.676360 |

**1_methylacrylate_TS_3**

| Datum                                           | Value      |
|-------------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -744.675796|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.573833|
| Number of Imaginary Frequencies                  | 1          |

**Frequencies** (Top 3 out of 45)

1. -197.4724 cm⁻¹
2. 35.7148 cm⁻¹
3. 60.7509 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 0.776154 | 1.270970 | 0.836846 |
| C | -0.164375 | 1.395449 | -0.163126 |
| C | -1.317410 | 0.557294 | -0.278580 |
| O | -1.404329 | -0.396664 | 0.690119  |
| O | -2.188431 | 0.641317  | -1.139113 |
| C | -2.542659 | -1.242297 | 0.625185  |
| H | -2.564012 | -1.794563 | -0.313411 |
| H | -2.454040 | -1.931890 | 1.459518  |
| H | -3.462631 | -0.666177 | 0.714802  |
| H | 0.525373  | 0.715623  | 1.726718  |
| H | 1.498396  | 2.061470  | 0.974572  |
| H | -0.031733 | 2.103887  | -0.969088 |
| S | 2.515598  | -0.280340 | 0.293930  |
| C | 1.672278  | -1.045297 | -1.102893 |
| H | 2.312335  | -1.087193 | -1.983047 |
| H | 1.330893  | -2.054389 | -0.873330 |
| H | 0.793999  | -0.435264 | -1.352252 |

1_methylacrylate_TS_4_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.676976 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.575035 |

Number of Imaginary Frequencies

1

Frequencies (Top 3 out of 45)

1. -183.2223 cm⁻¹
2. 36.7422 cm⁻¹
3. 62.1898 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 0.973727 | -1.522436 | -0.110974 |
| C | -0.156310 | -1.014789 | -0.708972 |
### 1_methylacrylate_TS_5_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.672055 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.569857 |

**Number of Imaginary Frequencies**

1

**Frequencies (Top 3 out of 45)**

1. -156.2791 cm⁻¹
2. 34.9206 cm⁻¹
3. 50.6356 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -1.74265 | -0.392935 | 0.081364 |
|-------|----------|-----------|----------|
| O     | -2.21955 | 0.056181  | -0.671547|
| O     | -1.18031 | -0.246990 | 1.297718 |
| C     | -3.27138 | 0.687319  | 0.043172 |
| H     | -4.00616 | 0.984159  | -0.699392|
| H     | -3.72258 | 0.001669  | 0.759213 |
| H     | -2.90733 | 1.563960  | 0.577487 |
| H     | 1.64516  | -2.143769 | -0.683432|
| H     | 0.95316  | -1.710134 | 0.951712 |
| H     | -0.26947 | -0.987431 | 1.783249 |
| S     | 2.68164  | 0.148260  | 0.190980 |
| C     | 1.67358  | 1.559350  | -0.297690|
| H     | 0.71250  | 1.185643  | -0.67667 |
| H     | 1.47002  | 2.225434  | 0.540352 |
| H     | 2.14526  | 2.135720  | -1.092471|

| Datum | Value |
|-------|-------|
| C     | 0.653206 | -1.272157 | -0.948381 |
| C     | -0.481016 | -0.526058 | -0.853946 |
| C     | -1.230030 | -0.524642 | 0.383220 |
| O     | -2.363429 | 0.220732  | 0.468546 |
| O     | -0.928009 | -1.152386 | 1.385228 |
| C     | -2.806916 | 0.994076  | -0.637777|
| H     | -2.075480 | 1.758115  | -0.901668|
| H     | -3.727382 | 1.473423  | -0.318310|
| H     | -3.009408 | 0.364151  | -1.503530|
| H     | 0.872411  | -2.013616 | -0.197030|
| H     | 1.165531  | -1.367597 | -1.892585 |
| H     | -0.776222 | 0.117276  | -1.666883|
### 1_methylacrylate_TS_6_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -744.672076 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -744.570571 |

Number of Imaginary Frequencies 2

**Frequencies (Top 3 out of 45)**

1. -222.3206 cm⁻¹
2. -4.1784 cm⁻¹
3. 38.6979 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       |       |       |
|-------|-------|-------|
| C     | 0.801005 | 0.895433 | 0.498157 |
| C     | -0.453855 | 1.079573 | -0.033651 |
| C     | -1.481273 | 0.112130 | 0.192824 |
| O     | -2.659181 | 0.451534 | -0.406031 |
| O     | -1.393325 | -0.923909 | 0.841304 |
| C     | -3.736643 | -0.452305 | -0.212025 |
| H     | -3.496027 | -1.437050 | -0.610332 |
| H     | -4.583307 | -0.032868 | -0.747440 |
| H     | -3.977526 | -0.550336 | 0.845740 |
| H     | 1.512217  | 1.708589  | 0.481911  |
| H     | 0.920449  | 0.189302  | 1.308284  |
| H     | -0.671809 | 1.898463  | -0.703667 |
| S     | 2.372858  | -0.426317 | -0.740896 |
| C     | 3.683855  | -0.130873 | 0.479115  |
| H     | 4.280785  | -1.026399 | 0.645725  |
| H     | 4.351808  | 0.672015  | 0.168468  |
| H     | 3.239193  | 0.154605  | 1.436938  |

### 1_methylacrylate_TS_7_reopt
| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -744.67108    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -744.570567   |
| Number of Imaginary Frequencies                                      | 1             |

**Frequencies (Top 3 out of 45)**

1. -222.6992 cm\(^{-1}\)
2. 21.4457 cm\(^{-1}\)
3. 49.9683 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C          | C          | C          | O          | O          | C          | H          | H          | H          | H          | H          |
|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|   | -0.669978  | -0.761509  | 0.739626   |            |            |            |            |            |            |            |            |
| C | 0.487415   | -1.318569  | 0.242845   |            |            |            |            |            |            |            |            |
| C | 1.679322   | -0.572821  | -0.013479  |            |            |            |            |            |            |            |            |
| C | 2.729756   | -1.023361  | -0.459514  |            |            |            |            |            |            |            |            |
| O | 1.578454   | 0.751554   | 0.289903   |            |            |            |            |            |            |            |            |
| O | 2.748721   | 1.526555   | 0.076529   |            |            |            |            |            |            |            |            |
| C | 2.495578   | 2.541493   | 0.368612   |            |            |            |            |            |            |            |            |
| H | 3.575619   | 1.159728   | 0.683253   |            |            |            |            |            |            |            |            |
| H | 3.044511   | 1.503915   | -0.971347  |            |            |            |            |            |            |            |            |
| H | 0.628019   | 0.201545   | 1.227259   |            |            |            |            |            |            |            |            |
| H | 1.459463   | -1.415407  | 1.082740   |            |            |            |            |            |            |            |            |
| H | -2.353302  | 1.897361   | -0.800387  |            |            |            |            |            |            |            |            |
| S | 3.448942   | 0.441078   | 0.521823   |            |            |            |            |            |            |            |            |
| H | -4.086563  | 1.300060   | 0.318079   |            |            |            |            |            |            |            |            |
| H | -4.085870  | 1.304220   | 0.648628   |            |            |            |            |            |            |            |            |
| H | -2.936910  | 0.624461   | 1.470424   |            |            |            |            |            |            |            |            |

**1_methylacrylate_TS_8_reopt**

| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -744.672055   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -744.569858   |
| Number of Imaginary Frequencies                                      | 1             |

**Frequencies (Top 3 out of 45)**
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 0.653058 | -1.272234 | -0.948358 |
| C       | -0.481154 | -0.526132 | -0.853833 |
| C       | -1.229994 | -0.524614 | 0.383438  |
| O       | -2.363381 | 0.220764  | 0.468863  |
| O       | -0.927837 | -1.152285 | 1.385452  |
| C       | -2.806998 | 0.994065  | -0.637438 |
| H       | -2.075579 | 1.758074  | -0.901462 |
| H       | -3.727410 | 1.473448  | -0.317871 |
| H       | -3.009621 | 0.364104  | -1.503134 |
| H       | 0.872382  | -2.013599 | -0.196948 |
| H       | 1.165233  | -1.367787 | -1.892632 |
| H       | -0.776495 | 0.117108  | -1.666797 |
| S       | 2.667419  | 0.055130  | -0.032826 |
| C       | 1.675876  | 1.478653  | 0.467093  |
| H       | 0.632721  | 1.318717  | 0.160543  |
| H       | 1.684917  | 1.622471  | 1.547510  |
| H       | 2.020158  | 2.399116  | -0.003935 |

### 2_tert-butylacrylate_1

| Datum                        | Value             |
|------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -424.402886     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -424.254255     |

**Number of Imaginary Frequencies**: 0

### Frequencies (Top 3 out of 57)

| Frequency | cm⁻¹ |
|-----------|------|
| 1.        | 65.9392 |
| 2.        | 86.3067 |
| 3.        | 135.2275 |
2_tert-butylacrylate_2

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -424.402309 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -424.253871 |
| Number of Imaginary Frequencies                                      | 0           |

**Frequencies** (Top 3 out of 57)

1. 46.5934 cm\(^{-1}\)
2. 97.3909 cm\(^{-1}\)
3. 119.6199 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 3.473369 | 0.195015 | -0.000000 |
| C   | 2.268878 | 0.745238 | 0.000000  |
| C   | 1.047083 | -0.104774| -0.000000 |
| O   | -0.046208| 0.654047 | 0.000001  |
| O   | 1.057747 | -1.312329| -0.000001 |
| C   | -1.389415| 0.075262 | 0.000000  |
| C   | -2.288478| 1.301331 | 0.000002  |
| C   | -1.665051| -0.742835| -1.264997 |
| C   | -1.605051| -0.742838| 1.264996  |
| H   | 3.584402 | -0.881767| 0.000001  |
| H   | 4.369460 | 0.799456 | 0.000000  |
| H   | 2.119222 | 1.815928 | 0.000001  |
| H   | -2.655135| -1.029248| -1.324342 |
| H   | -1.364673| -0.144117| -2.143926 |
| H   | -0.996588| -1.642712| -1.266947 |
| H   | -3.332427| 0.990762 | 0.000001  |
| H   | -2.104093| 1.907821 | 0.886324  |
| H   | -2.104093| 1.907823 | -0.886320 |
| H   | -2.655135| -1.029250| 1.323431  |
| H   | -0.996588| -1.642715| 1.266944  |
| H   | -1.364672| -0.144121| 2.143926  |

C           3.473369        0.195015       -0.000000
C           2.268878        0.745238       0.000000
C           1.047083       -0.104774       -0.000000
O          -0.046208        0.654047        0.000001
O           1.057747       -1.312329       -0.000001
C           -1.389415       0.075262       0.000000
C           -2.288478       1.301331       0.000002
C           -1.665051       -0.742835      -1.264997
C           -1.605051       -0.742838       1.264996
H           3.584402        -0.881767      0.000001
H           4.369460        0.799456       0.000000
H           2.119222        1.815928       0.000001
H           -2.655135       -1.029248      -1.324342
H           -1.364673       -0.144117      -2.143926
H           -0.996588       -1.642712      -1.266947
H           -3.332427       0.990762       0.000001
H           -2.104093       1.907821       0.886324
H           -2.104093       1.907823      -0.886320
H           -2.655135       -1.029250       1.323431
H           -0.996588       -1.642715      1.266944
H           -1.364672       -0.144121       2.143926

C           -2.830945       1.169512       -0.000002
C           -2.473274       -0.106303      -0.000001
C           -1.063511       -0.576574       0.000000
O           -0.185476       0.419796       -0.000001
O          -0.782025       -1.752804       0.000002

B

2.288478  1.301331  0.000002
-1.605051 -0.742838  1.264996
3.584402  -0.881767  0.000001
4.369460   0.799456  0.000000
2.119222   1.815928  0.000001
-2.655135 -1.029248 -1.324342
-1.364673 -0.144117 -2.143926
-0.996588 -1.642712 -1.266947
-3.332427  0.990762  0.000001
-2.104093  1.907821  0.886324
-2.104093  1.907823 -0.886320
-2.655135 -1.029250  1.323431
-0.996588 -1.642715  1.266944
-1.364672 -0.144121  2.143926

C           -2.830945       1.169512       -0.000002
C           -2.473274       -0.106303      -0.000001
C           -1.063511       -0.576574       0.000000
O           -0.185476       0.419796       -0.000001
O           -0.782025       -1.752804       0.000002
2_ tert-butylacrylate_3

| Datum                                   | Value        |
|-----------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy   | -424.390976  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -424.241606 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 57)

1.  -13.0175 cm⁻¹
2.   67.5495 cm⁻¹
3.  117.3289 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | 2.972020 | -0.888454 | 0.000959 |
| C      | 1.657588 | -0.715065 | -0.000644 |
| C      | 1.096064 | 0.666021  | -0.000463 |
| O      | -0.221986| 0.869902  | -0.000744 |
| O      | 1.810934 | 1.641055  | -0.000175 |
| C      | -1.310778| -0.106578 | -0.000012 |
| C      | -1.298708| -0.938737 | -1.275503 |
| C      | -1.296968| -0.938928 | 1.275341  |
| C      | -2.540428| 0.793407  | 0.000887  |
| H      | 3.643146 | -0.040265 | 0.002457  |
| H      | 3.401711 | -1.880357 | 0.000821  |
| H     | 0.997835 | -1.564131 | -0.002125 |
|-------|----------|-----------|-----------|
| H     | -0.478879| -1.652558 | 1.320077  |
| H     | -1.237130| -0.283017 | 2.143583  |
| H     | -2.228957| -1.500445 | 1.335195  |
| H     | -2.230604| -1.500553 | -1.334000 |
| H     | -1.240414| -0.282677 | -2.143734 |
| H     | -0.480453| -1.652088 | -1.321631 |
| H     | -3.443281| 0.184627  | 0.001348  |
| H     | -2.543106| 1.426777  | 0.887122  |
| H     | -2.544196| 1.427039  | -0.885156 |

### 2_tertbutylacrylate_HEI_1_reopt

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -862.61594  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.433315 |
| Number of Imaginary Frequencies                            | 0           |

**Frequencies** (Top 3 out of 72)

1. 33.6536 cm⁻¹
2. 58.6897 cm⁻¹
3. 71.1736 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 1.991132 | 0.715458 | -0.979528 |
|-------|----------|----------|-----------|
| C     | 1.126388 | 1.568758 | -0.145519 |
| C     | -0.197507| 1.298035 | 0.153114  |
| O     | -0.692281| 0.171775 | -0.511053 |
| O     | -0.964066| 1.954401 | 0.896437  |
| C     | -1.933627| -0.439394| -0.138658 |
| C     | -1.996866| -1.682559| -1.019968 |
| C     | -1.921676| -0.858546| 1.328711  |
| C     | -3.124532| 0.462524 | -0.454941 |
| H     | 1.414045 | 0.094148 | -1.660819 |
| H     | 2.712725 | 1.284704 | -1.567422 |
| H     | 1.559341 | 2.435004 | 0.337885  |
| H     | -2.838323| -1.401473| 1.564753  |
| H     | -1.074271| -1.519568| 1.517786  |
| H     | -1.845255| 0.011545 | 1.975453  |
| H     | -2.909733| -2.244014| -0.819322 |
| H     | -1.139432| -2.327442| -0.824387 |
### 2_tertbutylacrylate_HEI_2_reopt

| Datum                                                                 | Value            |
|----------------------------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -862.617443      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -862.434634      |
| Number of Imaginary Frequencies                                      | 0                |

**Frequencies (Top 3 out of 72)**

1. 38.6737 cm⁻¹  
2. 48.1383 cm⁻¹  
3. 61.8116 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|            |                |                |                |
|------------|----------------|----------------|----------------|
| C          | 2.299763       | -1.211609      | 0.079350       |
| C          | 0.925878       | -1.160503      | -0.456763      |
| C          | -0.130519      | -0.748527      | 0.325474       |
| O          | -1.371425      | -0.872757      | -0.328142      |
| O          | -0.117775      | -0.342884      | 1.511276       |
| C          | -2.358317      | 0.156096       | -0.161729      |
| C          | -3.068670      | 0.040753       | 1.184847       |
| C          | -1.732440      | 1.536382       | -0.336776      |
| C          | -3.355731      | -0.104896      | -1.284687      |
| H          | 2.289248       | -1.229708      | 1.168629       |
| H          | 2.878790       | -2.072834      | -0.271511      |
| H          | 0.744223       | -1.431617      | -1.487043      |
| H          | -2.510149      | 2.300887       | -0.322067      |
| H          | -1.023277      | 1.740715       | 0.463613       |
| H          | -1.211488      | 1.593569       | -1.294313      |
| H          | -2.382561      | 0.258431       | 1.997603       |
| H          | -3.910162      | 0.735360       | 1.220816       |
| H          | -3.455062      | -0.971976      | 1.312141       |
### 2_tertbutylacrylate_HEI_3

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.61508 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.432617 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 72)

1. 39.3772 cm\(^{-1}\)
2. 42.2028 cm\(^{-1}\)
3. 60.2225 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -1.784034 | 0.307639 | -1.167524 |
| C     | -1.017228 | 1.373441 | -0.491562 |
| C     | 0.324679  | 1.289339 | -0.173848 |
| O     | 0.923975  | 0.113014 | -0.641221 |
| O     | 1.034146  | 2.133340 | 0.421500  |
| C     | 2.023289  | -0.477245| 0.066468  |
| C     | 2.137928  | -1.870797| -0.541477 |
| C     | 3.319747  | 0.292411 | -0.171535 |
| C     | 1.712933  | -0.592127| 1.555752  |
| H     | -2.632606 | 0.710539 | -1.721933 |
| H     | -1.176490 | -0.274654| -1.858124 |
| H     | -1.529303 | 2.279838 | -0.197703 |
| H     | 4.160520  | -0.258093| 0.254780  |
| H     | 3.492031  | 0.403107 | -1.243559 |
| H     | 3.264865  | 1.278187 | 0.280333  |
| H     | 1.215310  | -2.430044| -0.380002 |
| H     | 2.317252  | -1.799221| -1.614904 |
| H     | 2.964005  | -2.418231| -0.86831  |
| H     | 2.494262  | -1.169229| 2.052164  |
2_tertbutylacrylate_HEI_4_reopt

**Datum**

| Datum                                      | Value           |
|--------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -862.616928     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.43426      |
| Number of Imaginary Frequencies            | 0               |

**Frequencies (Top 3 out of 72)**

1. 39.3121 cm⁻¹
2. 48.6453 cm⁻¹
3. 76.5104 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|             | X       | Y       | Z         |
|-------------|---------|---------|-----------|
| C           | 2.186903| -1.089926| -0.477085 |
| C           | 0.894003| -0.979983| 0.225951  |
| C           | -0.090322| -0.122521| -0.217016 |
| O           | -1.181044| -0.045483| 0.668076  |
| O           | -0.109795| 0.580835 | -1.254203 |
| C           | -2.515407| 0.037785 | 0.145550  |
| C           | -3.400841| -0.256644| 1.351038  |
| C           | -2.829114| 1.435570 | -0.383380 |
| C           | -2.737994| -1.021612| -0.928793 |
| H           | 2.570283 | -2.110443| -0.525133 |
| H           | 2.106145 | -0.708038| -1.494270 |
| H           | 0.744902 | -1.514972| 1.153418  |
| H           | -3.891239| 1.509394 | -0.624781 |
| H           | -2.600038| 2.179030 | 0.382100  |
| H           | -2.238864| 1.651102 | -1.268638 |
| H           | -4.453585| -0.209731| 1.071040  |
| H           | -3.186825| -1.250693| 1.744600  |
| H           | -3.218425| 0.475598 | 2.138565  |
| H           | -2.108445| -0.827922| -1.795175 |
| H           | -2.502498| -2.011161| -0.533419 |
### 2_tertbutylacrylate_HEI_5

| Datum                                                                 | Value               |
|-----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -862.614766         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -862.432771         |
| Number of Imaginary Frequencies                                       | 0                   |
| **Frequencies** (Top 3 out of 72)                                     |                     |
| 1. 18.0610 cm⁻¹                                                       |                     |
| 2. 41.5752 cm⁻¹                                                       |                     |
| 3. 59.1559 cm⁻¹                                                       |                     |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -1.689989 | -0.135950 | 1.042030  |
|-------|-----------|-----------|-----------|
| C     | -0.992826 | 1.087206  | 0.598764  |
| C     | 0.254497  | 1.104980  | 0.005752  |
| O     | 0.785888  | -0.174270 | -0.201582 |
| O     | 0.917377  | 2.099815  | -0.370848 |
| C     | 2.197123  | -0.399854 | -0.064440 |
| C     | 2.319186  | -1.918512 | -0.011067 |
| C     | 2.972423  | 0.130509  | -1.267672 |
| C     | 2.712763  | 0.205836  | 1.236784  |
| H     | -0.994761 | -0.923502 | 1.328106  |
| H     | -2.355193 | 0.055682  | 1.885402  |
| H     | -1.505065 | 2.037257  | 0.675662  |
| H     | 4.014079  | -0.190187 | -1.205838 |
| H     | 2.545299  | -0.271235 | -2.188074 |
| H     | 2.927088  | 1.214605  | -1.303153 |
| H     | 3.364940  | -2.213661 | 0.079165  |
| H     | 1.910865  | -2.359797 | -0.921083 |
| H     | 1.768742  | -2.313336 | 0.843570  |
| H     | 3.756043  | -0.073943 | 1.388359  |
| H     | 2.638622  | 1.291016  | 1.209886  |
| H     | 2.130009  | -0.170146 | 2.079812  |
### 2_tertbutylacrylate_HEI_6

| Datum | Value                          |
|-------|-------------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.616393 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.43404 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 72)

1. 25.9747 cm\(^{-1}\)
2. 44.7451 cm\(^{-1}\)
3. 56.3557 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -3.928551 | 0.350700 | -0.539341 |
|-------|-----------|----------|-----------|
| H     | -3.384661 | 1.232337 | -0.875080 |
| H     | -4.613875 | 0.032836 | -1.321663 |
| H     | -4.498127 | 0.595049 | 0.356758  |
| S     | -2.774868 | -0.993552| -0.216078 |
| Datum                                                                 | Value        |
|----------------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -862.615288  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -862.433379  |
| Number of Imaginary Frequencies                                       | 0            |

**Frequencies (Top 3 out of 72)**

1. 37.8453 cm⁻¹  
2. 43.0621 cm⁻¹  
3. 56.8470 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C  | -1.795706  | 0.782493  | -0.734376 |
| C  | -0.745707  | 1.708152  | -0.249937 |
| C  | 0.590784   | 1.383234  | -0.132623 |
| O  | 0.894196   | 0.105183  | -0.622021 |
| O  | 1.524327   | 2.097867  | 0.302321  |
| C  | 1.935992   | -0.675934 | -0.019586 |
| C  | 1.697730   | -2.079080 | -0.566044 |
| C  | 3.318543   | -0.189561 | -0.446754 |
| C  | 1.798531   | -0.687531 | 1.499557  |
| H  | -2.614264  | 1.310426  | -1.226431 |
| H  | -1.403471  | 0.037030  | -1.424250 |
| H  | -1.033634  | 2.703418  | 0.062326  |
| H  | 4.080912   | -0.890527 | -0.101725 |
| H  | 3.370760   | -0.136052 | -1.535525 |
| H  | 3.519189   | 0.795433  | -0.036238 |
| H  | 2.449277   | -2.770313 | -0.183735 |
| H  | 0.710069   | -2.434970 | -0.269820 |
| H  | 1.752798   | -2.073062 | -1.655318 |
| H  | 2.519955   | -1.383430 | 1.929853  |
| H  | 1.975867   | 0.304180  | 1.909345  |
| H  | 0.795914   | -1.014844 | 1.780860  |
| C  | -3.798190  | -1.132099 | -0.284456 |
| H  | -4.345866  | -1.759157 | 0.415523  |
2_tertbutylacrylate_HEI_8_reopt

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -862.616417 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.434929 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 72)

1. 18.7681 cm⁻¹
2. 40.8049 cm⁻¹
3. 53.8019 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -2.131571 | -0.564184 | 0.795230 |
|-------|-----------|-----------|----------|
| C     | -0.732774 | -0.196248 | 1.109210 |
| C     | 0.305327  | -0.619837 | 0.309589 |
| O     | 1.568577  | -0.277202 | 0.823712 |
| O     | 0.250560  | -1.288189 | -0.748993|
| C     | 2.585968  | 0.194929  | -0.073070|
| C     | 3.629407  | 0.816503  | 0.848060 |
| C     | 3.220671  | -0.949701 | -0.859572|
| C     | 2.022860  | 1.259137  | -1.009128|
| H     | -2.176957 | -1.489544 | 0.219904 |
| H     | -2.749945 | -0.677804 | 1.687206 |
| H     | -0.521404 | 0.423023  | 1.968548 |
| H     | 4.095189  | -0.584932 | -1.401778|
| H     | 3.545835  | -1.732914 | -0.172626|
| H     | 2.509141  | -1.373115 | -1.562099|
| H     | 4.466734  | 1.205194  | 0.267862 |
| H     | 3.190444  | 1.633944  | 1.420697 |
| H     | 4.008198  | 0.068094  | 1.545204 |
| H     | 1.565697  | 2.063688  | -0.430797|
| H     | 2.824936  | 1.682752  | -1.614726|
| H     | 1.273242  | 0.829879  | -1.671613|
| C     | -4.604431 | -0.029082 | -0.409724|
| H     | -5.070409 | -0.164858 | 0.565303 |
| H     | -5.223362 | 0.636032  | 1.007846 |
## 2_tertbutylacrylate_TS_1_reopt

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -862.608577 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -862.426568 |
| Number of Imaginary Frequencies                                      | 1           |

**Frequencies (Top 3 out of 72)**

1. -207.5432 cm\(^{-1}\)
2.  43.8929 cm\(^{-1}\)
3.  46.2867 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|    | x       | y       | z       |
|----|---------|---------|---------|
| C  | 1.797103| 0.973513| -1.182995|
| C  | 1.041807| 1.654744| -0.245373|
| C  | -0.262500| 1.248085| 0.178376|
| O  | -0.683726| 0.104966| -0.428473|
| O  | -0.961659| 1.843522| 0.995635|
| C  | -1.964700| -0.495679| -0.133799|
| C  | -1.973702| -1.736155| -1.017600|
| C  | -2.047541| -0.905328| 1.332074|
| C  | -3.106465| 0.432834| -0.530477|
| H  | 1.298664 | 0.292407| -1.854731|
| H  | 2.669457 | 1.460756| -1.593369|
| H  | 1.450104 | 2.504190| 0.285134|
| H  | -2.945913| -1.503844| 1.488081|
| H  | -1.181142| -1.513196| 1.596750|
| H  | -2.083563| -0.035780| 1.981762|
| H  | -2.901443| -2.290249| -0.877392|
| H  | -1.135430| -2.385573| -0.763499|
| H  | -1.890313| -1.453819| -2.067287|
| H  | -4.051629| -0.106312| -0.455021|
| H  | -3.144120| 1.305869| 0.114474|
| H  | -2.980306| 0.757232| -1.564351|
| C  | 2.248887 | -0.838139| 1.327786|
| H  | 1.636609 | -1.734740| 1.420928|
| H  | 2.954288 | -0.809413| 2.156986|
2_tertbutylacrylate_TS_2

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.609398
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.427887

Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 72)

1. -203.1837 cm⁻¹
2. 24.5195 cm⁻¹
3. 41.2576 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C  |  -2.156400 |  -1.499056 |  0.258673 |
| C  |  -0.950859 |  -1.106068 |  0.804678 |
| C  |   0.124667 |  -0.686297 | -0.040656 |
| O  |   1.221263 |  -0.317453 |  0.683472 |
| O  |   0.113996 |  -0.649819 | -1.267032 |
| C  |   2.414412 |   0.198195 |  0.051032 |
| C  |   3.055943 |  -0.856372 | -0.843360 |
| C  |   2.189028 |   1.483525 | -0.710116 |
| C  |   3.330306 |   0.501782 |  1.229525 |
| H  |  -2.174410 |  -1.782152 | -0.783027 |
| H  |  -2.881292 |  -1.996672 |  0.885129 |
| H  |  -0.818992 |  -1.007371 |  1.872608 |
| H  |   3.044499 |   1.943209 | -1.031191 |
| H  |   1.492567 |   1.287965 | -1.582785 |
| H  |   1.589482 |   2.186479 | -0.056954 |
| H  |   2.436794 |  -1.064247 | -1.710961 |
| H  |   4.030887 |  -0.499985 | -1.178211 |
| H  |   3.204713 |  -1.779383 | -0.281189 |
| H  |   4.278545 |   0.902487 |  0.872232 |
| H  |   2.867580 |   1.235223 |  1.890008 |
| H  |   3.527578 |  -0.406203 |  1.799591 |
| C  |  -2.419777 |   1.628276 |  0.160276 |
| H  |  -2.150714 |   2.152382 | -0.756553 |
| H  |  -2.791902 |   2.354805 |  0.881266 |
2_tertbutylacrylate_TS_3

**Datum** | **Value**
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.608577
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.426568

Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 72)

1. -207.5367 cm⁻¹
2. 43.8975 cm⁻¹
3. 46.2941 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -1.797097 | 0.973549 | -1.182953 |
|-------|-----------|----------|-----------|
| C     | -1.041795 | 1.654741 | -0.245318 |
| C     | 0.262524  | 1.248081 | 0.178403  |
| O     | 0.683706  | 0.104924 | -0.428396 |
| O     | 0.961717  | 1.843553 | 0.995613  |
| C     | 1.964714  | -0.495694| -0.133804 |
| C     | 1.973693  | -1.736166| -1.017609 |
| C     | 3.106435  | 0.432843 | -0.530554 |
| C     | 2.047657  | -0.905334| 1.332062  |
| H     | -2.669443 | 1.460812 | -1.593318 |
| H     | -1.298690 | 0.292411 | -1.854677 |
| H     | -1.450064 | 2.504212 | 0.285171  |
| H     | 4.051592  | -0.106349| -0.455349 |
| H     | 2.980094  | 0.757386 | -1.564359 |
| H     | 3.144243  | 1.305790 | 0.114507  |
| H     | 1.135392  | -2.385554| -0.763529 |
| H     | 1.890339  | -1.453825| -2.067298 |
| H     | 2.901411  | -2.290292| -0.877382 |
| H     | 2.946177  | -1.503632| 1.488059  |
| H     | 2.083484  | -0.035776| 1.981748  |
| H     | 1.181412  | -1.513414| 1.596749  |
| C     | -2.248871 | -0.838214| 1.327728  |
| H     | -1.590736 | 0.036901 | 1.411079  |
| H     | -2.954229 | -0.809706| 2.156972  |
### 2 tertbutylacrylate_TS_4

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -862.609398    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -862.427885    |
| Number of Imaginary Frequencies                                      | 1              |

**Frequencies** (Top 3 out of 72)

1. -203.1495 cm⁻¹
2. 24.5833 cm⁻¹
3. 41.2776 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 2.156396   | -1.499079  | 0.258804   |
| C       | 0.950848   | -1.106030  | 0.804735   |
| C       | -0.124667  | -0.686279  | -0.040636  |
| O       | -1.221275  | -0.317426  | 0.683462   |
| O       | -0.113958  | -0.649807  | -1.267014  |
| C       | -2.414433  | 0.198196   | 0.051013   |
| C       | -3.330399  | 0.501642   | 1.229485   |
| C       | -2.189063  | 1.483590   | -0.710029  |
| C       | -3.055874  | -0.856325  | -0.843501  |
| H       | 2.881289   | -1.996585  | 0.885344   |
| H       | 2.174483   | -1.782248  | -0.782873  |
| H       | 0.818947   | -1.007295  | 1.872658   |
| H       | -3.044513  | 1.943012   | -1.031539  |
| H       | -1.589990  | 2.186706   | -0.056666  |
| H       | -1.492168  | 1.288148   | -1.582419  |
| H       | -4.278566  | 0.902515   | 0.872187   |
| H       | -3.527817  | -0.406431  | 1.799360   |
| H       | -2.867656  | 1.234909   | 1.890148   |
| H       | -2.436748  | -1.063998  | -1.711163  |
| H       | -3.204496  | -1.779438  | -0.281458  |
| H       | -4.030881  | -0.500010  | -1.178243  |
| C       | 2.419821   | 1.628235   | 0.160470   |
| H       | 1.508869   | 1.174847   | 0.574930   |
| H       | 2.791975   | 2.354576   | 0.881637   |
2_tertbutylacrylate_TS_5_reopt

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.608577
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.426571

**Number of Imaginary Frequencies**

**Frequencies** (Top 3 out of 72)

1. -207.5527 cm⁻¹
2.  43.8507 cm⁻¹
3.  46.1623 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C | 1.797111 | 0.973626 | -1.182895 |
| C | 1.041802 | 1.654781 | -0.245236 |
| C | -0.262507 | 1.248081 | 0.178477 |
| O | -0.683702 | 0.104983 | -0.428425 |
| O | -0.961688 | 1.843479 | 0.995744 |
| C | -1.964696 | -0.495669 | -0.133847 |
| C | -1.973697 | -1.736055 | -1.017774 |
| C | -2.047577 | -0.905468 | 1.331980 |
| C | -3.106437 | 0.432902 | -0.530460 |
| H |  1.298698 | 0.292518 | -1.854647 |
| H |  2.669454 | 1.460906 | -1.593248 |
| H |  1.450882 | 2.504208 | 0.285315 |
| H | -2.946014 | -1.503904 | 1.487924 |
| H | -1.181246 | -1.513462 | 1.596588 |
| H | -2.083509 | -0.035993 | 1.981770 |
| H | -2.901435 | -2.290166 | -0.877617 |
| H | -1.135423 | -2.385498 | -0.763741 |
| H | -1.890315 | -1.453613 | -2.067433 |
| H | -4.051605 | -0.106253 | -0.455128 |
| H | -3.144122 | 1.305848 | 0.114608 |
| H | -2.980220 | 0.757440 | -1.564282 |
| C |  2.248671 | -0.838470 | 1.327614 |
| H |  1.590468 | 0.036587 | 1.411023 |
| H |  1.636313 | -1.735059 | 1.420351 |
### 2_tertbutylacrylate_TS_6_reopt

#### Datum

|               | Value          |
|---------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.609398   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.427882   |

#### Number of Imaginary Frequencies

1

#### Frequencies (Top 3 out of 72)

1. -203.1607 cm⁻¹
2. 24.6706 cm⁻¹
3. 41.2816 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |         |         |         |
|---|---------|---------|---------|
| C | -2.156332 | -1.499065 | 0.258658 |
| C | -0.950848 | -1.105946 | 0.804705 |
| C | 0.124630  | -0.686044 | -0.040639 |
| O | 1.221205  | -0.317122 | 0.683470 |
| O | 0.113901  | -0.64912 | -1.267008 |
| C | 2.414507  | 0.198157  | 0.051014  |
| C | 2.109473  | 1.48366  | -0.710477 |
| C | 3.303622  | 0.501822  | 1.229517 |
| C | 3.055880  | -0.85676 | -0.843083 |
| H | -2.174282 | -1.782138 | -0.783049 |
| H | -2.881202 | -1.996750 | 0.885084 |
| H | -0.818991 | -1.007273 | 1.872638 |
| H | 4.278657  | 0.902392  | 0.872223 |
| H | 2.867662  | 1.235398  | 1.889867 |
| H | 3.527518  | -0.406899 | 1.799725 |
| H | 3.045077  | 1.942733  | -1.031618 |
| H | 1.493017  | 1.287724  | -1.583131 |
| H | 1.590865  | 2.186621  | -0.057529 |
| H | 2.436741  | -1.064704 | -1.710674 |
| H | 4.030916  | -0.500647 | -1.177960 |
| H | 3.204424  | -1.779666 | -0.280687 |
| C | -2.428015 | 1.628214  | 0.160532 |
| H | -1.509179 | 1.174930  | 0.573559 |
| H | -2.150706 | 2.152347  | -0.756208 |
H          -2.792388        2.354711        0.881428
S          -3.617132        0.315688       -0.136783

2_tertbutylacrylate_TS_7_reopt

| Datum                                            | Value        |
|--------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -862.603501  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423177  |
| Number of Imaginary Frequencies                  | 1            |

**Frequencies** (Top 3 out of 72)

1.  -233.9947 cm⁻¹
2.   25.3806 cm⁻¹
3.   32.5538 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -1.688319 | 0.928356 | -0.797237 |
|-------|-----------|----------|------------|
| C     | -0.687404 | 1.754437 | -0.325180 |
| C     | 0.639210  | 1.311502 | -0.025874 |
| O     | 0.831943  | -0.009633 | -0.288836 |
| O     | 1.538141  | 2.021311 | 0.418835  |
| C     | 2.090654  | -0.670712 | -0.027450 |
| C     | 1.819683  | -2.108155 | -0.452161 |
| C     | 3.205880  | -0.079378 | -0.881623 |
| C     | 2.425819  | -0.625556 | 1.458838  |
| H     | -2.595403 | 1.377327 | -1.177669 |
| H     | -1.419881 | -0.011906 | -1.257026 |
| H     | -0.898161 | 2.780544 | -0.056875 |
| H     | 4.097703  | -0.700425 | -0.788728 |
| H     | 2.905374  | -0.068708 | -1.930252 |
| H     | 3.444608  | 0.933079 | -0.569743 |
| H     | 2.706971  | -2.719860 | -0.291218 |
| H     | 0.996683  | -2.524295 | 0.129380  |
| H     | 1.555129  | -2.147317 | -1.509019 |
| H     | 3.285283  | -1.268093 | 1.653699  |
| H     | 2.659642  | 0.385740 | 1.778471  |
| H     | 1.581421  | -0.997936 | 2.040830  |
| C     | -4.014818 | -1.030854 | -0.488123 |
| H     | -4.974803 | -0.522354 | -0.570665 |
| H     | -3.518401 | -0.970585 | -1.461029 |
| Datum                                      | Value          |
|-------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -862.604234    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423904 |
| Number of Imaginary Frequencies           | 1              |

**Frequencies (Top 3 out of 72)**

1. -235.9450 cm\(^{-1}\)
2. 34.5894 cm\(^{-1}\)
3. 41.4428 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 1.974457 | -1.076030 | 0.061863 |
|-----|----------|-----------|----------|
| C   | 0.705821 | -1.089571 | -0.475554 |
| C   | -0.356442 | -0.371991 | 0.160564 |
| O   | -1.528686 | -0.495537 | -0.524948 |
| O   | -0.273088 | 0.282853  | 1.194250  |
| C   | -2.750603 | 0.131559  | -0.072478 |
| C   | -3.764154 | -0.277278 | -1.133390 |
| C   | -3.172991 | -0.418682 | 1.284910  |
| C   | -2.607800 | 1.649203  | -0.052484 |
| H   | 2.090811  | -0.788020 | 1.097813  |
| H   | 2.716072  | -1.768557 | -0.310343 |
| H   | 0.502411  | -1.552023 | -1.430419 |
| H   | -4.172571 | -0.054473 | 1.525222  |
| H   | -3.206014 | -1.508504 | 1.250436  |
| H   | -2.485947 | -0.108166 | 2.066569  |
| H   | -4.741746 | 0.142317  | -0.897604 |
| H   | -3.454609 | 0.087042  | -2.113049 |
| H   | -3.850922 | -1.363087 | -1.175745 |
| H   | -2.244078 | 2.000935  | -1.018934 |
| H   | -3.584513 | 2.099426  | 0.128911  |
| H   | -1.920107 | 1.970233  | 0.724316  |
| C   | 4.794468  | 0.014975  | 0.420852  |
| H   | 4.410124  | -0.601244 | 1.237670  |
| H   | 5.425122  | -0.615109 | -0.206690 |
### 3_methylcrotonate_1

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -345.784109 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -345.688853 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

1. 73.6615 cm⁻¹
2. 146.0981 cm⁻¹
3. 159.5768 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          | 1.871906 | 0.283441 | 0.000002 |
|----------|----------|----------|----------|
| C        | 0.770252 | -0.459914| -0.000002|
| C        | -0.566043| 0.168318 | -0.000000|
| C        | -1.534744| -0.753625| -0.000004|
| O        | -0.790902| 1.355779 | 0.000004 |
| C        | -2.872637| -0.253728| -0.000002|
| H        | -3.516873| -1.125991| -0.000003|
| H        | -3.049539| 0.349977 | 0.887649 |
| H        | -3.049540| 0.349977 | -0.887650|
| H        | 1.754526 | 1.362842 | 0.000007 |
| C        | 3.260286 | -0.252874| 0.000001 |
| H        | 0.805396 | -1.541425| -0.000006|
| H        | 3.803356 | 0.108356 | 0.875070 |
| H        | 3.271897 | -1.340784| -0.000004|
| H        | 3.803358 | 0.108364 | -0.875063|

### 3_methylcrotonate_2

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -345.783427 |
| Datum                                                                 | Value                      |
|----------------------------------------------------------------------|----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -345.688127                |
| Number of Imaginary Frequencies                                      | 0                          |

**Frequencies (Top 3 out of 39)**

```
1.  85.3381 cm⁻¹
2.  139.7822 cm⁻¹
3.  161.0840 cm⁻¹
```

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

```
C           1.664156       -0.400580       -0.000004
C           0.836520        0.640264        0.000004
C          -0.633754        0.524921        0.000005
O          -1.078546       -0.734111       -0.000004
O          -1.375323        1.480870        0.000013
C          -2.497419       -0.892965       -0.000005
H          -2.676728       -1.962471       -0.000011
H          -2.928733       -0.435156        0.887702
H          -2.928733       -0.435147       -0.887708
H           1.241780       -1.399512       -0.000011
C           3.149552       -0.295272       -0.000005
H           1.203816        1.658578        0.000011
H           3.562600       -0.799937       -0.875125
H           3.480016        0.741313        0.000003
H           3.562601       -0.799950        0.875107
```

---

**3 methylcrotonate_3**

| Datum                                                                 | Value                      |
|----------------------------------------------------------------------|----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -345.775611                |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -345.680396                |
| Number of Imaginary Frequencies                                      | 0                          |

**Frequencies (Top 3 out of 39)**

```
1.  51.1125 cm⁻¹
2.  135.6901 cm⁻¹
```
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     | C      | C      | O      | O      | C      | H      | H      | H      | H      | C      | H      | H      | H        |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|----------|
|     | 1.724753 | 0.213489 | 0.000005 | 0.490686 | -0.285024 | -0.000009 | -1.905048 | 0.103742 | 0.000001 | -2.116810 | -1.308103 | 0.000001 | -3.193526 | -1.440717 | 0.000011 |
|     | -0.672681 | 0.631716 | -0.000000 | -0.577324 | 1.836078 | 0.000005 | -1.695993 | -1.765901 | -0.893209 | -1.695977 | -1.765903 | 0.893203 | 1.836642 | 1.292957 | 0.000022 |
|     | -2.116810 | -1.308103 | 0.000001 | -3.193526 | -1.440717 | 0.000011 | -1.695993 | -1.765901 | -0.893209 | -1.695977 | -1.765903 | 0.893203 | 1.836642 | 1.292957 | 0.000022 |
|     | 2.968701 | -0.601743 | -0.000003 | 0.335163 | -1.353541 | -0.000026 | 3.574942 | -0.359561 | 0.874750 | 2.754886 | -1.668371 | -0.000020 | 3.574949 | -0.359534 | -0.874743 |

3_methylcrotonate_HEI_1

| Datum                                         | Value            |
|-----------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy         | -783.995001      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.866194 |
| Number of Imaginary Frequencies               | 0                |

Frequencies (Top 3 out of 54)

1.  60.2649 cm-1
2.  70.6865 cm-1
3.  81.3294 cm-1

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     | C      | C      | O      | O      | C      | O      | C      | C      | O      |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|     | 1.139143 | 0.749575 | 0.304819 | -0.149978 | 0.776021 | -0.405889 | -1.291098 | 0.221226 | 0.137687 |
|     | -2.409533 | 0.333180 | -0.700323 |
### 3_methylcrotonate_HEI_2

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -783.991845 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.863401 |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 54)**

1. 37.8713 cm\(^{-1}\)
2. 46.8032 cm\(^{-1}\)
3. 83.2227 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|            |              |              |              |
|------------|--------------|--------------|--------------|
| C          | -0.799975    | 0.535410     | -0.647598    |
| C          | 0.177098     | 0.918394     | 0.392286     |
| C          | 1.479812     | 0.463530     | 0.455629     |
| O          | 1.817066     | -0.416030    | -0.578188    |
| O          | 2.367251     | 0.739982     | 1.294586     |
| C          | 3.155402     | -0.863273    | -0.597414    |
| H          | 3.413004     | -1.406255    | 0.312521     |
| H          | 3.242660     | -1.529714    | -1.453193    |
| H          | 3.856307     | -0.035133    | -0.711274    |
| H          | -0.295126    | 0.274118     | -1.577501    |
| C          | -1.828321    | 1.630025     | -0.912548    |
### 3_methylcrotonate_HEI_3

| Datum                                                      | Value          |
|-------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -783.988922    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.860235    |
| Number of Imaginary Frequencies                             | 0              |

#### Frequencies (Top 3 out of 54)

1. 31.4725 cm\(^{-1}\)
2. 64.1989 cm\(^{-1}\)
3. 85.9684 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | -0.955382 | 0.555704 | -0.815677 |
|---------|-----------|----------|-----------|
| C       | 0.125486  | -0.413010| -1.116850 |
| C       | 1.352240  | -0.537145| -0.488184 |
| O       | 1.581012  | 0.393171 | 0.525679  |
| O       | 2.258740  | -1.369223| -0.722039 |
| C       | 2.852314  | 0.342333 | 1.136833  |
| H       | 3.653086  | 0.496595 | 0.412600  |
| H       | 2.869820  | 1.144029 | 1.872395  |
| H       | 3.022978  | -0.611708| 1.636669  |
| H       | -1.701527 | 0.474365 | -1.608246 |
| C       | -0.576110 | 2.029971 | -0.685120 |
| H       | -0.094479 | -1.187218| -1.839655 |
| H       | -1.466368 | 2.652075 | -0.577101 |
| H       | 0.071893  | 2.192777 | 0.172579  |
| H       | -0.038716 | 2.346271 | -1.580126 |
| S       | -1.963114 | 0.187479 | 0.735173  |
| C       | -2.456951 | -1.503402| 0.369784  |
| H       | -3.108026 | -1.539416| -0.503201 |
### 3_methylcrotonate_HEI_4

| Datum                                               | Value                  |
|-----------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy               | -783.994467            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.865886            |
| Number of Imaginary Frequencies                     | 0                      |

**Frequencies (Top 3 out of 54)**

1. 42.9921 cm⁻¹  
2. 55.8435 cm⁻¹  
3. 79.4335 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|      | C             | O             | H             |
|------|---------------|---------------|---------------|
| C    | 0.903260      | 0.600634      | 0.287067      |
| C    | -0.447233     | 0.773049      | -0.295485     |
| C    | -1.521547     | 0.026486      | 0.141213      |
| O    | -2.712956     | 0.325395      | -0.532535     |
| O    | -1.562642     | -0.844276     | 1.038733      |
| C    | -3.859945     | -0.365224     | -0.087921     |
| H    | -4.685035     | -0.019385     | -0.707481     |
| H    | -3.751558     | -1.444706     | -0.199757     |
| H    | -4.080716     | -0.151029     | 0.958991      |
| H    | 0.827074      | 0.207996      | 1.303004      |
| C    | 1.722479      | 1.883657      | 0.284350      |
| H    | -0.582129     | 1.477660      | -1.105141     |
| H    | 2.731832      | 1.732748      | 0.667504      |
| H    | 1.796732      | 2.279030      | -0.730249     |
| H    | 1.230897      | 2.633599      | 0.906987      |
| S    | 1.800987      | -0.730742     | -0.649187     |
| C    | 3.339402      | -0.913013     | 0.298766      |
| H    | 3.110900      | -0.980105     | 1.362246      |
| H    | 3.817791      | -1.839001     | -0.013897     |
| H    | 4.026702      | -0.087420     | 0.127252      |

### 3_methylcrotonate_HEI_5_reopt3
### Data

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -783.988159   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -783.85847    |
| Number of Imaginary Frequencies                           | 0             |

#### Frequencies (Top 3 out of 54)

1. 46.4774 cm⁻¹
2. 72.9766 cm⁻¹
3. 88.4450 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|                  | x     | y     | z     |
|------------------|-------|-------|-------|
| C                | 1.109704 | -1.053900 | 0.088031 |
| C                | -0.109914 | -1.113017 | -0.754981 |
| C                | -1.328022 | -0.488703 | -0.561172 |
| O                | -1.451177 | 0.205721 | 0.643667 |
| O                | -2.321929 | -0.491439 | -1.326613 |
| C                | -2.645571 | 0.935375 | 0.817144 |
| H                | -2.579151 | 1.400944 | 1.798689 |
| H                | -2.756522 | 1.711065 | 0.057034 |
| H                | -3.524479 | 0.291624 | 0.778789 |
| H                | 1.738233 | -1.908350 | -0.169992 |
| C                | 0.940253  | -1.049480 | 1.606018 |
| H                | 1.902800 | -1.209948 | 2.091861 |
| H                | 0.523084 | -0.109801 | 1.958026 |
| H                | 0.257869 | -1.847022 | 1.906487 |
| S                | 2.296348 | 0.341664 | -0.376200 |
| H                | 1.193437 | 1.759959 | -0.269692 |
| H                | 1.738139 | 2.628834 | -0.633083 |
| H                | 0.319764 | 1.586196 | -0.896587 |
| H                | 0.870075 | 1.937959 | 0.753883 |

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### 3_methylcrotonate_HEI_6

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -783.994667   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -783.864234   |
| Number of Imaginary Frequencies                           | 0             |
**Frequencies** (Top 3 out of 54)

1. 54.6686 cm⁻¹
2. 78.5247 cm⁻¹
3. 101.5193 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.962432 | 0.731130 | 0.419627 |
|-------|----------|----------|----------|
| C     | -0.417351| 0.595028 | -0.092916|
| C     | -1.345409| -0.184093| 0.566497 |
| O     | -2.640897| -0.291339| 0.050492 |
| O     | -1.194100| -0.837637| 1.626835 |
| C     | -2.965388| 0.375219 | -1.146154|
| H     | -2.848941| 1.457422 | -1.048415|
| H     | -2.346472| 0.031085 | -1.978478|
| H     | -4.007593| 0.147513 | -1.360367|
| H     | 1.004803 | 0.383056 | 1.451177 |
| C     | 1.511245 | 2.150908 | 0.322983 |
| H     | -0.651902| 1.099734 | -1.018030|
| H     | 2.549293 | 2.212024 | 0.654263 |
| H     | 1.460182 | 2.507068 | -0.707788|
| H     | 0.909839 | 2.819270 | 0.939590 |
| S     | 2.217831 | -0.322096| -0.490965|
| C     | 1.456794 | -1.944431| -0.330822|
| H     | 1.959467 | -2.622000| -1.017558|
| H     | 1.548826 | -2.326543| 0.683972 |
| H     | 0.403234 | -1.865859| -0.596830|

**3_methylcrotonate_HEI_7**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -783.993038   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.864016 |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 54)

1. 48.9703 cm⁻¹
2. 70.5437 cm⁻¹
3. 84.6283 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| C     | 0.785376  | 0.576758  | 0.384364  |
| C     | -0.434748 | 1.115828  | -0.263262 |
| C     | -1.673870 | 0.507050  | -0.244086 |
| O     | -1.702570 | -0.691479 | 0.476546  |
| O     | -2.743628 | 0.891840  | -0.769462 |
| C     | -2.960837 | -1.323424 | 0.569412  |
| H     | -3.356567 | -1.580025 | -0.413689 |
| H     | -2.804517 | -2.232909 | 1.146033  |
| H     | -3.692127 | -0.693818 | 1.078098  |
| H     | 0.525990  | -0.069569 | 1.223675  |
| C     | 1.734863  | 1.672767  | 0.849107  |
| H     | -0.346343 | 2.030782  | -0.835530 |
| H     | 2.656681  | 1.272670  | 1.271518  |
| H     | 1.995296  | 2.322705  | 0.011800  |
| H     | 1.246359  | 2.280428  | 1.613153  |
| S     | 1.665422  | -0.553615 |-0.806535  |
| C     | 3.019013  | -1.212516 | 0.197878  |
| H     | 3.811786  | -0.482274 | 0.344835  |
| H     | 2.638212  | -1.534406 | 1.167026  |
| H     | 3.429292  | -2.077411 | -0.319504 |

3_methylcrotonate_HEI_8_reopt

| Datum                                                                 | Value            |
|-----------------------------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -783.990291      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -783.860872      |

Number of Imaginary Frequencies: 0

Frequencies (Top 3 out of 54)

1. 64.1062 cm⁻¹
2. 73.0587 cm⁻¹
3. 91.6012 cm⁻¹
### 3_methylcrotonate_TS_1

| Datum                                                      | Value     |
|------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -783.987906 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.859366 |
| Number of Imaginary Frequencies                            | 1         |

**Frequencies (Top 3 out of 54)**

1. -198.8273 cm⁻¹
2. 57.2731 cm⁻¹
3. 63.9246 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

C  
1.011671  
0.894023  
-0.531480

C  
0.208162  
0.480034  
-0.934116

C  
1.248815  
0.203382  
-0.070354

O  
2.414538  
-0.191219  
-0.755623

O  
1.311563  
0.258671  
1.177261

C  
3.539477  
-0.454065  
0.051828

H  
3.352514  
-1.265149  
0.757268

H  
4.341905  
-0.743332  
-0.624291

H  
3.846869  
0.426216  
0.618894

H  
-1.610131  
1.464069  
-1.344912

C  
-1.267972  
1.718303  
0.747362

H  
-0.380251  
0.296839  
-1.986214

H  
-2.287407  
2.080394  
0.880040

H  
-0.979768  
1.132207  
1.616130

H  
-0.593231  
2.575087  
0.694303

S  
-2.389212  
-0.533121  
-0.438286

C  
-1.552630  
-1.595192  
0.750838

H  
-2.018178  
-2.577552  
0.711738

H  
-0.503235  
-1.673790  
0.468718

H  
-1.627923  
-1.203568  
1.763329
3_methylcrotonate_TS_2

| Datum | Value                  |
|-------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -783.986773 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.858417 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 54)

1. -211.3018 cm⁻¹
2. 31.6181 cm⁻¹
3. 56.7624 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        |        |        |
|--------|--------|--------|
| C      | -0.906469 | 1.017228 | -0.384916 |
| C      | 0.091814  | 1.103555 | 0.571932  |
| C      | 1.394880  | 0.549137 | 0.418127  |
| O      | 1.588043  | -0.087157 | -0.774994 |
| O      | 2.311468  | 0.604463 | 1.236068  |
| C      | 2.865044  | -0.675463 | -0.962684 |
| H      | 3.063138  | -1.427558 | -0.199661 |
| H      | 2.841562  | -1.141811 | -1.943821 |
| H      | 3.653161  | 0.075597  | -0.927265 |
| H      | -0.593743 | 0.743803  | -1.382266 |
| C      | -2.085098 | 1.949649  | -0.320227 |
| H      | -0.112056 | 1.550595  | 1.536800  |
| H      | -2.907243 | 1.605534  | -0.945347 |
3_methylcrotonate_TS_3_reopt

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -783.981629 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.852733 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 54)

1.  -201.4286 cm⁻¹  
2.    35.2728 cm⁻¹  
3.    71.1061 cm⁻¹  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C    | 0.818835 | 0.980229 | 0.836074 |
| C    | -0.190475| 0.127029 | 1.275071 |
| C    | -1.396688| -0.241172| 0.611114 |
| O    | -1.560979| 0.299399 | -0.630348|
| O    | -2.262171| -0.988268| 1.065495 |
| C    | -2.763979| -0.043034| -1.301429|
| H    | -3.634645| 0.280636 | -0.732715|
| H    | -2.732623| 0.472740 | -2.256944|
| H    | -2.829853| -1.118362| -1.461517|
| H    | 1.562757 | 1.177531 | 1.597440 |
| C    | 0.623907 | 2.154174 | -0.089885|
| H    | -0.032887| -0.415450| 2.197625 |
| H    | 1.584059 | 2.612482 | -0.323222|
| H    | 0.135867 | 1.871800 | -1.015925|
| H    | 0.001679 | 2.903898 | 0.408552 |
| S    | 2.412000 | -0.162521| -0.469123 |
| C    | 1.762286 | -1.832862| -0.279709 |
| H    | 2.438424 | -2.477434| 0.280773 |
| H    | 0.813766 | -1.767185| 0.268779 |
| H    | 1.563335 | -2.295546| -1.245482|
### 3_methylcrotonate_TS_4

| Datum                                           | Value          |
|-------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -783.983201    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.855557    |
| Number of Imaginary Frequencies                 | 1              |

**Frequencies (Top 3 out of 54)**

1. -247.1072 cm⁻¹  
2.  41.0215 cm⁻¹  
3.  56.3149 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |        |        |        |        |
|-----|--------|--------|--------|--------|
| C   | 0.710980 | 0.836518 | 0.309397 |
| C   | -0.563496 | 0.946625 | -0.216044 |
| C   | -1.600002 | 0.053436 | 0.176184 |
| O   | -2.779076 | 0.304139 | -0.471713 |
| O   | -1.533031 | -0.859235 | 0.994255 |
| C   | -3.869798 | -0.530930 | -0.117409 |
| H   | -4.708793 | -0.208391 | -0.727319 |
| H   | -3.643896 | -1.576961 | -0.320376 |
| H   | -4.117425 | -0.424562 | 0.938296 |
| H   | 0.809877  | 0.247573 | 1.214113 |
| C   | 1.673869  | 1.981675 | 0.166049 |
| H   | -0.778936 | 1.660199 | -0.999871 |
| H   | 2.694370  | 1.694439 | 0.408085 |
| H   | 1.652762  | 2.377935 | -0.848817 |
| H   | 1.376097  | 2.785467 | 0.846091 |
| S   | 2.023179  | -0.852132 | -0.752883 |
| C   | 3.324406  | -0.908299 | 0.511367 |
| H   | 2.935984  | -0.518857 | 1.457193 |
| H   | 3.660494  | -1.929189 | 0.688303 |
| H   | 4.189704  | -0.306924 | 0.232829 |

### 3_methylcrotonate_TS_5
| Datum                                                                 | Value          |
|-----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -783.981629    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -783.852732    |
| Number of Imaginary Frequencies                                        | 1              |

**Frequencies (Top 3 out of 54)**

1. -201.3974 cm⁻¹
2. 35.3289 cm⁻¹
3. 71.1130 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Datum | Value |
|-------|-------|
| C     | -0.818768 0.980189 -0.836189 |
| C     | 0.190482 0.126884 -1.275054 |
| C     | 1.396721 -0.241255 -0.611067 |
| O     | 1.561031 0.299431 0.630332 |
| O     | 2.262183 -0.988397 -1.065402 |
| C     | 2.764046 -0.042937 1.301425 |
| H     | 2.732772 0.473041 2.256832 |
| H     | 2.829852 -1.118237 1.461739 |
| H     | 3.634699 0.280557 0.732594 |
| H     | -1.562726 1.177364 -1.597552 |
| C     | -0.623887 2.154188 0.089782 |
| H     | 0.032874 -0.415711 -2.197536 |
| H     | -1.584060 2.612443 0.323048 |
| H     | -0.135796 1.871883 1.015738 |
| H     | -0.001724 2.903930 -0.408788 |
| S     | -2.412023 -0.162433 0.469214 |
| C     | -1.762452 -1.832821 0.279711 |
| H     | -2.438516 -2.477249 -0.281029 |
| H     | -0.813791 -1.767181 -0.268542 |
| H     | -1.563789 -2.295665 1.245466 |

**3_methylcrotonate_TS_6**

| Datum                                                                 | Value          |
|-----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -783.9836      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -783.855044    |
| Number of Imaginary Frequencies                                        | 1              |
**Frequencies** (Top 3 out of 54)

1. -172.3500 cm\(^{-1}\)
2. 17.5161 cm\(^{-1}\)
3. 54.4248 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 0.761052 | 1.165619 | 0.349467 |
| C | -0.468998 | 0.803333 | -0.141018 |
| C | -1.352258 | 0.007194 | 0.662478 |
| O | -2.564623 | -0.358506 | 0.152454 |
| O | -1.122529 | -0.385436 | 1.799358 |
| C | -2.935410 | 0.018362 | -1.164102 |
| H | -2.970396 | 1.102617 | -1.270806 |
| H | -2.249082 | -0.39096 | -1.901614 |
| H | -3.928485 | -0.390629 | -1.326413 |
| H | 0.927747 | 1.014390 | 1.406274 |
| C | 1.573180 | 2.242018 | -0.306033 |
| H | -0.732194 | 1.059347 | -1.155917 |
| H | 2.620294 | 2.188167 | -0.017214 |
| H | 1.507273 | 2.176198 | -1.391549 |
| H | 1.186387 | 3.219563 | -0.002675 |
| S | 2.377158 | -0.704332 | -0.055053 |
| C | 1.162303 | -1.935225 | -0.570140 |
| H | 1.447540 | -2.412878 | -1.506959 |
| H | 1.015333 | -2.710865 | 0.181516 |
| H | 0.199049 | -1.433773 | -0.732197 |

**3_methylcrotonate_TS_7**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -783.981995 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.854066 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 54)

1. -248.6699 cm\(^{-1}\)
2. 52.5395 cm\(^{-1}\)
3. 72.5029 cm\(^{-1}\)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 0.598040 | 0.834971 | 0.424058 |
| C   | -0.572200 | 1.237499 | -0.196204 |
| C   | -1.777571 | 0.480064 | -0.206719 |
| O   | -1.704988 | -0.690607 | 0.491267 |
| O   | -2.826900 | 0.794478 | -0.764350 |
| C   | -2.894586 | -1.462604 | 0.531448 |
| H   | -3.205031 | -1.755428 | -0.470635 |
| H   | -2.661460 | -2.345616 | 1.119559 |
| H   | -3.705651 | -0.907460 | 1.001323 |
| H   | 0.521189 | 0.038468 | 1.153858 |
| C   | 1.673185 | 1.853588 | 0.686089 |
| H   | -0.589245 | 2.144292 | -0.786909 |
| H   | 2.621095 | 1.393075 | 0.954122 |
| H   | 1.825517 | 2.485308 | -0.188696 |
| H   | 1.360899 | 2.496537 | 1.514477 |
| S   | 1.878372 | -0.686187 | -0.891473 |
| C   | 3.018459 | -1.192852 | 0.426949 |
| H   | 3.951885 | -0.630764 | 0.397717 |
| H   | 2.553465 | -1.020844 | 1.402199 |
| H   | 3.256524 | -2.253552 | 0.357490 |

3_methylcrotonate_TS_8_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -783.983668 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.854279 |
| Number of Imaginary Frequencies | 2 |

Frequencies (Top 3 out of 54)

1. -196.0135 cm⁻¹
2. -18.0050 cm⁻¹
3. 60.4262 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
4_methylmethacrylate_1

| Datum                                             | Value      |
|---------------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy             | -345.781977 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -345.686401 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 39)

1. 55.5385 cm⁻¹
2. 133.7581 cm⁻¹
3. 184.2183 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C       | 0.994902  | 1.028900  | 0.727328  |
|---------|-----------|-----------|-----------|
| C       | -0.225059 | 0.427302  | 1.008388  |
| C       | -1.282729 | 0.262646  | 0.068091  |
| O       | -2.367938 | -0.363378 | 0.627491  |
| O       | -1.318359 | 0.595105  | -1.112649 |
| C       | -3.469429 | -0.581409 | -0.238368 |
| H       | -3.186589 | -1.210625 | -1.081780 |
| H       | -4.228399 | -1.081150 | 0.356890  |
| H       | -3.860338 | 0.360827  | -0.621055 |
| H       | 1.633088  | 1.155837  | 1.592290  |
| C       | 1.178051  | 2.105772  | -0.309799 |
| H       | -0.363703 | -0.059312 | 1.963630  |
| H       | 2.234437  | 2.329402  | -0.449100 |
| H       | 0.742586  | 1.822074  | -1.262061 |
| H       | 0.679615  | 3.018092  | 0.033318  |
| S       | 2.513202  | -0.543313 | -0.201071 |
| C       | 1.464019  | -2.006247 | -0.115324 |
| H       | 1.878417  | -2.771600 | 0.539967  |
| H       | 0.487549  | -1.703182 | 0.284818  |
| H       | 1.303942  | -2.442953 | -1.100421 |
### 4_methylmethacrylate_2

| Datum                                      | Value               |
|--------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -345.781618         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -345.686015         |
| Number of Imaginary Frequencies            | 0                   |

**Frequencies** (Top 3 out of 39)

1. 46.3408 cm⁻¹
2. 146.4326 cm⁻¹
3. 172.9723 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|      |         |         |         |
|------|---------|---------|---------|
| C    | -2.107648 | -0.923423 | 0.000000 |
| C    | -1.186849 | 0.033369  | 0.000001 |
| C    | 0.246950  | -0.394877 | 0.000001 |
| O    | 1.076821  | 0.648847  | -0.000003|
| O    | 0.633141  | -1.538554 | 0.000005 |
| C    | 2.471255  | 0.337820  | -0.000003|
| H    | 2.988866  | 1.290546  | -0.000000|
| H    | 2.727641  | -0.236128 | 0.887795 |
| H    | 2.727640  | -0.236128 | -0.887800|
| H    | 1.820874  | -1.965858 | 0.000000 |
| H    | -3.162218 | -0.682545 | 0.000000 |
| C    | -1.495808 | 1.499864  | 0.000000 |
| H    | -1.068072 | 1.987185  | -0.876210|
| H    | -2.572003 | 1.656879  | 0.000001 |
| H    | -1.068071 | 1.987185  | 0.876210 |
4_methylmethacrylate_3

| Datum                                           | Value          |
|------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -345.769113    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -345.674082    |
| Number of Imaginary Frequencies                | 0              |

Frequencies (Top 3 out of 39)

1. 48.2441 cm⁻¹
2. 120.7213 cm⁻¹
3. 172.4030 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|        |        |        |        |
|--------|--------|--------|--------|
| C      | -0.705098 | -1.467959 | -0.813545 |
| C      | -0.838914 | -0.363613 | -0.090615 |
| C      | 0.188558  | 0.724030  | -0.186450 |
| O      | 1.486408  | 0.439721  | -0.047005 |
| O      | -0.130942 | 1.863143  | -0.418706 |
| C      | 1.948615  | -0.781960 | 0.540165  |
| H      | 2.897525  | -0.540428 | 1.008825  |
| H      | 1.250179  | -1.148441 | 1.287318  |
| H      | 2.101372  | -1.537208 | -0.226342 |
| H      | 0.170859  | -1.655609 | -1.419706 |
| H      | -1.491203 | -2.211437 | -0.836361 |
| C      | -2.046728 | -0.030009 | 0.731333  |
| H      | -2.506105 | 0.889268  | 0.368633  |
| H      | -2.774301 | -0.836735 | 0.683883  |
| H      | -1.770652 | 0.134747  | 1.774114  |

4_methylmethacrylate_HEI_1_reopt

| Datum                                           | Value          |
|------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -783.991114    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.863091    |
| Number of Imaginary Frequencies                | 0              |

Frequencies (Top 3 out of 54)

1. 48.2441 cm⁻¹
2. 120.7213 cm⁻¹
3. 172.4030 cm⁻¹
1. 32.6006 cm⁻¹  
2. 59.7670 cm⁻¹  
3. 87.6195 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | -1.165592 | 0.436021  | 1.059507  |
| C    | 0.071501  | 0.803286  | 0.347978  |
| C    | 1.125295  | -0.088915 | 0.359941  |
| O    | 2.218253  | 0.314203  | -0.423086 |
| O    | 1.230740  | -1.181696 | 0.971361  |
| C    | 3.363221  | -0.504891 | -0.345757 |
| H    | 3.158637  | -1.521148 | -0.684092 |
| H    | 4.108846  | -0.050945 | -0.996016 |
| H    | 3.755903  | -0.557219 | 0.671167  |
| H    | -0.994652 | -0.375600 | 1.762922  |
| H    | -1.620852 | 1.276349  | 1.591282  |
| C    | 0.042949  | 2.040276  | -0.503920 |
| H    | -0.486889 | 2.852064  | 0.007104  |
| H    | 1.045561  | 2.395399  | -0.735903 |
| H    | -0.478739 | 1.894499  | -1.460260 |
| C    | -1.758288 | -1.402223 | -0.977777 |
| H    | -0.791981 | -1.026411 | -1.314241 |
| H    | -1.607383 | -2.294507 | -0.372877 |
| H    | -2.375169 | -1.649298 | -1.838786 |
| S    | -2.586234 | -0.106535 | -0.041020 |

**4_methylmethacrylate_HEI_2**

| Datum | Value  |
|-------|--------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -783.991178 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.863254 |

Number of Imaginary Frequencies  

0  

**Frequencies** (Top 3 out of 54)

1. 32.2468 cm⁻¹  
2. 44.8667 cm⁻¹  
3. 76.7734 cm⁻¹
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |    |    |
|----|----|----|
| C  | -0.983207 | 0.298279 | -1.076062 |
| C  | 0.031138  | 1.020860 | -0.286742 |
| C  | 1.253403  | 0.465553 | 0.035180  |
| O  | 1.468671  | -0.810843 | -0.510241 |
| O  | 2.180374  | 0.953677 | 0.728845  |
| C  | 2.716090  | -1.398448 | -0.220144 |
| H  | 2.714039  | -2.374534 | -0.702107 |
| H  | 3.545475  | -0.805921 | -0.609647 |
| H  | 2.863925  | -1.525938 | 0.853272  |
| H  | -0.561356 | -0.522112 | -1.650043 |
| H  | -1.526535 | 0.957270  | -1.759297 |
| C  | -0.361956 | 2.349620  | 0.290231  |
| H  | 0.500279  | 2.852534  | 0.725898  |
| H  | -0.787659 | 3.012913  | -0.472281 |
| H  | -1.123439 | 2.263973  | 1.077273  |
| C  | -1.445615 | -1.521087 | 1.001641  |
| H  | -2.101635 | -1.868026 | 1.796800  |
| H  | -1.048717 | -2.376857 | 0.458505  |
| H  | -0.620263 | -0.952465 | 1.429356  |
| S  | -2.394099 | -0.443261 | -0.085074 |

### 4_methylmethacrylate_HEI_3

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -783.988881 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.860743 |

Number of Imaginary Frequencies  0

**Frequencies (Top 3 out of 54)**

1. 42.3674 cm⁻¹
2. 61.4810 cm⁻¹
3. 77.9003 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |    |    |
|----|----|----|
| C  | -1.061221 | -0.284539 | 1.078202 |
| C  | 0.116624  | 0.448510  | 0.571912 |
### 4_methylmethacrylate_HEI_4_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -783.988774 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.860216 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

1. 45.8043 cm⁻¹
2. 70.8177 cm⁻¹
3. 93.2099 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.806889 | -0.215120 | 1.073685 |
|-------|----------|-----------|----------|
| C     | -0.084132 | 0.775729  | 0.435670 |
| C     | -1.337955 | 0.440061  | -0.028516|
| O     | -1.682831 | -0.907246 | 0.151493 |
| O     | -2.183117 | 1.188599  | -0.578630|
| C     | -2.995613 | -1.259728 | -0.223103|
| H     | -3.094700 | -2.325672 | -0.026561|
| H     | -3.742790 | -0.715708 | 0.357570 |
| H     | -3.180370 | -1.067864 | -1.280554|
### 4_methylmethacrylate_HEI_5

| Datum                                                  | Value               |
|--------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                  | -783.989792         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.861989         |
| Number of Imaginary Frequencies                        | 0                   |

**Frequencies (Top 3 out of 54)**

1. 48.9600 cm\(^{-1}\)
2. 55.5320 cm\(^{-1}\)
3. 77.2881 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | -1.037550 | 0.117362 | 0.760124 |
|---------|-----------|----------|----------|
| C       | 0.288263  | 0.636186 | 0.356711 |
| C       | 1.320430  | -0.264655| 0.201831 |
| O       | 2.536104  | 0.312348 | -0.198136|
| O       | 1.307210  | -1.509501| 0.379585 |
| C       | 3.621519  | -0.577135| -0.330647|
| H       | 3.853660  | -1.077270| 0.610652 |
| H       | 3.428816  | -1.342744| -1.083346|
| H       | 4.474690  | 0.024518 | -0.638770|
| H       | -0.960803 | -0.844994| 1.263669 |
| H       | -1.575224 | 0.817304 | 1.406795 |
| C       | 0.392018  | 2.105430 | 0.057925 |
| H       | 0.015194  | 2.713567 | 0.889586 |
| H       | 1.422116  | 2.403757 | -0.124883|
| H       | -0.193494 | 2.402911 | -0.822085|
| C       | -3.693263 | -0.560467| 0.157617 |
| Datum                                                                 | Value       |
|-----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -783.989833 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -783.861945 |
| Number of Imaginary Frequencies                                       | 0           |

**Frequencies** (Top 3 out of 54)

1. 50.0531 cm⁻¹  
2. 57.8527 cm⁻¹  
3. 80.5713 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | 0.332313 | 0.907000 | 0.297453 |
|------------|----------|----------|----------|
| C          | 1.530257 | 0.289633 | 0.005411 |
| O          | 1.512954 | -1.104274 | 0.184274 |
| O          | 2.607993 | 0.803130 | -0.386364 |
| C          | 2.746704 | -1.761286 | 0.002669 |
| H          | 3.502411 | -1.408378 | 0.706855 |
| H          | 2.558843 | -2.819013 | 0.178428 |
| H          | 3.133883 | -1.626068 | -1.007848 |
| H          | -1.462027 | 0.729155 | 1.453477 |
| H          | -0.610948 | -0.804937 | 1.192910 |
| C          | 0.170960 | 2.384894 | 0.084374 |
| H          | 1.116666 | 2.833733 | -0.215949 |
| H          | -0.567281 | 2.622557 | -0.692385 |
| H          | -0.168275 | 2.899293 | 0.992295 |
| C          | -3.424692 | -0.884543 | 0.252203 |
| H          | -4.200539 | -1.153087 | -0.461397 |
| H          | -3.134239 | -1.773568 | 0.810220 |
| H          | -3.820341 | -0.139645 | 0.941342 |
| S          | -2.017634 | -0.217722 | -0.662049 |
4_methylmethacrylate_TS_1

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -783.984906 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.856529 |
| Number of Imaginary Frequencies                            | 1           |

**Frequencies** (Top 3 out of 54)

1. -226.9363 cm⁻¹
2.  50.3544 cm⁻¹
3.  59.7216 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C       |  1.022812 |  0.822892 |  1.118926 |
|---------|----------|----------|----------|
| C       |  0.108629 |  0.965619|  0.326522|
| C       |  1.129713 | -0.022813|  0.443896|
| O       |  2.175011 |  0.185149| -0.418252|
| O       |  1.158650 | -0.984957|  1.212201|
| C       |  3.233640 | -0.754966| -0.345502|
| H       |  2.882642 | -1.758917| -0.582312|
| H       |  3.970505 | -0.439263| -1.078833|
| H       |  3.681076 | -0.766800|  0.647681|
| H       | -0.959515 |  0.166405|  1.973731|
| H       | -1.674861 |  1.676609|  1.243759|
| C       |  0.169640 |  2.014736| -0.750654|
| H       | -0.580161 |  2.784172| -0.561329|
| H       |  1.144074 |  2.501722| -0.800152|
| H       | -0.032329 |  1.606410| -1.747671|
| C       | -1.627243 | -1.203835| -1.154048|
| H       | -0.634072 | -0.740381| -1.112544|
| H       | -1.514935 | -2.267929| -0.949531|
| H       | -2.016104 | -1.079427| -2.163824|
| S       | -2.680313 | -0.388371|  0.059037|

4_methylmethacrylate_TS_2

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -783.985082 |
### Datum | Value
---|---
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.857114

Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 54)

| # | Frequency (cm⁻¹) |
|---|---|
| 1. | -230.3728 |
| 2. | 51.3551 |
| 3. | 66.6325 |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | X | Y | Z |
|---|---|---|---|
| C | -0.795335 | 0.475986 | -1.286773 |
| C | 0.104954 | 1.065783 | -0.408033 |
| C | 1.286459 | 0.389229 | 0.012536 |
| O | 1.470437 | -0.840796 | -0.562475 |
| O | 2.121938 | 0.816539 | 0.810808 |
| C | 2.642755 | -1.534412 | -0.171050 |
| H | 2.628546 | -2.479028 | -0.707684 |
| H | 3.538976 | -0.973385 | -0.434001 |
| H | 2.648991 | -1.718958 | 0.902898 |
| H | -0.466307 | -0.365705 | -1.875675 |
| H | -1.519374 | 1.114572 | -1.775099 |
| C | -0.227025 | 2.360630 | 0.279496 |
| H | 0.649782 | 3.001186 | 0.382437 |
| H | -0.983482 | 2.906959 | -0.285513 |
| H | -0.626560 | 2.205687 | 1.289115 |
| C | -1.546382 | -0.991403 | 1.333940 |
| H | -2.139164 | -0.731782 | 2.209910 |
| H | -1.228576 | -2.029838 | 1.420954 |
| H | -0.651545 | -0.357646 | 1.328368 |
| S | -2.461428 | -0.685805 | -0.187691 |

### 4_methylmethacrylate_TS_3_reopt

| Datum | Value |
|---|---|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -783.984906 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.856525 |
| Number of Imaginary Frequencies | 1 |
**Frequencies (Top 3 out of 54)**

1. -226.7038 cm\(^{-1}\)
2.  50.3637 cm\(^{-1}\)
3.  59.7119 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C      | 1.022633 | 0.823060 | -1.118917 |
|--------|----------|----------|------------|
| C      | -0.108671| 0.965650 | -0.326466  |
| C      | -1.129748| -0.022877| -0.443931  |
| O      | -2.175027| 0.185046 | 0.418167   |
| O      | -1.158587| -0.984991| 1.212272   |
| C      | -3.233525| -0.755247| 0.345577   |
| H      | -2.882334| -1.759112| 0.582458   |
| H      | -3.970385| -0.439584| 1.078926   |
| H      | -3.681018| -0.767237| -0.647574  |
| H      |  0.959504| 0.166305 | -1.973520  |
| H      |  1.674745| 1.676727 | 1.243721   |
| C      | -0.170164| 2.014857 | 0.750599   |
| H      |  0.579988| 2.784079 | 0.561809   |
| H      | -1.144521| 2.502096 | 0.799288   |
| H      |  0.30887 | 1.606518 | 1.747760   |
| C      |  1.627272| -1.203702| 1.153952   |
| H      |  2.015761| -1.079003| 2.163838   |
| H      |  0.639008| -0.740434| 1.111976   |
| H      |  1.515167| -2.267868| 0.949684   |
| S      |  2.680645| -0.388336| -0.058935  |

**4_methylmethacrylate_TS_4_reopt**

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy       | -783.985082   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.857112 |

Number of Imaginary Frequencies

1

**Frequencies (Top 3 out of 54)**

1. -230.5716 cm\(^{-1}\)
2.  51.3820 cm\(^{-1}\)
3.  66.6349 cm\(^{-1}\)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | -0.795672 | 0.475729 | -1.286543 |
| C    | 0.104865  | 1.065673  | -0.407996  |
| C    | 1.286366  | 0.389249  | 0.012444   |
| O    | 1.470379  | -0.840867 | -0.562483  |
| O    | 2.121980  | 0.816638  | 0.810603   |
| C    | 2.642752  | -1.534321 | -0.170962  |
| H    | 2.628476  | -2.479162 | -0.707203  |
| H    | 3.538946  | -0.973413 | -0.434271  |
| H    | 2.649173  | -1.718426 | 0.903062   |
| H    | -0.466491 | -0.365778 | -1.875637  |
| H    | -1.519521 | 1.114444  | -1.774995  |
| C    | -0.226992 | 2.360608  | 0.279427   |
| H    | 0.649563  | 3.001731  | 0.381078   |
| H    | -0.984407 | 2.906291  | -0.284923  |
| H    | -0.625227 | 2.205878  | 1.289596   |
| C    | -1.546400 | -0.991356 | 1.334025   |
| H    | -1.228600 | -2.029786 | 1.421070   |
| H    | -0.651606 | -0.357543 | 1.328501   |
| H    | -2.139301 | -0.731719 | 2.209906   |
| S    | -2.461212 | -0.685761 | -0.187720  |

4_methylmethacrylate_TS_5_reopt

| Datum | Value    |
|-------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -783.979739 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.853053 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 54)

1.  -251.7318 cm⁻¹
2.   35.0702 cm⁻¹
3.   53.5001 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
4_methylmethacrylate_TS_6

| Datum                                             | Value    |
|---------------------------------------------------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy             | -783.979973 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -783.853631 |
| Number of Imaginary Frequencies                   | 1        |

**Frequencies (Top 3 out of 54)**

1. -257.3413 cm⁻¹
2. 32.3660 cm⁻¹
3. 58.6917 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| X     | Y     | Z     |
|-------|-------|-------|
| C     | -0.710746 | 0.381996 | 0.815353 |
| C     | 0.453389  | 0.983814 | 0.364932 |
| C     | 1.606577  | 0.213685 | 0.034613 |
| O     | 1.481538  | -1.128162 | 0.271350 |
| O     | 2.659535  | 0.654611 | -0.425482 |
| C     | 2.623956  | -1.915606 | -0.019834 |
**5_methyltiglate_1**

| Datum                                                      | Value          |
|------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -385.094038    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.97239     |
| Number of Imaginary Frequencies                            | 0              |

**Frequencies (Top 3 out of 48)**

1. 49.6713 cm⁻¹
2. 124.2600 cm⁻¹
3. 133.7189 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C | 1.705103 | -0.633504 | -0.000020 |
| C | 0.684477 | 0.226314  | 0.000008  |
| C | -0.682110| -0.374401 | 0.000009  |
| O | -1.636593| 0.560915  | 0.00017   |
| O | -0.935981| -1.556432 | -0.00039  |
| C | -2.981280| 0.081538  | -0.00006  |
| H | -3.612202| 0.963581  | 0.000078  |
| H | -3.167178| -0.519565 | -0.887526 |
| H | -3.167154| -0.519720 | 0.887413  |
| H | 1.447008 | -1.687159 | -0.00053  |
| C | 3.162405 | -0.323801 | -0.00013  |
| C | 0.783835 | 1.723307  | 0.00057   |
| H | 0.288074 | 2.142495  | 0.875740  |
5_methyltiglate_2

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -385.094139   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.97299    |
| Number of Imaginary Frequencies                            | 0             |

**Frequencies (Top 3 out of 48)**

1. 48.4999 cm⁻¹  
2. 110.5146 cm⁻¹  
3. 115.5529 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 1.361073 | -0.852407 | 0.000010 |
| C   | 0.724579 | 0.321389  | -0.000011|
| C   | -0.764157| 0.354631  | -0.000005|
| O   | -1.348809| -0.846546 | 0.000020 |
| O   | -1.401171| 1.383270  | -0.000021|
| C   | -2.775897| -0.843582 | 0.000033 |
| H   | -3.153243| -0.34003  | 0.887582 |
| H   | -3.153259| -0.340049 | -0.887535|
| H   | -3.075099| -1.886021 | 0.000063 |
| H   | 0.750890 | -1.747546 | 0.000033 |
| C   | 2.833478 | -1.086421 | 0.000008 |
| C   | 1.362116 | 1.678742  | -0.000039|
| H   | 1.046479 | 2.247044  | 0.875292 |
| H   | 2.445565 | 1.617780  | -0.000013|
| H   | 1.046517 | 2.246993  | -0.875418|
| H   | 3.113356 | -1.677318 | -0.874244|
| H   | 3.418106 | -0.171604 | -0.000071|
| H   | 3.113380 | -1.677183 | 0.874345 |
## 5_methyltiglate_3

| Datum | Value                  |
|-------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -385.080926 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.960136 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 48)

1. 50.7450 cm⁻¹  
2. 99.1487 cm⁻¹  
3. 118.0540 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |    |    |    |
|----|----|----|----|
| C  | -1.160761 | -0.628756 | -0.406362 |
| C  | -0.475904 | 0.407925  | 0.076416  |
| C  | 0.974018  | 0.531829  | -0.265739 |
| O  | 1.782617  | -0.535510 | -0.197770 |
| O  | 1.444910  | 1.577328  | -0.642746 |
| C  | 1.495260  | -1.677000 | 0.616040  |
| H  | 2.450042  | -2.004457 | 1.017088  |
| H  | 0.820513  | -1.423377 | 1.428695  |
| H  | 1.063366  | -2.471442 | 0.012302  |
| H  | -0.609846 | -1.384991 | -0.956048 |
| C  | -2.630086 | -0.871317 | -0.311677 |
| C  | -1.036970 | 1.589616  | 0.811402  |
| H  | -0.912813 | 2.493817  | 0.215581  |
| H  | -2.090717 | 1.463698  | 1.038574  |
| H  | -0.499556 | 1.745839  | 1.747910  |
| H  | -2.816397 | -1.832364 | 0.171177  |
| H  | -3.156985 | -0.099065 | 0.240585  |
| H  | -3.061172 | -0.935982 | -1.312221 |

## 5_methyltiglate_4

| Datum | Value                  |
|-------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -385.081265 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.959662 |
| Datum                                      | Value            |
|-------------------------------------------|------------------|
| Number of Imaginary Frequencies           | 0                |

**Frequencies** (Top 3 out of 48)

1. 63.5213 cm⁻¹  
2. 114.5190 cm⁻¹  
3. 142.4851 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C          |          | O           |          | C          |          | O           |          | C          |          | H           |          | H           |          | H           |          | H           |          | H           |          | H           |          | C          |          | C          |          | H           |          | H           |          | H           |          |
|---|------------|----------|-------------|----------|------------|----------|-------------|----------|------------|----------|-------------|----------|-------------|----------|-------------|----------|-------------|----------|-------------|----------|-------------|----------|-------------|----------|-------------|----------|-------------|----------|
|   | -1.527943  | 0.507370 | -0.377373   |          | -0.466410  | -0.019315| 0.231970    |          | 0.800884   | 0.769975 | 0.172470    |          | 1.943835    | 0.123913 | -0.107703   |          | 0.858182   | 1.956103 | 0.384644    |          | 1.940445   | -1.165533| -0.725190   |          | 2.824568   | -1.199050| -1.354375   |          | 1.999308   | -1.947156| 0.028439    |          | 1.053600   | -1.303417| -1.340328   |          | -1.400690  | 1.462374 | -0.876147   |          | 2.885614   | -0.104649| -0.450992   |          | -0.477270  | -1.315221| 1.004684    |          | 0.402078   | -1.401187| 1.640586    |          | -1.354365  | -1.355581| 1.648142    |          | -0.503862  | -2.187206| 0.350070    |          | -3.184039  | -0.230846| -1.493054   |          | -2.935294  | -1.072777| 0.040996    |          | -3.621986  | 0.558950 | 0.006725    |          |

**5_methyltiglate_HEI_1**

| Datum                                      | Value            |
|-------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.299953      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.144884 |
| Number of Imaginary Frequencies           | 0                |

**Frequencies** (Top 3 out of 63)
|   |   |   |
|---|---|---|
|   | 1. 49.2463 cm⁻¹ |   |
|   | 2. 52.1951 cm⁻¹ |   |
|   | 3. 82.4748 cm⁻¹ |   |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
|   | C -1.125600 | 0.465283 | -0.635048 |
|   | C 0.138742 | 0.707966 | 0.092471 |
|   | C 1.266271 | 0.027787 | -0.321977 |
|   | O 2.417623 | 0.308927 | 0.432515 |
|   | O 1.391954 | -0.786136 | -1.271779 |
|   | C 3.595510 | -0.347763 | 0.022176 |
|   | H 3.488480 | -1.432699 | 0.054325 |
|   | H 3.885862 | -0.065043 | -0.990946 |
|   | H 4.374884 | -0.040765 | 0.717432 |
|   | H -0.910994 | -0.038064 | -1.575695 |
|   | C -1.966775 | 1.711613 | -0.893118 |
|   | C 0.100294 | 1.601399 | 1.300953 |
|   | H 1.016850 | 1.521123 | 1.881173 |
|   | H -0.037707 | 2.662054 | 1.056451 |
|   | H -0.733189 | 1.331195 | 1.961778 |
|   | H -1.389158 | 2.430450 | -1.476626 |
|   | H -2.879070 | 1.472827 | -1.441807 |
|   | H -2.251528 | 2.192493 | 0.043929 |
|   | S -2.304050 | -0.708950 | 0.262256 |
|   | C -1.296888 | -2.114164 | 0.522923 |
|   | H -1.681007 | -2.783965 | 1.238953 |
|   | H -1.023832 | -2.649356 | -0.406072 |
|   | H -0.263923 | -1.752102 | 0.924836 |

5_methyltiglate_HEI_2

|   |   |   |
|---|---|---|
|   | Datum | Value |
|   | M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.300044 |
|   | M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.144707 |
|   | Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 63)

|   |   |   |
|---|---|---|
|   | 1. 43.3060 cm⁻¹ |   |
|   | 2. 57.8526 cm⁻¹ |   |
|   | 3. 92.3374 cm⁻¹ |   |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 0.976682 | -0.254071 | -0.725029 |
| C | -0.035673 | -0.930042 | 0.114665 |
| C | -1.358484 | -0.533461 | 0.138329 |
| O | -1.664123 | 0.520935 | -0.738130 |
| O | -2.304445 | -0.995535 | 0.824563 |
| C | -2.992795 | 0.987565 | -0.696245 |
| H | -3.054746 | 1.799502 | -1.418791 |
| H | -3.706925 | 0.208658 | -0.966542 |
| H | -3.258302 | 1.364768 | 0.292926 |
| H | 0.496451 | 0.347775 | -1.491800 |
| C | 1.989821 | -1.192820 | -1.373870 |
| C | 0.429061 | -1.997167 | 1.065432 |
| H | -0.363288 | -2.243684 | 1.770776 |
| H | 0.727310 | -2.929422 | 0.570172 |
| H | 1.300847 | -1.666256 | 1.643934 |
| H | 1.468768 | -1.912907 | -2.006841 |
| H | 2.706763 | -0.645715 | -1.987678 |
| H | 2.545927 | -1.751040 | -0.619401 |
| S | 2.046076 | 0.986878 | 0.225147 |
| C | 0.762683 | 2.036495 | 0.925187 |
| H | 1.220235 | 2.675979 | 1.676952 |
| H | 0.294983 | 2.653420 | 0.160256 |
| H | 0.005527 | 1.406684 | 1.391410 |

5_methyltiglate_HEI_3_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.298578 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.143052 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 63)

1. 55.1829 cm⁻¹
2. 65.5468 cm⁻¹
3. 85.6906 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C          | 0.922559 | 0.234411 | 0.553382 |
|---|------------|---------|---------|---------|
|   | C          | -0.414884 | 0.628651 | 0.032275 |
|   | C          | -1.456236 | -0.242556 | 0.227289 |
|   | O          | -2.691119 | 0.205744 | -0.292223 |
|   | O          | -1.464373 | -1.359179 | 0.807040 |
|   | C          | -3.791229 | -0.651851 | -0.090972 |
|   | H          | -3.634513 | -1.628778 | -0.550276 |
|   | H          | -3.997645 | -0.804476 | 0.969577 |
|   | H          | -4.646945 | -0.166787 | -0.557350 |
|   | H          | 0.802193  | -0.544352 | 1.305756 |
|   | C          | 1.737208  | 1.386188  | 1.128292 |
|   | C          | -0.527391 | 1.916988  | -0.736069 |
|   | H          | 0.244057  | 1.992913  | -1.512600 |
|   | H          | -1.493669 | 1.992789  | -1.229740 |
|   | H          | -0.411813 | 2.809959  | -0.108724 |
|   | H          | 1.176149  | 1.860421  | 1.936776 |
|   | H          | 2.690822  | 1.047788  | 1.533332 |
|   | H          | 1.939536  | 2.140852  | 0.367361 |
|   | S          | 1.871905  | -0.590143 | -0.823743 |
|   | C          | 3.433310  | -1.037416 | -0.026830 |
|   | H          | 4.075502  | -0.172780 | 0.125790 |
|   | H          | 3.238275  | -1.518017 | 0.931656 |
|   | H          | 3.945472  | -1.746266 | -0.674420 |

5_methyltiglate_HEI_4

| Datum | Value   |
|-------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.294761 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139482 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 63)

1. 20.9913 cm⁻¹
2. 71.8347 cm⁻¹
3. 84.1060 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.294385   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -823.138231   |
| Number of Imaginary Frequencies                                      | 0             |

**Frequencies** (Top 3 out of 63)

1. 36.1335 cm⁻¹
2. 70.0752 cm⁻¹
3. 90.3460 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C      | 0.632106 | -0.471027 | 0.544044 |
|--------|----------|-----------|----------|
| C      | -0.285681| 0.658932  | 0.211401 |
| C      | -1.621011| 0.449557  | -0.068798|
### 5_methyltiglate_HEI_6

| Datum                                      | Value             |
|--------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.298384       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.14299       |
| Number of Imaginary Frequencies            | 0                 |

**Frequencies (Top 3 out of 63)**

1. 45.8415 cm\(^{-1}\)
2. 61.1048 cm\(^{-1}\)
3. 86.4789 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|    |    |    |    |
|----|----|----|----|
| C  | 0.764701 | 0.178909 | 0.555434 |
| C  | -0.435817 | 0.880471 | 0.023563 |
| C  | -1.661867 | 0.259216 | -0.089382 |
| O  | -1.672823 | -1.081221 | 0.333266 |
| O  | -2.746802 | 0.731895 | -0.513514 |
| C  | -2.933159 | -1.712227 | 0.334585 |
| H  | -2.766720 | -2.727668 | 0.689815 |
### 5_methyltiglate_TS_1

| Datum | Value         |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.29476 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140365 |

Number of Imaginary Frequencies 1

**Frequencies** (Top 3 out of 63)

1. -213.8843 cm⁻¹
2. 40.2382 cm⁻¹
3. 55.6738 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|      | X           | Y           | Z           |
|------|-------------|-------------|-------------|
| H    | -3.637520   | -1.209119   | 0.999429    |
| H    | -3.371870   | -1.745507   | -0.663246   |
| H    | 0.468803    | -0.700347   | 1.124138    |
| C    | 1.664700    | 1.058928    | 1.415231    |
| C    | -0.274181   | 2.289396    | -0.476763   |
| H    | 0.571736    | 2.385868    | -1.168521   |
| H    | -1.173121   | 2.598904    | -1.008128   |
| H    | -0.098260   | 3.021581    | 0.321345    |
| H    | 2.509313    | 0.502816    | 1.821614    |
| H    | 2.055251    | 1.899444    | 0.840628    |
| H    | 1.088364    | 1.458212    | 2.252871    |
| S    | 1.739799    | -0.503658   | -0.883469   |
| C    | 3.141150    | -1.313143   | -0.074453   |
| H    | 3.867769    | -0.594138   | 0.297515    |
| H    | 2.789024    | -1.932488   | 0.750298    |
| H    | 3.624296    | -1.953718   | -0.809555   |
| C    | -1.012455   | 0.784983    | -0.688348   |
| C    | 0.141159    | 0.833068    | 0.093246    |
| C    | 1.284089    | 0.133855    | -0.391960   |
| O    | 2.380513    | 0.222771    | 0.429214    |
| O    | 1.375127    | -0.505317   | -1.442467   |
| C    | 3.542423    | -0.453533   | -0.018522   |
| H    | 3.359253    | -1.522452   | -0.123718   |
| H    | 3.880715    | -0.062132   | -0.977336   |
| H    | 4.302766    | -0.282393   | 0.738697    |
| H    | -0.866865   | 0.422881    | -1.696788   |
| C    | -2.082159   | 1.834211    | -0.544938   |
### 5_methyltiglate_TS_2

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.294927 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140417 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 63)

1. -224.8927 cm⁻¹
2. 47.1365 cm⁻¹
3. 64.7576 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 0.852983 | -0.540859 | -0.854271 |
| C | -0.072728 | -0.999384 | 0.085840  |
| C | -1.395842 | -0.476267 | 0.131402  |
| O | -1.654069 | 0.483105  | -0.816272 |
| O | -2.294238 | -0.802452 | 0.911510  |
| C | -2.962129 | 1.026424  | -0.804770 |
| H | -2.993092 | 1.756240  | -1.609362 |
| H | -3.712360 | 0.255238  | -0.976532 |
| H | -3.176701 | 1.515569  | 0.145180  |
| H | 0.445374  | 0.025688  | -1.678365 |
| C | 2.040550  | -1.392145 | -1.221697 |
| C | 0.355747  | -1.939539 | 1.178674  |
| H | -0.456386 | -2.096094 | 1.885557  |
| H | 0.664594  | -2.918562 | 0.801549  |
| H | 1.210862  | -1.531402 | 1.731081  |
### 5_methyltiglate_TS_3

| Datum                                           | Value          |
|-------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -823.289187    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy       | -823.134588    |
| (Quasiharmonic)                                 |                |
| Number of Imaginary Frequencies                 | 1              |

**Frequencies** (Top 3 out of 63)

1. -256.5346 cm⁻¹
2. 57.8545 cm⁻¹
3. 60.9238 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C      | 0.769545 | 0.510130 | 0.605734 |
|--------|----------|----------|----------|
| C      | -0.507087| 0.778438 | 0.112446 |
| C      | -1.491573| -0.237272| 0.273517 |
| O      | -2.712636| 0.080233 | -0.267394|
| O      | -1.352986| -1.325162| 0.836449 |
| C      | -3.730756| -0.891988| -0.107164|
| C      | -3.457666| -1.830782| -0.587863|
| H      | -3.928511| -1.085016| 0.946743 |
| H      | -4.618801| -0.480910| -0.579634|
| H      | 0.839053 | -0.308967| 1.311519 |
| C      | 1.734107 | 1.641327 | 0.838469 |
| C      | -0.762489| 2.019185 | -0.701498|
| H      | -0.152610| 2.034916 | -1.613258|
| H      | -1.803875| 2.088250 | -1.003043|
| H      | -0.516601| 2.930436 | -0.149579|
| H      | 1.353042 | 2.277394 | 1.644648 |
| H      | 2.718172 | 1.280315 | 1.128931 |
| H      | 1.841856 | 2.261388 | -0.049883|
| S      | 2.043862 | -0.729369| -0.907179|
### 5_methyltiglate_TS_4_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.29476     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140366 |

**Number of Imaginary Frequencies**

1

**Frequencies (Top 3 out of 63)**

1. -213.8492 cm⁻¹
2. 40.2952 cm⁻¹
3. 55.7054 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | 3.403219 | -1.131773 | 0.225897 |
|--------|----------|-----------|----------|
| H      | 4.211890 | -0.403486 | 0.167277 |
| H      | 3.034211 | -1.145617 | 1.255073 |
| H      | 3.813219 | -2.116870 | 0.007096 |

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.29476     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140366 |

**Number of Imaginary Frequencies**

1

**Frequencies (Top 3 out of 63)**

1. -213.8492 cm⁻¹
2. 40.2952 cm⁻¹
3. 55.7054 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | -1.012441 | 0.784977 | -0.688383 |
|--------|-----------|----------|-----------|
| C      | 1.284123  | 0.133849 | -0.391984 |
| O      | 2.380506  | 0.222722 | 0.429240  |
| O      | 1.375184  | -0.505328| -1.442481 |
| C      | 3.542409  | -0.453637| -0.018432 |
| H      | 3.359233  | -1.522571| -0.123473 |
| H      | 3.880678  | -0.062373| -0.977308 |
| H      | 4.302768  | -0.282391| 0.738748  |
| H      | -0.866922 | 0.422779 | -1.696797 |
| C      | -2.082193 | 1.834150 | -0.544937 |
| C      | 0.099770  | 1.455846 | 1.462501  |
| H      | -0.111975 | 2.528297 | 1.429296  |
| H      | -0.693660 | 0.999060 | 2.067012  |
| H      | 1.039129  | 1.320831 | 1.991715  |
| H      | -1.714655 | 2.785150 | -0.943465 |
| H      | -2.981306 | 1.560745 | -1.095490 |
| H      | -2.354277 | 1.989251 | 0.497822  |
| S      | -2.314267 | -1.037534| -0.070295 |
| C      | -1.060980 | -1.984340| 0.811136  |
| H      | -0.772222 | -2.887462| 0.274383  |
| H      | -0.172198 | -1.350825| 0.922666  |
| H      | -1.403102 | -2.262935| 1.807105  |
5_methyltiglate_TS_5_reopt2

| Datum                                              | Value          |
|----------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy               | -823.294927    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140419    |
| Number of Imaginary Frequencies                    | 1              |

**Frequencies (Top 3 out of 63)**

1. -224.9045 cm⁻¹  
2.  47.0836 cm⁻¹  
3.  64.7386 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| C | -0.852958 | 0.540871 | -0.854256 |
| C | 0.072744  | 0.999371 | 0.085871  |
| C | 1.395857  | 0.476229 | 0.131447  |
| O | 1.654083  | -0.483107| -0.816263 |
| O | 2.294246  | 0.802376 | 0.911578  |
| C | 2.962147  | -1.026416| -0.804804 |
| H | 2.993118  | -1.756160| -1.609461 |
| H | 3.712371  | -0.255210| -0.976498 |
| H | 3.176720  | -1.515643| 0.145103  |
| H | -0.445336 | -0.025675| -1.678345 |
| C | -2.040476 | 1.392221 | -1.221711 |
| C | -0.355735 | 1.939533 | 1.178697  |
| H | -0.664780 | 2.918476 | 0.801527  |
| H | -1.210721 | 1.531325 | 1.731253  |
| H | 0.456465  | 2.096271 | 1.885461  |
| H | -1.702001 | 2.262360 | -1.792827 |
| H | -2.749281 | 0.838079 | -1.835750 |
| H | -2.563500 | 1.753046 | -0.337737 |
| S | -2.036650 | -1.255882| -0.018308 |
| C | -0.872911 | -1.774509| 1.254687  |
| H | -0.342499 | -2.687069| 0.984324  |
| H | -0.136663 | -0.972515| 1.385951  |
| H | -1.376122 | -1.931119| 2.207825  |
5 methyltiglate_TS_6

| Datum                                                                 | Value                   |
|-----------------------------------------------------------------------|-------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -823.289318             |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -823.135108             |
| Number of Imaginary Frequencies                                       | 1                       |

**Frequencies** (Top 3 out of 63)

1.  -262.7267 cm⁻¹
2.   51.7949 cm⁻¹
3.   66.2136 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C  | 0.621193 | 0.473646 | 0.637072 |
| C  | -0.558196| 0.989190 | 0.095764 |
| C  | -1.715579| 0.175366 | -0.052576|
| O  | -1.578824| -1.095414| 0.446395 |
| O  | -2.790231| 0.503532 | -0.561399|
| C  | -2.724466| -1.922798| 0.350730 |
| H  | -2.444065| -2.878486| 0.785427 |
| H  | -3.564071| -1.499082| 0.901273 |
| H  | -3.024152| -2.062976| -0.687230|
| H  | 0.534383 | -0.454687| 1.186789 |
| C  | 1.666977 | 1.420690 | 1.164090 |
| C  | -0.581733| 2.367616 | -0.506924|
| H  | 0.134940 | 2.460663 | -1.332014|
| H  | -1.570796| 2.591260 | -0.900394|
| H  | -0.325878| 3.145739 | 0.217286 |
| H  | 2.575494 | 0.898431 | 1.455853 |
| H  | 1.925658 | 2.178990 | 0.427109 |
| H  | 1.271291 | 1.934864 | 2.046499 |
| S  | 1.907488 | -0.608754| -0.969384|
| C  | 3.103285 | -1.372960| 0.161810 |
| H  | 3.981790 | -0.745655| 0.311421 |
| H  | 2.635912 | -1.539319| 1.136078 |
| H  | 3.433252 | -2.339117| -0.217717|

7 isobutylacrylate_1

| Datum                                                                 | Value                   |
|-----------------------------------------------------------------------|-------------------------|
### Frequencies (Top 3 out of 57)

1. 51.8686 cm⁻¹
2. 60.5986 cm⁻¹
3. 80.0092 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 1.295189| -0.243411| 0.145602|
| C    | 2.541934| 0.562178 | 0.157949|
| C    | 3.625037| 0.137228 | -0.474723|
| O    | 1.161425| -1.307455| -0.408312|
| O    | 0.327920| 0.361317 | 0.838688 |
| C    | -0.947850| -0.296367| 0.894955 |
| C    | -1.790669| -0.013333| -0.338472|
| C    | -2.031974| 1.481967 | -0.510319|
| C    | -3.106396| -0.774976| -0.216977|
| H    | 2.513474 | 1.496393 | 0.701258 |
| H    | 4.539861 | 0.712780 | -0.474729|
| H    | 3.614761 | -0.804129| -1.009006|
| H    | -0.788610| -1.366051| 1.023536 |
| H    | -1.429701| 0.107280 | 1.785209 |
| H    | -1.244519| -0.389892| -1.206714|
| H    | -2.621989| 1.674141 | -1.406549|
| H    | -2.581952| 1.877830 | 0.346889 |
| H    | -1.094813| 2.031095 | -0.595840|
| H    | -3.730450| -0.602831| -1.093511|
| H    | -2.939952| -1.848557| -0.122813|
| H    | -3.662493| -0.438663| 0.661177 |
**Data**

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 57)

1. 51.8688 cm⁻¹  
2. 60.5986 cm⁻¹  
3. 80.0092 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -1.295189 | -0.243411 | 0.145602 |
| C | -2.541935 | 0.562178  | 0.157948 |
| C | -3.625037 | 0.137227  | -0.474724 |
| O | -1.161425 | -1.307455 | -0.408310 |
| O | -0.327920 | 0.361318  | 0.838687 |
| C | 0.947850  | -0.296367 | 0.894955 |
| C | 1.790669  | -0.013333 | -0.216977 |
| C | 3.106396  | 1.481967  | -0.510319 |
| H | -2.513474 | 1.496394  | 0.701256 |
| H | -4.539861 | 0.712779  | -0.474730 |
| H | -3.614761 | -0.804130 | -1.009005 |
| H | 1.429700  | 0.107280  | 1.785209 |
| H | 0.788609  | -1.366050 | 1.023536 |
| H | 1.244518  | -0.389891 | -1.206714 |
| H | 3.730449  | -0.602833 | -1.093512 |
| H | 3.662493  | -0.438665 | 0.661176 |
| H | 2.939950  | -1.848558 | -0.122814 |
| H | 2.621991  | 1.674140  | -1.406549 |
| H | 1.094815  | 2.031096  | -0.595839 |
| H | 2.581955  | 1.877830  | 0.346888 |

**7_isobutylacrylate_3**

**Datum**

**Value**

M06-2X/def2tzvpp-IEFPCM(water) Energy  
-424.398575

M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  
-424.249314

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 57)
1.  49.7953 cm⁻¹
2.  60.2993 cm⁻¹
3. 102.4427 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|    |        |        |        |
|----|--------|--------|--------|
| C  | -1.375996 | 0.285378 | 0.000003 |
| C  | -2.300652 | -0.875789 | 0.000003 |
| C  | -3.612320 | -0.692879 | -0.000005 |
| O  | -1.713505 | 1.444705 | -0.000001 |
| O  | -0.103907 | 0.110218 | 0.000010 |
| C  | 0.891763  | 0.925979 | 0.000010 |
| C  | 2.261459  | 0.274208 | -0.000002 |
| C  | 2.484437  | -0.556065 | -1.260357 |
| C  | 2.484455  | -0.556076 | 1.260341 |
| H  | -1.849590 | -1.858355 | 0.000009 |
| H  | -4.297937 | -1.528413 | -0.000005 |
| H  | -4.026841 | 0.307053 | -0.000010 |
| H  | 0.745190  | 1.546157 | 0.885260 |
| H  | 0.745201  | 1.546145 | 0.885291 |
| H  | 2.973996  | 1.103794 | -0.000003 |
| H  | 3.497806  | -0.956873 | -1.279341 |
| H  | 1.789667  | -1.396264 | -1.293059 |
| H  | 2.337697  | 0.042756 | -2.160134 |
| H  | 2.337697  | 0.042736 | 2.160126 |
| H  | 1.789687  | -1.396277 | 1.293045 |

**7_isobutylacrylate_4**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -424.398068   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -424.248614 |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 57)

1.  41.7586 cm⁻¹
2.  54.8351 cm⁻¹
3.  90.4747 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|  |  |  |
|---|---|---|
| C | -1.306599 | -0.632626 | -0.073016 |
| C | -2.664362 | -0.081386 | -0.297447 |
| C | -3.059072 | 1.105835 | 0.139536 |
| O | -0.954762 | -1.703475 | -0.509364 |
| O | -0.524805 | 0.163784 | 0.655343 |
| C | 0.823138 | -0.274169 | 0.887266 |
| C | 1.736631 | 0.046934 | -0.284779 |
| C | 1.753973 | 1.543275 | -0.575595 |
| C | 3.136231 | -0.471699 | 0.028449 |
| H | -3.316835 | -0.732974 | -0.862559 |
| H | -4.060132 | 1.465005 | -0.05471 |
| H | -2.393427 | 1.747349 | 0.700647 |
| H | 1.141544 | 0.268498 | 1.777139 |
| H | 0.817061 | -1.342478 | 1.098817 |
| H | 1.352294 | -0.483053 | -1.159628 |
| H | 0.755505 | 1.918864 | -0.797914 |
| H | 2.140380 | 2.092139 | 0.286647 |
| H | 2.397120 | 1.760371 | -1.428552 |
| H | 3.536915 | 0.023195 | 0.916145 |
| H | 3.813575 | -0.269651 | -0.800871 |
| H | 3.132897 | -1.546736 | 0.211280 |

7_isobutylacrylate_5

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -424.398068 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -424.248614 |

Number of Imaginary Frequencies 0

**Frequencies** (Top 3 out of 57)

| Rank | Frequency |
|------|-----------|
| 1. | 41.7586 cm⁻¹ |
| 2. | 54.8352 cm⁻¹ |
| 3. | 90.4747 cm⁻¹ |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### 7_isobutylacrylate_6

| Datum                                                | Value               |
|------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                | -424.398166         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -424.248959         |
| Number of Imaginary Frequencies                      | 0                   |

**Frequencies (Top 3 out of 57)**

1. 42.4624 cm\(^{-1}\)
2. 59.3915 cm\(^{-1}\)
3. 109.4919 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|         |             |             |             |
|---------|-------------|-------------|-------------|
| C       | -1.513521   | -0.564884   | 0.000002    |
| C       | -2.563082   | 0.482041    | -0.000001   |
| C       | -2.303148   | 1.781640    | -0.000001   |
| O       | -1.762511   | -1.747998   | -0.000003   |
| O       | -0.276823   | -0.076277   | 0.000010    |
### 7_isobutylacrylate_7

| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -424.398465 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -424.249459 |

Number of Imaginary Frequencies

0

**Frequencies** (Top 3 out of 57)

1. 43.2215 cm\(^{-1}\)
2. 63.0639 cm\(^{-1}\)
3. 104.6317 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        |        |        |
|--------|--------|--------|
| C      | -1.551253 | -0.632794 | 0.085951 |
| C      | -2.782795 | 0.184269  | -0.027365 |
| C      | 1.478362  | 1.4782851 | -0.312986 |
| O      | 0.500892  | -1.807345 | 0.371865  |
| O      | 0.050892  | 0.184269  | -0.027365 |
| C      | -0.676008 | -0.053633 | 0.085951  |
| C      | 0.279492  | -0.312986 | -0.027365 |
| C      | -0.501936 | -0.331603 | -0.333494 |
| C      | 1.431740  | 1.413740  | 0.684616  |
| H      | -0.366576 | 0.149298  | 0.085951  |
| H      | 2.032436  | -0.381009 | -0.333494 |
7_isobutylacrylate_8

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -424.397552 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -424.247897 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 57)

1. 40.8545 cm⁻¹
2. 72.5298 cm⁻¹
3. 85.8777 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -1.306779 | 0.509030 | -0.286904 |
|-------|-----------|----------|-----------|
| C     | -2.657407 | 0.119773 | 0.186255  |
| C     | -3.024099 | -1.131028| 0.425502  |
| O     | -0.987796 | 1.660223 | -0.467388 |
| O     | -0.500955 | -0.533961| -0.487770 |
| C     | 0.852173  | -0.291240| -0.903143 |
| C     | 1.815919  | -0.468387| 0.258525  |
| C     | 3.242341  | -0.321146| -0.261430 |
| C     | 1.532290  | 0.524003 | 1.380052  |
| H     | -3.330406 | 0.953962 | 0.330522  |
| H     | -4.021428 | -1.359857| 0.774995  |
| H     | -2.339367 | -1.955036| 0.279364  |
| H     | 1.051885  | -1.022839| -1.684325 |
| H     | 0.926832  | 0.712162 | -1.320465 |
| H     | 1.684306  | -1.483316| 0.643671  |
| H     | 3.455238  | -1.038968| -1.054321 |
| H     | 3.401286  | 0.683131 | -0.660374 |
### 7_isobutylacrylate_HEI_10_reopt

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzzvpp-IEFPCM(water) Energy                               | -862.6132           |
| M06-2X/def2tzzvpp-IEFPCM(water) Free Energy (Quasiharmonic)         | -862.429663         |
| Number of Imaginary Frequencies                                      | 0                   |
| **Frequencies** (Top 3 out of 72)                                    |                    |
| 1. 25.9963 cm⁻¹                                                     |                    |
| 2. 54.6172 cm⁻¹                                                     |                    |
| 3. 69.4906 cm⁻¹                                                     |                    |

### M06-2X/def2tzzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C       | 0.147524   | 1.439355 | 0.247521 |
| C       | 1.528709   | 1.445859 | 0.207612 |
| C       | 2.352113   | 0.673462 | -0.741368|
| O       | -0.605876  | 2.093992 | 1.003213 |
| O       | -0.439145  | 0.597656 | -0.709969|
| C       | -1.849413  | 0.552121 | -0.802701|
| C       | -2.413313  | -0.744402| -0.233912|
| C       | -3.898957  | -0.845224| -0.561929|
| C       | -2.176298  | -0.838278| 1.268186 |
| H       | 2.026167   | 2.056839 | 0.949365 |
| H       | 1.777157   | 0.355562 | -1.608499|
| H       | 3.221551   | 1.228601 | -1.097873|
| H       | -2.286366  | 1.485560 | -0.282440|
| H       | -2.100067  | 0.622092 | -1.864965|
| H       | -1.888465  | -1.570706| -0.724155|
| H       | -4.323332  | -1.770869| -0.171958|
| H       | -4.073594  | -0.818777| -1.638558|
| H       | -4.444813  | -0.012597| -0.111233|
| H       | -2.493076  | -1.808855| 1.653239 |
| H       | -1.122947  | -0.695986| 1.508832 |
| H       | -2.743160  | -0.062835| 1.788447 |
| S       | 3.154935   | -0.877642| -0.071409|
| C       | 1.675431   | -1.775800| 0.419029 |
7_isobutylacrylate_HEI_11

**Datum**                   **Value**
---                          ---
M06-2X/def2tzvpp-IEFPCM(water) Energy  -862.614553
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  -862.43118

Number of Imaginary Frequencies  0

**Frequencies** (Top 3 out of 72)

1. 29.1820 cm⁻¹  2. 52.0397 cm⁻¹  3. 60.7476 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| C  | 0.029542 | -1.159823 | 0.234005 |
| C  | -1.133702 | -0.819127 | 0.889142 |
| C  | -2.442309 | -0.989080 | 0.230731 |
| O  | 0.169516  | -1.609451 | -0.925610 |
| O  | 1.182293  | -0.998038 | 1.023263 |
| C  | 2.391410  | -0.808704 | 0.314328 |
| C  | 2.503373  | 0.585049  | -0.293949 |
| C  | 3.800652  | 0.692527  | -1.086908 |
| C  | 2.422774  | 1.663234  | 0.780153  |
| H  | -1.075658 | -0.387091 | 1.877416  |
| H  | -3.250236 | -1.158522 | 0.943463  |
| H  | -2.432204 | -1.818177 | -0.477022 |
| H  | 3.192106  | -0.952368 | 1.045220  |
| H  | 2.493986  | -1.563627 | -0.466635 |
| H  | 1.658582  | 0.706611  | -0.978440 |
| H  | 4.661709  | 0.544653  | -0.429830 |
| H  | 3.848084  | -0.058150 | -1.877175 |
| H  | 3.898960  | 1.676281  | -1.546902 |
| H  | 1.496550  | 1.581961  | 1.348656  |
| H  | 3.259424  | 1.566783  | 1.477533  |
| H  | 2.468126  | 2.659604  | 0.338183  |
| S  | -3.032526 | 0.433516  | -0.826133 |
| C  | -3.100515 | 1.705087  | 0.446890  |
| H  | -3.373303 | 2.646389  | -0.024573 |
### 7_sobutylacrylate_HEI_12

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.61287 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.429751 |

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 72)

1. 18.5018 cm⁻¹
2. 40.8544 cm⁻¹
3. 55.4328 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.072990 | 1.259361 | 0.120751 |
|-------|-----------|----------|----------|
| C     | 0.998807  | 1.208243 | -0.749262 |
| C     | 1.635280  | -0.036315 | -1.219255 |
| O     | -0.670341 | 2.269701 | 0.556543 |
| O     | -0.506886 | -0.004838 | 0.548792 |
| C     | -1.776988 | -0.107127 | 1.163905 |
| C     | -2.838453 | -0.598695 | 0.183024 |
| C     | -2.481288 | -1.976231 | -0.366092 |
| C     | -3.047694 | 0.400698 | -0.950099 |
| H     | 1.424012  | 2.157217 | -1.048772 |
| H     | 0.965877  | -0.889550 | -1.126605 |
| H     | 1.968979  | 0.023103 | -2.256562 |
| H     | -1.671510 | -0.829014 | 1.978042 |
| H     | -2.062064 | 0.856525 | 1.583829 |
| H     | -3.769190 | -0.681632 | 0.754147 |
| H     | -1.547115 | -1.924570 | -0.928320 |
| H     | -2.351726 | -2.702042 | 0.438713 |
| H     | -3.259703 | -2.345371 | -1.035183 |
| H     | -2.124521 | 0.518636 | -1.22106 |
| H     | -3.826297 | 0.056159 | -1.632314 |
| H     | -3.330037 | 1.381492 | -0.567127 |
| S     | 3.216348  | -0.534959 | -0.351083 |
| C     | 2.599387  | -0.66875 | 1.334781 |
| H     | 3.452921  | -0.767472 | 2.001797 |
7_isobutylacrylate_HEI_13_reopt

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -862.613682   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -862.430789   |
| Number of Imaginary Frequencies                            | 0             |

**Frequencies** (Top 3 out of 72)

1. 29.5364 cm⁻¹
2. 37.0532 cm⁻¹
3. 55.9963 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | -0.378130 | 1.559289 | -0.044705 |
| C | -1.662643 | 1.381771 | 0.432682  |
| C | -2.147687 | 0.149328 | 1.080865  |
| O | 0.100236  | 2.548094 | -0.648293 |
| O | 0.475392  | 0.482837 | 0.214337  |
| C | 1.760502  | 0.538696 | -0.368284 |
| C | 2.509862  | -0.737369| -0.022190 |
| C | 2.682994  | -0.886515| 1.485029  |
| C | 3.861165  | -0.741012| -0.728801 |
| H | -2.365915 | 2.179597 | 0.233622  |
| H | -2.884556 | 0.341668 | 1.862035  |
| H | -1.335320 | -0.427069| 1.519334  |
| H | 2.315163  | 1.406677 | 0.004159  |
| H | 1.677923  | 0.646457 | -1.453900 |
| H | 1.916824  | -1.579382| -0.392566 |
| H | 3.263482  | -0.048763| 1.880710  |
| H | 1.720809  | -0.048763| 1.93570   |
| H | 3.215701  | -1.807112| 1.72700   |
| H | 3.746982  | -0.660287| -1.810614 |
| H | 4.470233  | 0.100523 | -0.389717 |
| H | 4.410349  | -1.657641| -0.512466 |
| S | -3.073214 | -1.058866| -0.019319 |
| C | -1.788958 | -1.380300| 1.236884  |
| H | -2.236281 | -1.928759| -2.062850 |
### 7_isobutylacrylate_HEI_14

#### Datum

| Datum                              | Value       |
|------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.61448  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.431677 |

#### Frequencies (Top 3 out of 72)

1. 20.9879 cm⁻¹
2. 44.3110 cm⁻¹
3. 48.9233 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 0.002278 | -0.181689 | -0.068750 |
| C      | -1.034964 | 0.611830 | 0.375917 |
| C      | -2.170174 | 0.022559 | 1.108068 |
| O      | 0.174784 | -1.408993 | 0.102341 |
| O      | 0.957452 | 0.525206 | -0.816858 |
| C      | 2.209317 | -0.106249 | -0.998204 |
| C      | 3.086389 | -0.060681 | 0.247913 |
| C      | 3.339742 | 1.375322 | 0.691384 |
| C      | 4.396106 | -0.790713 | -0.026990 |
| H      | -1.044096 | 1.660027 | 0.114194 |
| H      | -2.632216 | 0.727479 | 1.800246 |
| H      | -1.869850 | -0.861389 | 1.670694 |
| H      | 2.069286 | -1.140617 | -1.315327 |
| H      | 2.701747 | 0.441312 | -1.806918 |
| H      | 2.546679 | -0.586690 | 1.039693 |
| H      | 3.947732 | 1.402867 | 1.596779 |
| H      | 3.874511 | 1.924165 | -0.088679 |
| H      | 2.403885 | 1.896652 | 0.891405 |
| H      | 5.037983 | -0.789846 | 0.854505 |
| H      | 4.220966 | -1.827458 | -0.318310 |
| H      | 4.942494 | -0.300901 | -0.837293 |
| S      | -3.589894 | -0.620646 | 0.074790 |
| C      | -4.055033 | 0.922872 | -0.727555 |
| H      | -4.411074 | 1.646825 | 0.004755 |
### 7_isobutylacrylate_HEI_15

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.614713 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430954 |
| Number of Imaginary Frequencies | 0 |

#### Frequencies (Top 3 out of 72)

1. 35.1935 cm⁻¹
2. 52.1688 cm⁻¹
3. 67.4290 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.075673 | -0.000996 | -0.005666 |
| C     | 1.057662 | -0.746704 | -0.624392 |
| C     | 2.256817 | -1.190393 | 0.108079  |
| O     | -0.010610 | 0.351701 | 1.190676  |
| O     | -0.940751 | 0.396108 | -0.895052 |
| C     | -2.144227 | 0.903938 | -0.354625 |
| C     | -3.251546 | -0.143888 | -0.348174 |
| C     | -4.560290 | 0.496081 | 0.101378  |
| C     | -2.884511 | -1.327794 | 0.538702  |
| H     | 0.976059 | -0.940019 | -1.685017 |
| H     | 2.587252 | -2.193952 | -0.164609 |
| H     | 2.084799 | -1.169781 | 1.183524  |
| H     | -1.972675 | 1.269712 | 0.659099  |
| H     | -2.443472 | 1.746947 | -0.983007 |
| H     | -3.370288 | -0.501382 | -1.375939 |
| H     | -4.466312 | 0.876740 | 1.121436  |
| H     | -4.840261 | 1.329783 | -0.544463 |
| H     | -5.374401 | -0.229263 | 0.090446  |
| H     | -1.935462 | -1.769744 | 0.233220  |
| H     | -2.784974 | -1.004442 | 1.577224  |
| H     | -3.654300 | -2.099829 | 0.494707  |
| S     | 3.808535 | -0.190161 | -0.181029 |
| C     | 3.214138 | 1.424529 | 0.349056  |
| H     | 3.110492 | 1.468899 | 1.431831  |
7_isobutylacrylate_HEI_16

| Datum | Value             | Datum | Value             |
|-------|-------------------|-------|-------------------|
|       |                   |       |                   |
|       |                   |       |                   |
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.615065 | M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.431104 |
| Number of Imaginary Frequencies | 0 | Frequencies (Top 3 out of 72) | |
| 1. | 32.0581 cm⁻¹ | 2. | 60.7387 cm⁻¹ |
| 3. | 67.8910 cm⁻¹ | |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -0.084204 | -1.027471 | 0.207853 |
|-------|-----------|-----------|----------|
| C     | -1.214661 | -1.178678 | -0.567483 |
| C     | -2.563324 | -1.051930 | 0.013773 |
| O     | 0.004731  | -0.760433 | 1.426363 |
| O     | 1.101474  | -1.251773 | -0.517705 |
| C     | 2.333628  | -0.913999 | 0.086682 |
| C     | 2.907820  | 0.375521  | -0.488559 |
| C     | 4.289574  | 0.630598  | 0.102642 |
| C     | 1.970654  | 1.549728  | -0.234505 |
| H     | -1.102641 | -1.385229 | -1.622669 |
| H     | -2.528138 | -1.153285 | 1.098140 |
| H     | -3.273687 | -1.784330 | -0.373574 |
| H     | 2.203154  | -0.813539 | 1.165223 |
| H     | 3.024425  | -1.739775 | -0.104725 |
| H     | 3.008168  | 0.237749  | -1.569815 |
| H     | 4.221328  | 0.760721  | 1.185525 |
| H     | 4.967939  | -0.201154 | -0.094016 |
| H     | 4.733089  | 1.535247  | -0.314347 |
| H     | 0.974186  | 1.343533  | -0.627479 |
| H     | 1.877683  | 1.735131  | 0.838175 |
| H     | 2.346179  | 2.459422  | -0.705342 |
| S     | -3.457150 | 0.553335  | -0.320710 |
| C     | -2.282470 | 1.694802  | 0.426835 |
| H     | -1.279112 | 1.416436  | 0.105245 |
| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy       | -862.612374 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.428421 |

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 72)

1. 30.9906 cm⁻¹  
2. 44.0641 cm⁻¹  
3. 65.9065 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | X     | Y     | Z     |
|-------|-------|-------|-------|
| -0.126524 | 1.197632 | -0.088496 |
| 0.992870  | 0.961557 | 0.686659 |
| 1.548543  | -0.379298 | 0.949808 |
| -0.675518 | 2.290264 | -0.350764 |
| -0.671208 | 0.028509 | -0.639715 |
| -1.980169 | 0.088684 | -1.175987 |
| -3.014411 | -0.450691 | -0.191151 |
| -3.622228 | 0.397997 | 1.075420 |
| -2.743446 | -1.913844 | 0.144134 |
| 1.504302  | 1.830323 | 1.077795 |
| 2.060566  | -0.427240 | 1.911931 |
| 0.782979  | -1.153942 | 0.933817 |
| -2.216018 | 1.115173 | -1.453290 |
| -1.976702 | -0.529257 | -2.077422 |
| -3.983644 | -0.383169 | -0.696348 |
| -2.095110 | 0.368842 | 1.582888 |
| -3.286734 | 1.439869 | 0.846662 |
| -3.818531 | 0.022058 | 1.766004 |
| -1.773346 | -2.013537 | 0.634332 |
| -3.504979 | -2.308734 | 0.817924 |
| -2.732199 | -2.530959 | -0.755971 |
| 2.806765  | -1.031187 | -0.273137 |
| 4.050018  | 0.258294 | -0.087238 |
| 4.462693  | 0.255161 | 0.921190 |
7_isobutylacrylate_HEI_18_reopt

| Datum                                                       | Value         |
|--------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                        | -862.613371   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  | -862.431212   |
| Number of Imaginary Frequencies                              | 0             |

**Frequencies** (Top 3 out of 72)

1. 26.5271 cm⁻¹  
2. 37.4094 cm⁻¹  
3. 49.5275 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.042014 | 1.755394 | -0.030793 |
| C     | 1.312404  | 1.729163 | 0.241181  |
| C     | 2.028723  | 0.538860 | 0.749321  |
| O     | -0.732007 | 2.697615 | -0.483364 |
| O     | -0.694120 | 0.554901 | 0.262848  |
| C     | -2.082408 | 0.504925 | 0.007529  |
| C     | -2.591422 | -0.884174| 0.355131  |
| C     | -1.907953 | -1.951604| -0.492203 |
| C     | -4.104963 | -0.931029| 0.175113  |
| H     | 1.877265  | 2.619197 | 0.000096  |
| H     | 2.892553  | 0.803595 | 1.361400  |
| H     | 1.379757  | -0.112857| 1.333051  |
| H     | -2.605687 | 1.261021 | 0.599255  |
| H     | -2.283903 | 0.720113 | -1.047447 |
| H     | -2.357180 | -1.068598| 1.408048  |
| H     | -2.122847 | -1.784259| -1.551072 |
| H     | -0.826932 | -1.929629| -0.359107 |
| H     | -2.268724 | -2.947120| -0.230228 |
| H     | -4.370502 | -0.735867| -0.866753 |
| H     | -4.497684 | -1.912896| 0.440252  |
| H     | -4.604842 | -0.186120| 0.795697  |
| S     | 2.785434  | -0.517387| -0.617097 |
| C     | 3.524856  | -1.803746| 0.350619  |
| H     | 2.804195  | -2.332262| 0.973210  |
### 7_isobutylacrylate_HEI_19

| Datum                                                   | Value          |
|---------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -862.614281    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -862.432315    |

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 72)

1. 26.9915 cm⁻¹
2. 30.8994 cm⁻¹
3. 45.5740 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.053914 | -0.493658 | 0.284177 |
|-------|-----------|-----------|----------|
| C     | -1.062362 | 0.13684   | 0.984291 |
| C     | -2.468298 | -0.290289 | 0.830351 |
| O     | -0.133748 | -1.461294 | -0.505943|
| O     | 1.212644  | 0.048268  | 0.531085 |
| C     | 2.300096  | -0.559891 | -0.135140|
| C     | 3.575820  | 0.181862  | 0.227712 |
| C     | 3.520433  | 1.634649  | -0.231126|
| C     | 4.772960  | -0.536863 | -0.385463|
| H     | -0.823309 | 0.989457  | 1.603472 |
| H     | -3.058088 | -0.146741 | 1.737216 |
| H     | -2.533149 | -1.338183 | 0.535799 |
| H     | 2.379641  | -1.612743 | 0.150278 |
| H     | 2.151443  | -0.527053 | -1.219969|
| H     | 3.673619  | 0.160308  | 1.317336 |
| H     | 3.422794  | 1.680094  | -1.319111|
| H     | 2.670580  | 2.155732  | 0.207167 |
| H     | 4.431720  | 2.166238  | 0.045944 |
| H     | 4.838873  | -1.569683 | -0.040882|
| H     | 4.692271  | -0.548898 | -1.475188|
| H     | 5.703882  | -0.032008 | -0.126371|
| S     | -3.355316 | 0.663503  | -0.488711|
| C     | -4.998345 | -0.076642 | -0.366511|
| H     | -5.414378 | 0.077271  | 0.628330 |
7_isobutylacrylate_HEI_1

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -862.613852 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430516 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 72)

1. 32.3512 cm\(^{-1}\)
2. 53.3114 cm\(^{-1}\)
3. 61.4203 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       |          |          |          |
|-------|----------|----------|----------|
| C     | -0.375813| 1.635447 | 0.038375 |
| C     | -1.677258| 1.436915 | -0.379282|
| C     | -2.150981| 0.221177 | -1.065535|
| O     | 0.094043 | 2.585630 | 0.707059 |
| O     | 0.510190 | 0.637065 | -0.385085|
| C     | 1.785324 | 0.622491 | 0.220850 |
| C     | 2.642396 | -0.436084| -0.453155|
| C     | 2.205108 | -1.817195| -0.356633|
| C     | 4.030440 | -0.432285| 0.169963 |
| H     | -2.401882| 2.179997 | -0.072721|
| H     | -2.941980| 0.418426 | -1.790511|
| H     | -1.343903| -0.297640| -1.578413|
| H     | 2.259492 | 1.602129 | 0.139025 |
| H     | 1.689526 | 0.391357 | 1.290448 |
| H     | 2.730047 | -0.164458| -1.509710|
| H     | 1.872959 | -2.098100| 0.692060 |
| H     | 1.027250 | -1.833543| -0.836197|
| H     | 2.635846 | -2.571122| -0.829705|
| H     | 3.977919 | -0.697900| 1.228424 |
| H     | 4.682255 | -1.158419| -0.321362|
| H     | 4.304155 | 0.549210 | 0.093357 |
| S     | -2.961470| -1.064491| 0.030382 |
| C     | -1.613141| -1.364749| 1.184822 |
| H     | -1.237771| -0.408724| 1.549957 |
### 7_isobutylacrylate_HEI_20

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -862.614093 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430949 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 72)

1. 27.7662 cm⁻¹
2. 34.9707 cm⁻¹
3. 59.6233 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.002991 | 0.028437 | -0.147228 |
|-------|-----------|----------|-----------|
| C     | 1.055326  | 0.068364 | 0.737893  |
| C     | 2.203731  | 0.961234 | 0.502691  |
| O     | -0.180761 | 0.707811 | -1.180541 |
| O     | -0.972853 | -0.926601| 0.204581  |
| C     | -2.222175 | -0.887117| -0.456059 |
| C     | -3.295792 | -0.221145| 0.397162  |
| C     | -4.646274 | -0.330315| -0.301967 |
| C     | -2.943328 | 1.232242 | 0.690700  |
| H     | 1.066866  | -0.616865| 1.572979  |
| H     | 2.686320  | 1.272403 | 1.429914  |
| H     | 1.914375  | 1.856275 | -0.049751 |
| H     | -2.124065 | -0.361297| -1.407056 |
| H     | -2.507167 | -1.922874| -0.658406 |
| H     | -3.345912 | -0.766122| 1.345183  |
| H     | -4.913998 | -1.370382| -0.494703 |
| H     | -5.436618 | 0.116787 | 0.301722  |
| H     | -4.621137 | 0.194279 | -1.268307 |
| H     | -3.682223 | 1.684861 | 1.353792  |
| H     | -1.962945 | 1.311588 | 1.161772  |
| H     | -2.918417 | 1.801950 | -0.236240 |
| S     | 3.597134  | 0.280764 | -0.544962 |
| C     | 4.038789  | -1.131798| 0.480507  |
| H     | 4.414561  | -0.804068| 1.449311  |
7_isobutylacrylate_HEI_21

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.613502 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430037 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 72)

1. 34.9832 cm\(^{-1}\)
2. 41.3798 cm\(^{-1}\)
3. 52.1070 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 0.084050 | -0.244806 | -0.273986 |
| C    | -0.871625 | 0.274631 | 0.575993 |
| C    | -2.051282 | -0.522384 | 0.956235 |
| O    | 0.134514 | -1.383649 | -0.785228 |
| O    | 1.101515 | 0.675202 | -0.579464 |
| C    | 2.292410 | 0.181854 | -1.164576 |
| C    | 3.391445 | -0.030964 | -1.164576 |
| C    | 2.995721 | -1.101372 | 0.885766 |
| C    | 3.747570 | 1.275317 | 0.576210 |
| H    | -0.778640 | 1.298033 | 0.909268 |
| H    | -2.434608 | -0.256870 | 1.942175 |
| H    | -1.833425 | -1.590385 | 0.951418 |
| H    | 2.084538 | -0.748386 | -1.692010 |
| H    | 2.616547 | 0.933115 | -1.889211 |
| H    | 4.270502 | -0.378964 | -0.679040 |
| H    | 2.103200 | -0.789431 | 1.432942 |
| H    | 2.769881 | -2.047293 | 0.393931 |
| H    | 3.796203 | -1.266103 | 1.608615 |
| H    | 4.047823 | 2.041978 | -0.140205 |
| H    | 2.886646 | 1.650237 | 1.131821 |
| H    | 4.566903 | 1.129071 | 1.281347 |
| S    | -3.540124 | -0.411348 | -0.170938 |
| C    | -3.852133 | 1.355977 | -0.026483 |
| H    | -4.129747 | 1.617522 | 0.994145 |
### 7_isobutylacrylate_HEI_22

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.61469 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430663 |

Number of Imaginary Frequencies

**Frequencies** (Top 3 out of 72)

1. 36.7471 cm⁻¹
2. 44.5457 cm⁻¹
3. 79.7286 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.253357 | 0.933039 | -0.125883 |
|-------|----------|----------|-----------|
| C     | -0.889002 | -0.081648 | -0.812188 |
| C     | -2.309159 | 0.056872 | -1.198392 |
| O     | -0.727635 | 2.039704 | 0.227626 |
| O     | 1.087455 | 0.782238 | 0.238491 |
| C     | 1.774785 | -0.408058 | -0.075890 |
| C     | 3.205770 | -0.305253 | 0.426057 |
| C     | 3.946637 | 0.843666 | -0.248006 |
| C     | 3.923427 | -1.629988 | 0.190429 |
| H     | -0.388244 | -1.008101 | -1.042723 |
| H     | -2.525578 | -0.347319 | -2.188696 |
| H     | -2.616334 | 1.101460 | -1.181774 |
| H     | 1.276205 | -1.266602 | 0.387179 |
| H     | 1.779208 | -0.570551 | -1.161450 |
| H     | 3.163571 | -0.114378 | 1.502521 |
| H     | 4.966048 | 0.924786 | 0.131220 |
| H     | 4.001931 | 0.672976 | -1.326413 |
| H     | 3.493765 | 1.792652 | -0.080538 |
| H     | 4.947336 | -1.587659 | 0.562199 |
| H     | 3.414345 | -2.455457 | 0.689616 |
| H     | 3.965766 | -1.855473 | -0.877934 |
| S     | -3.529040 | -0.861907 | -0.135128 |
| C     | -3.162420 | -0.185615 | 1.457074 |
| H     | -3.641361 | -0.698443 | 2.233093 |
# 7_isobutylacrylate_HEI_2_reopt3

## Datum

| Datum                                               | Value          |
|-----------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy               | -862.613682    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430792   |

### Frequencies (Top 3 out of 72)

1. 29.5556 cm⁻¹  
2. 36.9103 cm⁻¹  
3. 55.9776 cm⁻¹  

## M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.378187| 1.559293| -0.044908|
| C    | 1.662711| 1.381832| 0.432465 |
| C    | 2.147765| 0.149485| 1.000381|
| O    | -0.100150| 2.547957| -0.648751|
| O    | 0.482975 |        | 0.214500 |
| C    | -1.760335| 0.538498| -0.368535|
| C    | -2.509798| -0.737367| -0.021929|
| C    | -3.80867 | -0.741445| -0.728985|
| C    | -2.683428| -0.885603| 1.485322 |
| H    | 2.366060 | 2.179585 | 0.233198 |
| H    | 2.884689 | 0.341935| 1.861920 |
| H    | -1.335416| -0.426828| 1.519444 |
| H    | -2.315109| 1.406693 | 0.003231 |
| H    | -1.677420| 0.645623 | -1.454191|
| H    | -1.916631| -1.579597| -0.391603|
| H    | -4.410118| -1.657945| -0.512274|
| H    | -4.470051| 0.100293 | -0.390615|
| H    | -3.746327| -0.661379| -1.810810|
| H    | -1.720663| -0.900703| 1.994193 |
| H    | -3.264067| -0.047624| 1.880301 |
| H    | -3.216194| -1.806065| 1.727676 |
| S    | 3.073174 | -1.050939| -0.019227|
| C    | 1.788722 | -1.380661| -1.236501|
| H    | 1.390001 | -0.433495| -1.598751|
7_isobutylacrylate_HEI_3

| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.614797 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.432348 |

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 72)

1. 20.1296 cm⁻¹
2. 32.8254 cm⁻¹
3. 71.1114 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C  -0.235451  -0.719991  -0.027162
C  -1.252910  -0.605821  -0.953326
C  -2.640944  -0.953545  -0.604953
O  -0.281476  -1.145500  1.149301
O   1.005991  -0.299471  -0.522693
C   2.119349  -0.474245   0.328948
C   3.352365   0.097671  -0.351045
C   4.584896  -0.200615   0.495964
C   3.205897   1.596295  -0.589151
H  -1.031247  -0.189926  -1.926448
H  -2.668824  -1.594856   0.275391
H  -3.182452  -1.453708  -1.409545
H   1.955596   0.035068   1.284279
H   2.266801  -1.536314   0.547211
H   3.460938  -0.403428  -1.317706
H   4.494814   0.270183   1.477998
H   4.716555  -1.272864   0.646795
H   5.485966   0.189042   0.021724
H   2.328069   1.816294  -1.194843
H   3.099721   2.118383   0.365555
H   4.084269   1.998959  -1.095201
S  -3.775434   0.483809  -0.224052
C  -2.861745   1.215485   1.143645
H  -2.937445   0.601267   2.039195
**7_isobutylacrylate_HEI_4**

| Datum                                                                 | Value                |
|-----------------------------------------------------------------------|----------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -862.613222          |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -862.430036          |
| Number of Imaginary Frequencies                                        | 0                    |

**Frequencies (Top 3 out of 72)**

1. 42.5294 cm⁻¹  
2. 44.3282 cm⁻¹  
3. 68.6162 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | -0.177773 | 1.557013 | -0.015660 |
| C          | -1.477640 | 1.356075 | 0.411025  |
| C          | -1.936872 | 0.143422 | 1.113423  |
| O          | 0.301212  | 2.533436 | -0.635890 |
| O          | 0.686063  | 0.512071 | 0.320795  |
| C          | 2.028204  | 0.633745 | -0.103732 |
| C          | 2.783884  | -0.620631| 0.302072  |
| C          | 4.255160  | -0.470211| -0.069521 |
| C          | 2.181336  | -1.862222| -0.345412 |
| H          | -2.198155 | 2.116912 | 0.145015  |
| H          | -1.156892 | -0.305844| 1.726386  |
| H          | -2.796414 | 0.343887 | 1.754333  |
| H          | 2.072614  | 0.758359 | -1.191064 |
| H          | 2.491332  | 1.517044 | 0.344528  |
| H          | 2.704480  | -0.718077| 1.389127  |
| H          | 4.824316  | -1.349341| 0.233416  |
| H          | 4.364857  | -0.358219| -1.150963 |
| H          | 4.700892  | 0.404036 | 0.406881  |
| H          | 2.717626  | -2.761260| -0.038916 |
| H          | 1.131954  | -1.976246| -0.076563 |
| H          | 2.246535  | -1.786656| -1.434187 |
| S          | -2.482971 | -1.298786| 0.048308  |
| C          | -3.821978 | -0.485582| -0.839102 |
| H          | -4.218960 | -1.181826| -1.574174 |
7_isobutylacrylate_HEI_5_reopt2

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.613408 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430009 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 72)

1. 28.0450 cm⁻¹
2. 50.4420 cm⁻¹
3. 69.7126 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

```
C    -0.101867    -1.427328    -0.221692
C    -1.481012    -1.499949    -0.197299
C    -2.356324    -0.732442     0.707910
O     0.692190    -2.070167    -0.947781
O     0.442192    -0.530227     0.710210
C     1.853420    -0.492875     0.806424
C     2.503009     0.436285    -0.212303
C     4.018978     0.296311    -0.132071
C     2.075248     1.881554     0.010683
H    -1.937167    -2.153975    -0.929106
H    -3.200203    -1.315824     1.080502
H    -1.810365    -0.345099     1.565986
H     2.074302    -0.130224     1.815097
H     2.261749    -1.498205     0.701277
H     2.165540     0.109913    -1.198836
H     4.373699     0.558854     0.868268
H     4.336569    -0.725732    -0.343753
H     4.512075     0.959918    -0.843177
H     2.493165     2.537722    -0.754200
H     0.990336     1.975984    -0.011654
H     2.427493     2.234214     0.984020
S    -3.227440     0.740951    -0.045119
C    -1.784711     1.710279    -0.508799
H    -1.070656     1.057770    -1.012289
```
### 7_isobutylacrylate_HEI_6_reopt2

| Datum                                                      | Value          |
|-------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -862.613915    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.430834    |
| Number of Imaginary Frequencies                             | 0              |

**Frequencies** (Top 3 out of 72)

1. 20.9442 cm⁻¹
2. 35.3471 cm⁻¹
3. 38.5519 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| C | 0.028026 | 1.114386 | -0.396749 |
| C | 1.128379 | 0.749184 | -1.144975 |
| C | 1.816427 | -0.552243 | -1.045283 |
| O | -0.613405 | 2.191385 | -0.427998 |
| O | -0.392308 | 0.131118 | 0.512877 |
| C | -1.741088 | 0.200161 | 0.930959 |
| C | -2.716741 | -0.254975 | -0.148288 |
| C | -4.142521 | -0.162997 | 0.382796 |
| C | -2.392094 | -1.667719 | -0.618621 |
| H | 1.545326 | 1.508710 | -1.793882 |
| H | 1.168428 | -1.316653 | -0.620871 |
| H | 2.181387 | -0.912762 | -2.008535 |
| H | -1.816791 | -0.469045 | 1.792809 |
| H | -1.988042 | 1.212407 | 1.254138 |
| H | -2.607961 | 0.431866 | -0.992302 |
| H | -4.272355 | -0.826549 | 1.241739 |
| H | -4.384634 | 0.851782 | 0.702216 |
| H | -4.864369 | -0.460024 | -0.378617 |
| H | -2.491092 | -2.375300 | 0.209230 |
| H | -3.072240 | -1.982017 | -1.411550 |
| H | -1.371134 | -1.728602 | -0.995632 |
| S | 3.380413 | -0.580288 | -0.022267 |
| C | 2.714961 | -0.016400 | 1.552310 |
| H | 2.082190 | -0.776748 | 2.006140 |
7_isobutylacrylate_HEI_7_reopt

| Datum                                                      | Value                      |
|------------------------------------------------------------|----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                     | -862.614223                |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -862.431989                |

Number of Imaginary Frequencies

0

Frequencies (Top 3 out of 72)

1. 19.3613 cm⁻¹
2. 35.7226 cm⁻¹
3. 55.2159 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 0.146903 | -0.722046 | 0.244336 |
| C   | 1.222287 | -0.206833 | 0.752783 |
| C   | 2.573311 | -0.762627 | 0.531680 |
| O   | 0.127803 | -1.667830 | -0.574547|
| O   | -1.060687| -0.076846 | 0.531680 |
| C   | -2.10070 | -0.556313 | -0.135540|
| C   | -3.401298| 0.298428  | 0.264797 |
| C   | -4.670464| -0.276328 | -0.355229|
| C   | -3.203938| 1.752234  | -0.149477|
| H   | 1.072237 | 0.646415  | 1.585723 |
| H   | 2.544434 | -1.821554 | 0.495264 |
| H   | 3.200063 | -0.644088 | 1.637370 |
| H   | -2.06936 | -0.509428 | -1.220861|
| H   | -2.391601| -1.603328 | 0.123857 |
| H   | -3.490667| 0.252477  | 1.354410 |
| H   | -4.602398| -0.259631 | -1.445741|
| H   | -4.836001| -1.308414 | -0.043494|
| H   | -5.543517| 0.309820  | -0.067449|
| H   | -2.302782| 2.171374  | 0.295566 |
| H   | -3.110739| 1.822902  | -1.236480|
| H   | -4.055088| 2.363010  | 0.154294 |
| S   | 3.593194 | -0.041960 | -0.642612|
| C   | 3.642884 | 1.666743  | -0.877730|
| H   | 4.190766 | 1.748925  | 0.860494 |
### 7_isobutylacrylate_HEI_8

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.61516 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.431855 |
| Number of Imaginary Frequencies | 0 |

#### Frequencies (Top 3 out of 72)

1. 30.5233 cm⁻¹
2. 41.1038 cm⁻¹
3. 54.6499 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -0.068893 | 0.078219 | -0.002981 |
| C | -1.013994 | -0.913488 | -0.160193 |
| C | -2.196424 | -0.988943 | 0.717043 |
| O | 0.005183 | 0.969962 | 0.872938 |
| O | 0.924659 | 0.048148 | -0.998423 |
| C | 2.136332 | 0.709380 | -0.693691 |
| C | 3.006391 | -0.068191 | 0.287384 |
| C | 4.276161 | 0.722833 | 0.579438 |
| C | 3.332645 | -1.456873 | 0.248794 |
| H | -0.921316 | -1.594796 | 0.994778 |
| H | -2.031925 | 0.425812 | 1.635088 |
| H | -2.473824 | -2.008944 | 0.988129 |
| H | 2.665716 | 0.810924 | -1.645458 |
| H | 1.935049 | 1.708571 | 0.987156 |
| H | 2.432928 | -0.172591 | 1.212432 |
| H | 4.856082 | 0.863641 | -0.336470 |
| H | 4.047092 | 1.708571 | 0.987156 |
| H | 4.908984 | 0.198127 | 1.295871 |
| H | 2.422725 | -2.018102 | -0.459658 |
| H | 3.907470 | -1.380280 | -1.175819 |
| H | 3.927935 | -2.023228 | 0.468883 |
| S | -3.791379 | -0.342230 | -0.005928 |
| C | -3.287428 | 1.350332 | -0.356075 |
| H | -2.330283 | 1.331242 | -0.876056 |
7_isobutylacrylate_HEI_9_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.612336 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.428848 |

Number of Imaginary Frequencies
0

**Frequencies** (Top 3 out of 72)

1. 30.1691 cm\(^{-1}\)
2. 60.5368 cm\(^{-1}\)
3. 68.9161 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | -0.096524 | 1.589997 | 0.125913 |
| C    | -1.461244 | 1.505459 | -0.071194 |
| C    | -2.129111 | 0.497012 | -0.914037 |
| O    | 0.528938  | 2.407000 | 0.840432  |
| O    | 0.637712  | 0.633014 | -0.591559 |
| C    | 2.047667  | 0.751133 | -0.634885 |
| C    | 2.714809  | -0.52369 | -0.131034 |
| C    | 2.333017  | -1.72655 | -0.987266 |
| C    | 2.382323  | -0.76648 | 1.336767  |
| H    | -2.071471 | 2.190058 | 0.503579  |
| H    | -2.975709 | 0.897358 | -1.474640 |
| H    | -1.437970 | 0.044402 | -1.621582 |
| H    | 2.338049  | 0.929101 | -1.675957 |
| H    | 2.360281  | 1.602834 | -0.033712 |
| H    | 3.793265  | -0.359612 | -0.224507 |
| H    | 1.258128  | -1.903043 | -0.927635 |
| H    | 2.591260  | -1.563590 | -2.035074 |
| H    | 2.843885  | -2.628293 | -0.646960 |
| H    | 1.304631  | -0.889904 | 1.457589  |
| H    | 2.871213  | -1.669251 | 1.705511  |
| H    | 2.698192  | 0.072689  | 1.958035  |
| S    | -2.934634 | -0.925925 | -0.001786 |
| C    | -1.505811 | -1.537104 | 0.903821  |
| H    | -1.011288 | -0.692754 | 1.383645  |
### 7_isobutylacrylate_TS_10_reopt

| Datum                                                                 | Value                        |
|----------------------------------------------------------------------|------------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -862.605245                  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -862.421887                  |
| Number of Imaginary Frequencies                                      | 1                            |

#### Frequencies (Top 3 out of 72)

1. -202.7255 cm⁻¹
2.  26.2208 cm⁻¹
3.  54.0200 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C       | 0.033203 | 1.540348 | 0.316018 |
|---------|----------|----------|----------|
| C       | 1.451327 | 1.607303 | 0.147996 |
| C       | 2.125017 | 1.043917 | -0.918284|
| O       | -0.596954| 1.981687 | 1.271855 |
| O       | -0.604136| 0.933535 | -0.728099|
| C       | -1.999987| 0.674727 | -0.623982|
| C       | -2.257165| -0.801284| -0.356516|
| C       | -3.758836| -1.063789| -0.375483|
| C       | -1.633914| -1.237445|  0.963758|
| H       |  1.988417|  2.055185|  0.972241|
| H       |  1.577762|  0.801986| -1.815814|
| H       |  3.161577|  1.304986| -1.069329|
| H       | -2.431384|  1.286419|  0.168211|
| H       | -2.440563|  0.967794| -1.577985|
| H       | -1.788926| -1.367363| -1.167410|
| H       | -3.968996| -2.121643| -0.217684|
| H       | -4.204819| -0.766950| -1.325746|
| H       | -4.253465| -0.502132|  0.420481|
| H       | -1.781352| -2.305955|  1.125936|
| H       | -0.561836| -1.036678|  0.980592|
| H       | -2.092655| -0.699090|  1.796257|
| S       |  2.650648| -1.244182| -0.581909|
| C       |  2.279057| -1.292544|  1.180910|
| H       |  1.735137| -0.375186|  1.443717|
### 7_isobutylacrylate_TS_11_reopt

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -862.606932            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -862.423946            |
| Number of Imaginary Frequencies                                      | 1                      |

**Frequencies** (Top 3 out of 72)

1. -194.6938 cm⁻¹  
2.  31.8772 cm⁻¹  
3.  50.7309 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | -0.120667 | -1.212803 | -0.021102 |
|---------|-----------|-----------|-----------|
| C       | -1.319538 | -1.302908 |  0.753549 |
| C       | -2.548038 | -1.297520 |  0.132351 |
| O       | -0.036271 | -1.159185 | -1.242472 |
| O       |  1.001579 | -1.196946 |  0.759375 |
| C       |  2.240491 | -0.951323 |  0.101503 |
| C       |  2.455815 |  0.527954 | -0.189177 |
| C       |  3.785432 |  0.707662 | -0.913077 |
| C       |  2.408860 |  1.351945 |  1.092336 |
| H       | -1.225413 | -1.260861 |  1.829229 |
| H       | -3.434054 | -1.534043 |  0.701626 |
| H       | -2.591175 | -1.533852 | -0.920052 |
| H       |  3.088098 | -1.309399 |  0.790204 |
| H       |  2.291728 | -1.532822 | -0.818862 |
| H       |  1.646426 |  0.851825 | -0.848654 |
| H       |  4.611061 |  0.363951 | -0.284964 |
| H       |  3.812134 |  0.142109 | -1.845407 |
| H       |  3.960168 |  1.757764 | -1.147580 |
| H       |  1.459833 |  1.220879 |  1.611957 |
| H       |  3.212257 |  1.048318 |  1.768580 |
| H       |  2.535585 |  2.413090 |  0.874912 |
| S       | -3.331994 |  0.928632 | -0.300655 |
| C       | -1.791691 |  1.770930 |  0.104221 |
| H       | -1.312708 |  2.194946 | -0.778294 |
7_isobutylacrylate_TS_12_reopt

| Datum                                                                 | Value       |
|-----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -862.604452 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -862.421364 |
| Number of Imaginary Frequencies                                       | 1           |
| **Frequencies** (Top 3 out of 72)                                     |             |
| 1.  -194.4538 cm⁻¹                                                   |             |
| 2.   29.1393 cm⁻¹                                                   |             |
| 3.   40.2873 cm⁻¹                                                   |             |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          | 0.103576 | 1.76761 | 0.078485 |
|----------|----------|---------|----------|
| C        | -0.957203| 1.09143 | 1.035574 |
| C        | -1.476220| -0.099163| 1.496766 |
| O        | 0.623621 | 2.212907| -0.321636|
| O        | 0.513586 | -0.041493| -0.378256|
| C        | 1.679899 | -0.106896| -1.196016|
| C        | 2.888029 | -0.559421| -0.384636|
| C        | 2.671304 | -1.953529| 0.195386 |
| C        | 3.224571 | 0.443569 | 0.714139 |
| H        | -1.382731| 2.039345 | 1.334812 |
| H        | -0.910280| 1.006445 | 1.354242 |
| H        | -2.121977| -0.086721| 2.361885 |
| H        | 1.457671 | -0.834516| -1.977522|
| H        | 1.859990 | 0.864506 | -1.652008|
| H        | 3.723946 | -0.600074| -1.089388|
| H        | 1.833305 | -1.945804| 0.894552 |
| H        | 2.451862 | -2.679579| -0.588876|
| H        | 3.557110 | -2.291100| 0.734260 |
| H        | 2.400386 | 0.515593 | 1.427814 |
| H        | 4.113552 | 0.129267 | 1.261964 |
| H        | 3.401475 | 1.437942 | 0.304512 |
| S        | -3.257637| -0.930305| 0.126523 |
| C        | -2.933763| 0.143067 | -1.284565|
| H        | -3.840709| 0.640883 | -1.625007|
7_isobutylacrylate_TS_14_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.606259 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423554 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 72)

1. -188.5405 cm\(^{-1}\)
2. 34.3549 cm\(^{-1}\)
3. 39.3019 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.066561 | 0.242282 | 0.084560 |
|-------|----------|----------|----------|
| C     | -1.088791| 1.141976 | -0.355071|
| C     | -2.151795| 1.441750 | 0.465808 |
| O     | -0.005593| -0.329540| 1.166470 |
| O     | 0.901249 | 0.056964 | -0.861902|
| C     | 2.009978 | -0.763168| -0.506167|
| C     | 3.068189 | -0.003870| 0.282082 |
| C     | 3.588032 | 1.192561 | -0.506467|
| C     | 4.200635 | -0.958450| 0.644190 |
| H     | -1.035413| 1.502590 | -1.372278|
| H     | -2.810121| 2.256743 | 0.207075 |
| H     | -2.061812| 1.229537 | 1.520355 |
| H     | 1.660584 | -1.627403| 0.058442 |
| H     | 2.430522 | -1.105076| -1.453972|
| H     | 2.597796 | 0.352613 | 1.201712 |
| H     | 4.327754 | 1.746113 | 0.072817 |
| H     | 4.066354 | 0.857976 | -1.430666|
| H     | 2.780618 | 1.874877 | -0.770612|
| H     | 4.969924 | -0.445478| 1.221471 |
| H     | 3.838951 | -1.802056| 1.233486 |
| H     | 4.669887 | -1.353718| -0.260192|
| S     | -3.945290| -0.147166| 0.261307 |
| C     | -3.050494| -1.332443| -0.759217|
| H     | -3.596985| -1.573064| -1.670175|
### 7_isobutylacrylate_TS_15

| Datum                                                        | Value                  |
|--------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                        | -862.60588             |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  | -862.422716            |
| Number of Imaginary Frequencies                              |                         |
| Frequencies (Top 3 out of 72)                                |                         |
| 1. -185.7311 cm⁻¹                                           |                         |
| 2. 37.0086 cm⁻¹                                             |                         |
| 3. 47.6835 cm⁻¹                                             |                         |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.054393 | -0.240771 | -0.049438 |
|-------|----------|-----------|-----------|
| C     | 1.083312 | -0.824858 | -0.85504  |
| C     | 2.148744 | -1.465671 | -0.266967 |
| O     | -0.013596| -0.252386 | 1.172806  |
| O     | -0.905638| 0.367432  | -0.809493 |
| C     | -2.041032| 0.927255  | -0.156834 |
| C     | -3.267455| 0.042198  | -0.326885 |
| C     | -4.479810| 0.744005  | 0.275545  |
| C     | -3.054692| -1.329321 | 0.302527  |
| H     | 1.032494 | -0.667856 | -1.923402 |
| H     | 2.813132 | -2.061416 | -0.873703 |
| H     | 2.061844 | -1.765260 | 0.766385  |
| H     | -1.822294| 1.073735  | 0.900872  |
| H     | -2.212127| 1.899109  | -0.621767 |
| H     | -3.433109| -0.086684 | -1.400637 |
| H     | -4.337721| 0.895720  | 1.348114  |
| H     | -4.646889| 1.718928  | -0.184402 |
| H     | -5.380595| 0.145571  | 0.139498  |
| H     | -2.184307| -1.831419 | -0.121318 |
| H     | -2.897023| -1.232207 | 1.378765  |
| H     | -3.925683| -1.965482 | 0.141003  |
| S     | 3.938922 | 0.049102  | 0.287936  |
| C     | 3.026004 | 1.567908  | -0.039697 |
| H     | 2.811078 | 2.120869  | 0.874336  |
7_isobutylacrylate_TS_16

| Datum | Value                  |
|-------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -862.606336             |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423369             |
| Number of Imaginary Frequencies           | 1                       |

**Frequencies** (Top 3 out of 72)

1. -190.9112 cm⁻¹
2. 28.9688 cm⁻¹
3. 46.3142 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.074828 | -1.109294 | 0.122423 |
|-------|-----------|-----------|----------|
| C     | -1.266721 | -1.357649 | -0.630352|
| C     | -2.492474 | -1.387993 | -0.004437|
| O     | 0.000182  | -0.900346 | 1.326571 |
| O     | 1.043092  | -1.143074 | -0.664543|
| C     | 2.313445  | -0.914190 | -0.061927|
| C     | 2.841333  | 0.476384  | -0.383537|
| C     | 4.262916  | 0.608058  | 0.152486 |
| C     | 1.934818  | 1.560138  | 0.186659 |
| H     | -1.172945 | -1.446227 | -1.703116|
| H     | -2.518238 | -1.507261 | 1.067964 |
| H     | -3.350825 | -1.767301 | -0.537400|
| H     | 2.238840  | -1.049700 | 1.017051 |
| H     | 2.983676  | -1.672421 | -0.469470|
| H     | 2.865551  | 0.575181  | -1.472890|
| H     | 4.271576  | 0.496082  | 1.239270 |
| H     | 4.922199  | -0.150994 | -0.270690|
| H     | 4.676655  | 1.588082  | -0.085109|
| H     | 0.915194  | 1.464121  | -0.187073|
| H     | 1.900334  | 1.489565  | 1.275939 |
| H     | 2.304091  | 2.551060  | -0.080416|
| S     | -3.489863 | 0.787586  | 0.179263 |
| C     | -2.066684 | 1.709843  | -0.426392|
| H     | -1.324673 | 0.990002  | -0.799095|
### 7_isobutylacrylate_TS_17

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.604452 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.421377 |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 72)

1. -194.4723 cm⁻¹
2. 28.7388 cm⁻¹
3. 40.0847 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | 0.103593 | 1.176708 | 0.078642 |
| C    | 0.957171 | 1.091135 | 1.035732 |
| C    | 1.476162 | -0.099552 | 1.496675 |
| O    | -0.623589 | 2.212958 | -0.321298 |
| O    | -0.513671 | -0.041440 | -0.378318 |
| C    | -1.680003 | -0.106649 | -1.196062 |
| C    | -2.888099 | -0.559354 | -0.384735 |
| C    | -3.224686 | 0.443465 | 0.714184 |
| C    | -2.671289 | -1.953530 | 0.195095 |
| H    | 1.382702 | 2.038997 | 1.335184 |
| H    | 2.121872 | -0.087306 | 2.361833 |
| H    | 0.910199 | -1.006788 | 1.353947 |
| H    | -1.860107 | 0.864858 | -1.651826 |
| H    | -1.457805 | -0.834092 | -1.977741 |
| H    | -3.724023 | -0.599963 | -1.089931 |
| H    | -2.400478 | 0.515477 | 1.427832 |
| H    | -3.401703 | 1.437874 | 0.304691 |
| H    | -4.113616 | 0.129014 | 1.262007 |
| H    | -1.833337 | -1.945835 | 0.894319 |
| H    | -3.557102 | -2.291258 | 0.733858 |
| H    | -2.451728 | -2.679447 | -0.589259 |
| S    | 3.257623 | -0.930397 | 0.126378 |
| C    | 2.934150 | 0.143537 | -1.284369 |
| H    | 3.841182 | 0.641522 | -1.624336 |
### 7_isobutylacrylate_TS_18_reopt

**Datum**

|                     | Value          |
|---------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.601412 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.420067 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 72)

1. -226.4948 cm⁻¹
2. 23.6928 cm⁻¹
3. 37.8301 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |                     |                     |                     |
|---|---------------------|---------------------|---------------------|
| C | -0.221664           | 1.815384            | -0.049440           |
| C | 1.173055            | 1.912829            | 0.245071            |
| C | 1.914611            | 0.874290            | 0.766753            |
| O | -0.922460           | 2.703929            | -0.525896           |
| O | -0.763053           | 0.603581            | 0.253371            |
| C | -2.154418           | 0.442814            | 0.003105            |
| C | -2.549407           | -0.976155           | 0.368053            |
| C | -1.795161           | -1.994545           | -0.479549           |
| C | -4.057204           | -1.135257           | 0.203739            |
| H | 1.645078            | 2.836659            | -0.058664           |
| H | 2.908382            | 1.077693            | 1.140154            |
| H | 1.404759            | 0.051971            | 1.247915            |
| H | -2.718131           | 1.169065            | 0.592549            |
| H | -2.362440           | 0.635661            | -1.053276           |
| H | -2.291587           | -1.131348           | 1.419724            |
| H | -2.037736           | -1.856663           | -1.536422           |
| H | -0.717022           | -1.888669           | -0.362858           |
| H | -2.073710           | -3.011397           | -0.201116           |
| H | -4.346803           | -0.967861           | -0.836334           |
| H | -4.370766           | -2.142117           | 0.479067            |
| H | -4.604792           | -0.426150           | 0.825682            |
| S | 2.850305            | -0.763158           | -0.746392           |
| C | 3.675654            | -1.623331           | 0.582155            |
| H | 3.606749            | -2.698365           | 0.422822            |
### 7_isobutylacrylate_TS_1_reopt

| Datum | Value                  |
|-------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.60647 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423413 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 72)

1. -196.9032 cm\(^{-1}\)
2.  37.4793 cm\(^{-1}\)
3.  58.0061 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Carbon  |   X   |   Y   |   Z   |
|---------|-------|-------|-------|
|        C | -0.289308 | 1.647677 | 0.094431 |
|        C | -1.624379 | 1.574317 | -0.411979 |
|        C | -2.055257 | 0.592413 | -1.280937 |
|        O |  0.147277 | 2.497959 |  0.865942 |
|        O |  0.522195 | 0.654595 | -0.361936 |
|        C |  1.857903 | 0.644489 |  0.127446 |
|        C |  2.575609 | -0.562118 | -0.448657 |
|        C |  1.899320 | -1.861529 | -0.026143 |
|        C |  4.035016 | -0.534900 | -0.006760 |
|        H | -2.314808 | 2.294853 |  0.004116 |
|        H | -3.015013 | 0.708838 | -1.762141 |
|        H | -1.323484 | 0.035920 | -1.844775 |
|        H |  2.360634 | 1.570833 | -0.158216 |
|        H |  1.846468 | 0.593277 |  1.220311 |
|        H |  2.536412 | -0.481841 | -1.538908 |
|        H |  1.915296 | -1.956692 |  1.062821 |
|        H |  0.860713 | -1.893707 | -0.354106 |
|        H |  2.419991 | -2.722660 | -0.446280 |
|        H |  4.104594 | -0.599536 |  1.081645 |
|        H |  4.580557 | -1.379962 | -0.426425 |
|        H |  4.532401 |  0.382580 | -0.323589 |
|        S | -2.768157 | -1.386939 | -0.170533 |
|        C | -2.047387 | -0.988924 |  1.432043 |
|        H | -1.762453 |  0.071223 |  1.428039 |
7_isobutylacrylate_TS_20_reopt2

| Datum                                                        | Value         |
|--------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                        | -862.60588    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  | -862.422715   |
| Number of Imaginary Frequencies                              | 1             |

**Frequencies (Top 3 out of 72)**

1. -185.7784 cm⁻¹
2.  37.0520 cm⁻¹
3.  47.7003 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.054431 | -0.240799 | -0.049455 |
|-------|----------|-----------|-----------|
| C     | 1.083320 | -0.824820 | -0.85587  |
| C     | 2.148842 | -1.465579 | -0.267100 |
| O     | -0.013500| -0.252418 | 1.172782  |
| O     | -0.905689| 0.367357  | -0.809456 |
| C     | -2.041022| 0.927191  | -0.156702 |
| C     | -3.267494| 0.042193  | -0.326729 |
| C     | -4.479819| 0.744084  | 0.275660  |
| C     | -3.054824| -1.329330 | 0.302709  |
| H     | 1.032406 | -0.667856 | -1.923485 |
| H     | 2.813161 | -2.061363 | -0.873880 |
| H     | 2.061954 | -1.765229 | 0.766238  |
| H     | -1.822214| 1.073629  | 0.900996  |
| H     | -2.212122| 1.899074  | -0.621575 |
| H     | -3.433137| -0.086710 | -1.400480 |
| H     | -4.646834| 1.719005  | -0.184315 |
| H     | -5.380634| 0.145696  | 0.139612  |
| H     | -4.337741| 0.895818  | 1.348228  |
| H     | -3.925828| -1.965460 | 0.141127  |
| H     | -2.184433| -1.831469 | -0.121077 |
| H     | -2.897228| -1.232220 | 1.378960  |
| S     | 3.938951 | 0.049080  | 0.287631  |
| C     | 3.025972 | 1.567950  | -0.039538 |
| H     | 3.565811 | 2.222708  | -0.722338 |
### 7_isobutylacrylate_TS_21_reopt

| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.605388 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.422339 |

#### Number of Imaginary Frequencies

1

#### Frequencies (Top 3 out of 72)

1. -188.6273 cm⁻¹
2.  34.4227 cm⁻¹
3.  43.7481 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 0.023818 | -0.159680 | -0.106403 |
| C       | -0.875923 | -0.595932 | 0.918075 |
| C       | -1.953794 | -1.392268 | 0.605423 |
| O       | -0.042344 | -0.424034 | -1.299985 |
| O       | 1.024695 | 0.626028 | 0.393651 |
| C       | 2.058587 | 1.056581 | -0.489393 |
| C       | 3.325987 | 0.232853 | -0.294326 |
| C       | 3.093334 | -1.234872 | -0.637706 |
| C       | 3.871221 | 0.384197 | 1.122290 |
| H       | -0.721528 | -0.212913 | 1.916571 |
| H       | -2.508623 | -1.870728 | 1.397746 |
| H       | -1.953509 | -1.907147 | -0.343145 |
| H       | 1.708614 | 0.989768 | -1.517536 |
| H       | 2.249139 | 2.101794 | -0.242344 |
| H       | 4.058780 | 0.644168 | -0.995452 |
| H       | 2.350098 | -1.669458 | 0.034661 |
| H       | 2.730825 | -1.351950 | -1.658806 |
| H       | 4.016255 | -1.805410 | -0.528333 |
| H       | 4.059423 | 1.431181 | 1.364773 |
| H       | 3.156986 | -0.008995 | 1.847327 |
| H       | 4.885820 | -0.165449 | 1.238150 |
| S       | -3.885239 | -0.116479 | 0.048085 |
| C       | -3.054499 | 1.480700 | -0.130794 |
| H       | -3.559932 | 2.229582 | 0.477571 |
### 7_isobutylacrylate_TS_22

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.602044 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.419668 |

Number of Imaginary Frequencies

**Frequencies** (Top 3 out of 72)

1. -152.2033 cm\(^{-1}\)
2. 23.7336 cm\(^{-1}\)
3. 40.3353 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | -0.224094 | 1.040174 | 0.161615 |
|---------|-----------|----------|----------|
| C       | -0.864743 | 0.447851 | -0.990482|
| C       | -2.131470 | 0.825053 | -1.321278|
| O       | -0.732248 | 1.876436 | 0.892372 |
| O       | 1.040801  | 0.661508 | 0.482119 |
| C       | 1.739775  | -0.314962| -0.285370|
| C       | 3.130649  | -0.479501| 0.299751 |
| C       | 3.922590  | 0.820081 | 0.213082 |
| C       | 3.849786  | -1.610494| -0.427802|
| H       | -0.373529 | -0.342087| -1.535250|
| H       | -2.579791 | 0.478292 | -2.238789|
| H       | -2.562068 | 1.705293 | -0.871380|
| H       | 1.198153  | -1.263780| -0.252968|
| H       | 1.811930  | 0.011674 | -1.327408|
| H       | 3.013222  | -0.754554| 1.351651 |
| H       | 4.912344  | 0.697840 | 0.653580 |
| H       | 4.052959  | 1.111962 | -0.832041|
| H       | 3.413696  | 1.630984 | 0.731948 |
| H       | 4.846926  | -1.759163| -0.014103|
| H       | 3.303642  | -2.550848| -0.345968|
| H       | 3.960195  | -1.373001| -1.488368|
| S       | -3.841756 | -0.556813| -0.005814|
| C       | -2.598008 | -1.423884| 0.973625 |
| H       | -2.688579 | -2.505682| 0.878633 |
7_isobutylacrylate_TS_2

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.605656
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423295
Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 72)

1.  -199.0610 cm⁻¹
2.   28.9611 cm⁻¹
3.   42.1131 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | -0.309637 | 1.564078 | -0.033698 |
| C | -1.592539 | 1.429903 | -0.651034 |
| C | -1.970664 | 0.320784 | -1.379664 |
| O | 0.089880  | 2.532838 | 0.606711  |
| O | 0.494463  | 0.481491 | -0.214727 |
| C | 1.784431  | 0.530544 | 0.382531  |
| C | 2.496141  | -0.778357 | 0.093840 |
| C | 3.839226  | -0.791735 | 0.815717 |
| C | 2.676970  | -0.990164 | -1.405018 |
| H | -2.291369 | 2.227563 | -0.440632 |
| H | -2.872608 | 0.369831 | -1.971308 |
| H | -1.207025 | -0.339921 | -1.758674 |
| H | 2.350497  | 1.371876 | -0.028475 |
| H | 1.682491  | 0.689400 | 1.458039  |
| H | 1.873701  | -1.585520 | 0.491668  |
| H | 4.361023  | -1.732555 | 0.641071  |
| H | 4.476620  | 0.016737 | 0.450016  |
| H | 3.716304  | -0.665325 | 1.891998  |
| H | 1.719177  | -0.988665 | -1.923741 |
| H | 3.293912  | -0.191917 | -1.825664 |
| H | 3.174659  | -1.939676 | -1.604345 |
| S | -2.866125 | -1.425211 | -0.027169 |
| C | -2.331962 | -0.749333 | 1.555017  |
| H | -1.990323 | 0.281394 | 1.392439  |
### 7_isobutylacrylate_TS_3

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.606529 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.424176 |

#### Frequencies (Top 3 out of 72)

1. -186.7244 cm\(^{-1}\)
2. 27.1821 cm\(^{-1}\)
3. 41.0682 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -0.215736 | -0.876500 | -0.048053 |
| C    | -1.249590 | -0.804544 | -1.034179 |
| C    | -2.526823 | -1.222879 | -0.734492 |
| O    | -0.319785 | -1.290116 | 1.101296 |
| O    | 0.984214  | -0.425474 | -0.513281 |
| C    | 2.072489  | -0.455082 | 0.403709 |
| C    | 3.308083  | 0.089461  | -0.288488 |
| C    | 4.504481  | -0.039163 | 0.648663 |
| C    | 3.107249  | 1.536775  | -0.723323 |
| H    | -1.009403 | -0.339747 | -1.979642 |
| H    | -2.667876 | -1.858229 | 0.126834 |
| H    | -3.244940 | -1.348257 | -1.530195 |
| H    | 1.829254  | 0.152422  | 1.280625 |
| H    | 2.235784  | -1.479829 | 0.743327 |
| H    | 3.488243  | -0.524783 | -1.175476 |
| H    | 4.344102  | 0.550654  | 1.554215 |
| H    | 4.671322  | -1.075381 | 0.945023 |
| H    | 5.411460  | 0.327603  | 0.168318 |
| H    | 2.258360  | 1.634897  | -1.398460 |
| H    | 2.923614  | 2.169057  | 0.149148 |
| H    | 3.995379  | 1.914708  | -1.230675 |
| S    | -3.852649 | 0.501927  | 0.269894 |
| C    | -2.532910 | 1.717737  | 0.434490 |
| H    | -2.298124 | 1.925697  | 1.477914 |
### 7_isobutylacrylate_TS_4

| Datum | Value                  |
|-------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.60647 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423411 |
| Number of Imaginary Frequencies | 1 |

#### Frequencies (Top 3 out of 72)

1. -196.9031 cm\(^{-1}\)
2. 37.4937 cm\(^{-1}\)
3. 58.0789 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -2.047193 | -0.989180 | -1.431530 |
| S    | -2.768073 | -1.386971 | 0.171042  |
| C    | -2.047193 | -0.989180 | -1.431530 |
| C    | -0.289320 | 1.647743  | -0.094523 |
| C    | -1.629788 | 1.314427  | -0.044467 |
| C    | -2.783897 | 2.655818  | -0.058878 |
| O    | 0.147214  | 2.497927  | -0.866179 |
| O    | 0.522229  | 0.654748  | 0.361955  |
| H    | -2.314828 | 2.294857  | -0.004274 |
| H    | -1.323412 | 0.036152  | 1.844841  |
| H    | -3.014960 | 0.708931  | 1.762157  |
| H    | 1.846413  | 0.593573  | -1.220367 |
| H    | 2.360767  | 1.570817  | 0.158311  |
| H    | 4.580333  | -1.380340 | 0.425843  |
| H    | 4.104559  | -0.599149 | -1.081890 |
| H    | 4.532439  | 0.382258  | 0.323816  |
| H    | 2.419825  | -2.722753 | 0.445295  |
| H    | 0.860563  | -1.893719 | 0.353622  |
| H    | 1.914927  | -1.956281 | -1.063485 |
| S    | -2.768073 | -1.386971 | 0.171042  |
| C    | -2.047193 | -0.989180 | -1.431530 |
| H    | -1.154031 | -1.579233 | -1.636652 |
### 7_isobutylacrylate_TS_5_reopt

| Datum | Value            |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.611414 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.427134 |

Number of Imaginary Frequencies 1

**Frequencies (Top 3 out of 72)**

1. -118.0126 cm⁻¹
2. 35.5520 cm⁻¹
3. 51.7955 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 0.142657 | 1.580894 | -0.162995 |
| C | 1.519032 | 1.496137 | -0.090455 |
| C | 2.250861 | 0.589060 | 0.808567 |
| O | -0.550583 | 2.252350 | -0.960733 |
| O | -0.526884 | 0.835980 | 0.825635 |
| C | -1.921421 | 0.665146 | 0.666800 |
| C | -2.254569 | -0.574145 | -0.156140 |
| C | -3.743853 | -0.598287 | -0.479845 |
| C | -1.834409 | -1.843121 | 0.577733 |
| H | 2.072766 | 2.059350 | -0.830664 |
| H | 3.148545 | 1.030877 | 1.244622 |
| H | 1.617622 | 0.237114 | 1.618172 |
| H | -2.335187 | 0.553653 | 1.673590 |
| H | -2.354982 | 1.552270 | 0.206964 |
| H | -1.690330 | -0.497079 | -1.091463 |
| H | -4.332404 | -0.607066 | 0.441291 |
| H | -4.039052 | 0.277155 | -1.059705 |
| H | -4.007261 | -1.489861 | -1.049869 |
| H | -1.954453 | -2.724528 | -0.053940 |
| H | -0.793353 | -1.789762 | 0.896607 |
| H | -2.453353 | -1.980758 | 1.468327 |
| S | 2.972228 | -0.953165 | 0.005233 |
| C | 1.567776 | -1.515699 | -0.985439 |
| H | 1.711063 | -1.284723 | -2.038288 |
### 7_isobutylacrylate_TS_6

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.60529          |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.42249          |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 72)

1. \(-190.3994\) cm\(^{-1}\)
2. \(32.1608\) cm\(^{-1}\)
3. \(40.3573\) cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | -0.026686 | -0.932750 | -0.621886 |
| C          | -1.197439 | -0.596547 | -1.372615 |
| C          | -1.803639 | 0.640211  | -1.330188 |
| O          | 0.567454  | -2.006018 | -0.660202 |
| O          | 0.410336  | 0.076277  | 0.184103  |
| C          | 1.643533  | -0.125016 | 0.867479  |
| C          | 2.850240  | 0.161722  | -0.015219 |
| C          | 4.124257  | -0.090513 | 0.783466  |
| C          | 2.809915  | 1.587345  | -0.553351 |
| H          | -1.627731 | -1.410207 | -1.940024 |
| H          | -1.252582 | 1.481009  | -0.939427 |
| H          | -2.550958 | 0.880568  | -2.071340 |
| H          | 1.624026  | 0.574749  | 1.705279  |
| H          | 1.686706  | -1.142016 | 1.256363  |
| H          | 2.815183  | -0.536715 | -0.855019 |
| H          | 4.171529  | 0.577733  | 1.646859  |
| H          | 4.170334  | -1.117495 | 1.148141  |
| H          | 5.007613  | 0.092730  | 0.171648  |
| H          | 2.846582  | 2.304564  | 0.270741  |
| H          | 3.663436  | 1.779778  | -1.204239 |
| H          | 1.898279  | 1.770652  | -1.121733 |
| S          | -3.422452 | 0.826373  | 0.427610  |
| C          | -2.918868 | -0.659198 | 1.315077  |
| H          | -2.409952 | -0.425200 | 2.249745  |
### 7_isobutylacrylate_TS_7_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.606529 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.424175 |

Number of Imaginary Frequencies 1

**Frequencies** (Top 3 out of 72)

1. -186.7526 cm⁻¹
2. 27.1841 cm⁻¹
3. 41.0917 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.215754 | -0.876629 | 0.048049 |
| C     | 1.249600 | -0.804699 | 1.034160 |
| C     | 2.526889 | -1.222806 | 0.734401 |
| O     | 0.319819 | -1.290088 | -1.101355 |
| O     | -0.984234 | -0.425748 | 0.513342 |
| C     | -2.072500 | -0.455303 | -0.403654 |
| C     | -3.308050 | 0.089433 | 0.288472 |
| C     | -4.504343 | -0.038714 | -0.648879 |
| C     | -3.106922 | 1.536617 | 0.723605 |
| H     | 1.009373 | -0.340036 | 1.979680 |
| H     | 2.668009 | -1.858112 | -0.126951 |
| H     | 3.245015 | -1.348208 | 1.530096 |
| H     | -1.829187 | 0.152088 | -1.280625 |
| H     | -2.235914 | -1.480063 | -0.743181 |
| H     | -3.488507 | -0.524927 | 1.175320 |
| H     | -4.343845 | 0.551540 | -1.554125 |
| H     | -4.671171 | -1.074784 | -0.945763 |
| H     | -5.411372 | 0.327833 | -0.168459 |
| H     | -2.258254 | 1.634378 | 1.399070 |
| H     | -2.922768 | 2.168977 | -0.148701 |
| H     | -3.995126 | 1.914745 | 1.230681 |
| S     | 3.852492 | 0.502086 | -0.269940 |
| C     | 2.532626 | 1.717764 | -0.434422 |
| H     | 2.783501 | 2.655840 | 0.059011 |
### 7_isobutylacrylate_TS_8_reopt

| Datum | Value                |
|-------|----------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.606259 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.423555 |
| Number of Imaginary Frequencies | 1 |

#### Frequencies (Top 3 out of 72)

1. -188.5456 cm\(^{-1}\)
2.  34.3439 cm\(^{-1}\)
3.  39.2820 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.242373 | -0.084472 |
|-------|----------|-----------|
| C     | 1.142052 | 0.355098  |
| C     | 1.441762 | -0.465836 |
| O     | -0.329503| 1.166352  |
| O     | 0.057128 | 0.862002  |
| C     | -0.763083| 0.506329  |
| C     | -0.003944| -0.282095 |
| C     | -0.958626| -0.644135 |
| C     | 1.192578 | 0.506249  |
| H     | 1.502692 | 1.372299  |
| H     | 1.229546 | -1.520377 |
| H     | 2.256724 | -0.207141 |
| H     | -1.104856| 1.454165  |
| H     | -1.627397| -0.058128 |
| H     | 0.352424 | 1.201747  |
| H     | -1.353806| 0.260275  |
| H     | -1.802288| 1.233309  |
| H     | -0.445766| 1.221515  |
| H     | 1.874956 | 0.770360  |
| H     | 0.858104 | 1.430458  |
| H     | 1.746027 | -0.073167 |
| S     | -0.147204| -0.261447 |
| C     | -1.332434| 0.759235  |
| H     | -0.884602| 1.049568  |
### 7_isobutylacrylate_TS_9_reopt

#### Datum | Value
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -862.605619
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -862.421613

#### Frequencies

(Top 3 out of 72)

1. -203.9619 cm⁻¹
2. 40.1835 cm⁻¹
3. 62.8819 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | 0.192919 | 1.597396 | 0.141208 |
| C     | -1.227928 | 1.723368 | 0.054329 |
| C     | -2.003382 | 1.083400 | -0.895889 |
| O     | 0.916788  | 2.175606 | 0.946921 |
| O     | 0.717941  | 0.759958 | -0.800283 |
| C     | 2.123346  | 0.522554 | -0.804929 |
| C     | 2.461999  | -0.820331 | -0.168483 |
| C     | 1.745812  | -1.964017 | -0.880534 |
| C     | 2.151792  | -0.826497 | 1.324425 |
| H     | -1.682659 | 2.321056 | 0.832157 |
| H     | -3.021299 | 1.414857 | -1.036401 |
| H     | -1.523864 | 0.695345 | -1.780678 |
| H     | 2.419939  | 0.521758 | -1.854773 |
| H     | 2.632608  | 1.334343 | -0.288927 |
| H     | 3.541069  | -0.947233 | -0.301640 |
| H     | 0.664296  | -1.862704 | -0.768157 |
| H     | 1.976405  | -1.973863 | -1.947160 |
| H     | 2.041210  | -2.925662 | -0.459502 |
| H     | 1.085488  | -0.661877 | 1.489799 |
| H     | 2.416009  | -1.787760 | 1.767389 |
| H     | 2.697626  | -0.041031 | 1.847006 |
| S     | -2.714773 | -1.067581 | -0.247322 |
| C     | -1.796335 | -1.155016 | 1.298481 |
| H     | -1.274983 | -0.197275 | 1.437834 |
### 8_ethylmethacrylate_1

| Datum                                           | Value                  |
|-------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -385.093777            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.971744            |
| Number of Imaginary Frequencies                 | 0                      |

**Frequencies (Top 3 out of 48)**

1. 35.8850 cm⁻¹
2. 84.9653 cm⁻¹
3. 131.7870 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | X  | Y  | Z    |
|------|----|----|------|
| C    | 0.344125 | -0.560003 | 0.000006 |
| C    | 1.612188  | 0.235987  | -0.000002 |
| C    | 1.518264  | 1.731599  | 0.000012  |
| C    | 2.755364  | -0.439683 | -0.000021 |
| O    | 0.280986  | -1.766216 | 0.000012  |
| O    | 0.733536  | -0.223748 | 0.000003  |
| C    | -2.008782 | -0.439326 | 0.000006  |
| C    | -3.075968 | 0.626124  | -0.000015 |
| H    | 2.513299  | 2.170674  | 0.000009  |
| H    | 0.975648  | 2.086921  | -0.876080 |
| H    | 0.975661  | 2.086906  | 0.876118  |
| H    | 3.707292  | 0.074105  | -0.000028 |
| H    | 2.757521  | -1.520823 | -0.000030 |
| H    | -2.067647 | -1.076047 | -0.882188 |
| H    | -2.06756  | -1.076023 | 0.882216  |
| H    | -4.058552 | 0.156840  | -0.000013 |
| H    | -2.993161 | 1.254513  | 0.885516  |
| H    | -2.993152 | 1.254486  | -0.885564 |

### 8_ethylmethacrylate_2
| Datum                                                                 | Value       |
|---------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -385.093248 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)         | -384.9707   |

Number of Imaginary Frequencies

0

**Frequencies (Top 3 out of 48)**

1. 45.3074 cm\(^{-1}\)
2. 83.2996 cm\(^{-1}\)
3. 120.1157 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C         | -0.182047 | -0.407029 | -0.176780 |
|-----------|-----------|-----------|-----------|
| C         | -1.589890 | 0.043912  | 0.063191  |
| C         | -1.874670 | 1.514790  | 0.100777  |
| C         | -2.510671 | -0.898196 | 0.230860  |
| O         | 0.174901  | -1.559356 | -0.232953 |
| O         | 0.646692  | 0.626478  | -0.329767 |
| C         | 2.036676  | 0.326318  | -0.547883 |
| C         | 2.741551  | 0.044610  | 0.760574  |
| H         | -2.932840 | 1.688160  | 0.282927  |
| H         | -1.296818 | 2.002592  | 0.885835  |
| H         | -1.596239 | 1.988752  | -0.840505 |
| H         | -3.546384 | -0.641078 | 0.407981  |
| H         | -2.242359 | -1.944871 | 0.193451  |
| H         | 2.109532  | -0.516997 | -1.231435 |
| H         | 2.435385  | 1.214683  | -1.030398 |
| H         | 3.800855  | -0.128303 | 0.573832  |
| H         | 2.644602  | 0.893523  | 1.435998  |
| H         | 2.325835  | -0.839857 | 1.239643  |

**8_ethylmethacrylate_3**

| Datum                                                                 | Value       |
|---------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -385.093595 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)         | -384.971085 |

Number of Imaginary Frequencies

0

**Frequencies (Top 3 out of 48)**
1. 45.2374 cm$^{-1}$
2. 82.5778 cm$^{-1}$
3. 110.1466 cm$^{-1}$

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |          |          |
|----------|----------|----------|
| C        | -0.176615| -0.271849| -0.186268|
| C        | -1.557548| 0.243982 | 0.056454 |
| C        | -2.612813| -0.810401| 0.190645 |
| C        | -1.791060| 1.548982 | 0.143772 |
| O        | 0.076709 | -1.451823| -0.252927|
| O        | 0.740669 | 0.684649 | -0.327333|
| C        | 2.098708 | 0.261717 | -0.540600|
| C        | 2.768126 | -0.100118| 0.766781 |
| H        | -3.584835| -0.355903| 0.366519 |
| H        | -2.663906| -1.420402| -0.711560|
| H        | -2.380467| -1.483891| 1.015895 |
| H        | -2.792324| 1.918965 | 0.321945 |
| H        | -0.996526| 2.273523 | 0.041470 |
| H        | 2.100910 | -0.575187| -1.235995|
| H        | 2.579463 | 1.116669 | -1.008663|
| H        | 3.809704 | -0.361232| 0.582451 |
| H        | 2.741062 | 0.743600 | 1.455059 |
| H        | 2.275104 | -0.952622| 1.230252 |

8_ethylmethacrylate_4

| Datum                                      | Value   |
|--------------------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.081566 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.960304 |
| Number of Imaginary Frequencies            | 0       |

Frequencies (Top 3 out of 48)

1. 24.9000 cm$^{-1}$
2. 65.2684 cm$^{-1}$
3. 104.7491 cm$^{-1}$

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
8_ethylmethacrylate_5

| Datum                                      | Value    |
|--------------------------------------------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.081108 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.958971 |
| Number of Imaginary Frequencies            | 0        |

**Frequencies (Top 3 out of 48)**

1. 49.0212 cm⁻¹
2. 90.2755 cm⁻¹
3. 111.4752 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 0.283461 | 0.887410 | 0.120636 |
|-----|----------|----------|----------|
| C   | 1.069977 | -0.387930 | 0.187563 |
| C   | 1.931378 | -0.671091 | -1.006414 |
| C   | 1.086082 | -1.098055 | 1.308402 |
| O   | 0.811139 | 1.920793 | -0.207545 |
| O   | -1.005999 | 0.907854 | 0.472939 |
| C   | -1.837308 | -0.270216 | 0.429891 |
8_ethylmethacrylate_6

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.08076     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.959031   |
| Number of Imaginary Frequencies            | 0              |

**Frequencies (Top 3 out of 48)**

1. 44.3308 cm⁻¹
2. 95.9299 cm⁻¹
3. 109.4089 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -0.388829 | 0.888799 | -0.156737 |
|-------|-----------|----------|-----------|
| C     | -1.086533 | -0.442064| -0.142481 |
| C     | -1.849651 | -0.740204| 1.115363  |
| C     | -1.060855 | -1.216982| -1.216372 |
| O     | -0.918979 | 1.884110 | -0.580719 |
| O     | 0.832614  | 0.979432 | 0.371281  |
| C     | 1.578463  | -0.188468| 0.764440  |
| C     | 2.450082  | -0.666360| -0.372963 |
| H     | -1.197059 | -0.728669| 1.990288  |
| H     | -2.614672 | 0.021178 | 1.276701  |
| H     | -2.329536 | -1.713832| 1.046948  |
| H     | -1.598113 | -2.156519| -1.231621 |
| H     | -0.515155 | -0.938821| -2.108541 |
| H     | 2.176174  | 0.139248 | 1.611260  |
| H     | 0.901589  | -0.969886| 1.103034  |
| H     | 1.840983  | -1.004328| -1.210755 |
### 8_ethylmethacrylate_HEI_10_reopt

| Datum | Value            |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.300393     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.144423     |

**Number of Imaginary Frequencies**

0

**Frequencies (Top 3 out of 63)**

1. 35.2152 cm⁻¹
2. 52.5087 cm⁻¹
3. 68.5606 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.839409 | -0.258718 | -0.009594 |
|-------|----------|-----------|-----------|
| C     | -0.251323| 0.422232  | 0.486583  |
| C     | -0.338194| 1.927759  | 0.452967  |
| C     | -1.369650| -0.368231 | 1.040907  |
| O     | 1.041113 | -1.498331 | -0.055170 |
| O     | 1.827838 | 0.589261  | -0.538401 |
| C     | 3.087771 | 0.001977  | -0.806398 |
| C     | 3.909031 | -0.173897 | 0.457937  |
| H     | -1.182290| 2.267888  | 1.058321  |
| H     | 0.560387 | 2.405472  | 0.852673  |
| H     | -0.486022| 2.348677  | -0.549143 |
| H     | -1.898693| 0.172432  | 1.828797  |
| H     | -1.031283| -1.323306 | 1.441684  |
| H     | 2.954949 | -0.956243 | -1.307668 |
| H     | 3.588941 | 0.685639  | -1.492682 |
| H     | 4.890708 | -0.587350 | 0.222951  |
| H     | 4.050824 | 0.784888  | 0.957737  |
| H     | 3.400546 | -0.853550 | 1.140759  |
| C     | -3.245228| 0.720083  | -0.723072 |
| H     | -2.430371| 1.217833  | -1.244198 |
| H     | -3.571854| 1.339275  | 0.112514  |
| H     | -4.078151| 0.581208  | -1.408747 |
| S     | -2.719437| -0.902346 | -0.141276 |
8_ethylmethacrylate_HEI_11

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -823.30149          |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -823.147346         |
| Number of Imaginary Frequencies                                      | 0                   |

**Frequencies** (Top 3 out of 63)

1. 25.9999 cm⁻¹
2. 49.3823 cm⁻¹
3. 52.0689 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| C | -1.070293     | 0.963445      | -0.007700     |
| C | 0.248925      | 1.208775      | 0.311305      |
| C | 0.825633      | 2.584753      | 0.138577      |
| C | 1.171099      | 0.134791      | 0.743920      |
| O | -1.952304     | 1.772956      | -0.390624     |
| O | -1.447857     | -0.382943     | 0.126803      |
| C | 2.815169      | -0.677659     | -0.083655     |
| C | -1.994795     | -2.170067     | 0.062065      |
| H | 0.049009      | 3.290087      | -0.153725     |
| H | 1.286044      | 2.960063      | 1.061144      |
| H | 1.609879      | 2.622690      | -0.628672     |
| H | 0.652433      | -0.715918     | 1.180076      |
| H | 1.910706      | 0.501565      | 1.462017      |
| H | -3.434117     | -0.126741     | 0.632565      |
| H | -3.122885     | -0.366489     | -1.080619     |
| H | -2.386242     | -2.717603     | -0.623719     |
| H | -4.038324     | -2.445563     | -0.055812     |
| H | -2.699964     | -2.478201     | 1.099421      |
| C | 3.299955      | -1.622503     | 0.238354      |
| H | 3.895169      | -1.048377     | 0.947213      |
| H | 3.965849      | -2.100453     | -0.476745     |
| H | 2.745809      | -2.391578     | 0.773963      |
| S | 2.173534      | -0.539550     | -0.666770     |

8_ethylmethacrylate_HEI_12_reopt2
| Datum                                                                 | Value        |
|---------------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.300333  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -823.144765  |
| Number of Imaginary Frequencies                                     | 0            |

**Frequencies** (Top 3 out of 63)

1. 36.9777 cm⁻¹
2. 43.0164 cm⁻¹
3. 61.9617 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | 0.983136 | 0.907178 | -0.148228 |
| C    | -0.368750 | 1.076218 | -0.341100 |
| C    | -1.036658 | 2.263598 | 0.304129  |
| C    | -1.171535 | 0.130520 | -1.148594 |
| O    | 1.761579  | 1.621371 | 0.532610  |
| O    | 1.535436  | -0.187623| -0.840406 |
| C    | 2.732720  | -0.719371| -0.305030 |
| C    | 2.467341  | -1.534358| 0.947983  |
| H    | -1.105589 | 2.195432 | 1.396963  |
| H    | -0.506382 | 3.197347 | 0.092556  |
| H    | -2.058191 | 2.377746 | -0.066119 |
| H    | -0.599690 | -0.336078| -1.948345 |
| H    | -2.038316 | 0.624580 | -1.592343 |
| H    | 3.439491  | 0.082858 | -0.094590 |
| H    | 3.151133  | -1.350899| -1.089402 |
| H    | 1.767637  | -2.343096| 0.735193  |
| H    | 3.392761  | -1.967708| 1.329158  |
| H    | 2.038270  | -0.898919| 1.722998  |
| C    | -2.765275 | -0.509036| 1.056805  |
| H    | -3.518822 | 0.162342 | 0.645852  |
| H    | -3.254798 | -1.260104| 1.672725  |
| H    | -2.068685 | 0.060704 | 1.668322  |
| S    | -1.878801 | -1.356418| -0.262900 |

**8_ethylmethacrylate_HEI_1_reopt**

| Datum                                                                 | Value        |
|---------------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.302755  |
| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.147707 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

1. 40.5086 cm⁻¹
2. 54.4829 cm⁻¹
3. 71.0200 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C      | -0.646088 | -0.137978 | -0.567278 |
|--------|-----------|-----------|-----------|
| C      | 0.389029  | 0.771846  | -0.473490 |
| C      | 0.317153  | 2.022538  | 0.354939  |
| C      | 1.700970  | 0.401203  | -1.032530 |
| O      | -0.673133 | -1.246423 | -1.160007 |
| O      | -1.814768 | 0.266039  | 0.095325  |
| C      | -2.958983 | -0.543303 | -0.095936 |
| C      | -4.086496 | 0.054489  | 0.717664  |
| H      | 0.900831  | 2.827817  | -0.104871 |
| H      | -0.706014 | 2.377361  | 0.466585  |
| H      | 0.726655  | 1.892533  | 1.366959  |
| H      | 2.203134  | 1.229864  | -1.539717 |
| H      | 1.617313  | -0.435933 | -1.721049 |
| H      | -3.224300 | -0.578612 | -1.155998 |
| H      | -2.754948 | -1.568299 | 0.218715  |
| H      | -4.992777 | -0.539556 | 0.600749  |
| H      | -3.825427 | 0.078450  | 1.775803  |
| H      | -4.289809 | 1.073318  | 0.393529  |
| C      | 2.064211  | -1.318454 | 1.157393  |
| H      | 1.085098  | -0.908664 | 1.404748  |
| H      | 2.608867  | -1.545165 | 2.071143  |
| H      | 1.935096  | -2.230084 | 0.576956  |
| S      | 2.996863  | -0.083250 | 0.237458  |

**8_ethylmethacrylate_HEI_2**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.302939 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.148171 |
### Number of Imaginary Frequencies

| Datum                     | Value |
|---------------------------|-------|
| Number of Imaginary Frequencies | 0     |

### Frequencies (Top 3 out of 63)

| Frequency | Value   |
|-----------|---------|
| 1.        | 28.7281 cm\(^{-1}\) |
| 2.        | 50.4827 cm\(^{-1}\) |
| 3.        | 76.5432 cm\(^{-1}\) |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | C          | C          | C          | C          | O          | O          | C          | C          | H          | H          | H          | H          | H          | H          | H          | H          | H          | S          |
|------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|      | 0.595790   | 1.122257   | 0.042816   | -0.721349  | 1.097923   | -0.369137  | -1.661089  | 2.179409   | 0.079229   | -1.299605  | -0.045382  | -1.098899  | 1.182065   | 1.984772   | 0.744450   | 1.363749   | -0.417510  | 2.628075   | -0.131186  |
|      | 3.261840   | -1.369581  | 0.191002   |            |            |            |            |            |            |            |            |            |            |            |            |            |            |            |            |
|      | -1.108106  | 3.044978   | 0.442059   | -2.311165  | 2.513890   | -0.737616  | -2.330258  | 1.857065   | 0.888697   | -0.548705  | -0.649845  | -1.599977  | -2.045746  | 0.263816   | -1.835900  | 3.255893   | 0.022673   |            |            |
|      | -2.510780  | -0.240958  | 1.273262   | -4.243775  | -1.541539  | 0.035498   | -3.38314   | -1.257093  | -1.482665  | 2.642269   | -2.247256  | -0.219645  |            |            |            |            |            | -1.243588  |            |
|      | -1.000179  | -1.736179  | 1.109351   | -0.516839  | -0.842760  | 1.504548   | -0.253929  | -2.360876  | 0.621439   | -1.463459  | -2.290653  | 1.922340   |            |            |            |            |            |            |
|      | -2.290352  | -1.243588  | -0.046587  |            |            |            |            |            |            |            |            |            |            |            |            |            |            |            |

### 8_ethylmethacrylate_HEI_3_reopt

| Datum                                                                 | Value       |
|-----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -823.302744 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -823.147082 |
| Number of Imaginary Frequencies                                        | 0           |
**Frequencies** (Top 3 out of 63)

1. 37.2471 cm⁻¹
2. 50.0240 cm⁻¹
3. 61.9410 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 0.770749 | 0.386434 | 0.609652 |
| C | -0.357152 | 1.030510 | 0.150015 |
| C | -0.375867 | 2.006750 | -0.990607 |
| C | -1.653909 | 0.715575 | 0.783311 |
| O | 0.866035  | -0.482975 | 1.514202 |
| O | 1.966687  | 0.808046  | -0.007114 |
| C | 3.059134  | -0.086922 | 0.081868 |
| C | 2.891919  | -1.269054 | -0.855952 |
| H | -0.772547 | 2.985147  | -0.689488 |
| H | 0.619378  | 2.166999  | -1.398378 |
| H | -1.018225 | 1.660918  | -1.810408 |
| H | -2.277842 | 1.601977  | 0.931386 |
| H | -1.522443 | 0.217293  | 1.741381 |
| H | 3.938594  | 0.496369  | -0.193484 |
| H | 3.181066  | -0.431386 | 1.108388 |
| H | 3.754263  | -1.934179 | -0.795975 |
| H | 1.999552  | -1.833239 | -0.585070 |
| H | 2.790548  | -0.928559 | -1.886993 |
| C | -1.717210 | -1.820320 | -0.384084 |
| H | -0.717262 | -1.483315 | -0.657207 |
| H | -2.117883 | -2.458103 | -1.168767 |
| H | -1.668357 | -2.380281 | 0.548004 |
| S | -2.784788 | -0.378628 | -0.222832 |

**8_ethylmethacrylate_HEI_4_reopt**

| Datum                                    | Value       |
|------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -823.302663 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.147019 |
| Number of Imaginary Frequencies          | 0           |

**Frequencies** (Top 3 out of 63)
1. 46.0448 cm⁻¹
2. 50.2502 cm⁻¹
3. 68.7838 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | -0.756225 | -0.195854 | -0.160218 |
|--------|-----------|-----------|-----------|
| C      | 0.261530  | 0.728903  | -0.266712 |
| C      | 0.344248  | 1.972340  | 0.571456  |
| C      | 1.431420  | 0.395615  | -1.102516 |
| O      | -0.896375 | -1.290225 | -0.763918 |
| O      | -1.751264 | 0.161293  | 0.769850  |
| C      | -3.005562 | 0.102780  | -0.538361 |
| C      | -3.797028 | 2.794669  | 0.003533  |
| H      | -0.638025 | 2.298635  | 0.908067  |
| H      | 0.969471  | 1.846653  | 1.466706  |
| H      | 1.775193  | 1.235518  | -1.713371 |
| H      | 1.225700  | -0.451771 | -1.752480 |
| H      | -2.866442 | -1.549678 | 0.485026  |
| H      | -3.532037 | -0.313067 | 1.560519  |
| H      | -4.770458 | -0.382502 | -0.619528 |
| H      | -3.956241 | 1.172047  | -0.395661 |
| H      | -3.256716 | -0.048166 | 1.472608  |
| C      | 2.344310  | -1.293887 | 0.943844  |
| H      | 1.416696  | -0.935303 | 1.389931  |
| H      | 3.079469  | -1.476687 | 1.724238  |
| H      | 2.151380  | -2.220009 | 0.405177  |
| S      | 2.990822  | -0.020779 | -0.152517 |

8_ethylmethacrylate_HEI_5_reopt

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.300555   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.14554    |

Number of Imaginary Frequencies

**Frequencies** (Top 3 out of 63)

1. 35.8449 cm⁻¹
2. 44.6652 cm⁻¹
3. 71.4394 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          | X      | Y      | Z      |
|----------|--------|--------|--------|
| C        | -0.741290 | -0.474590 | 0.309503 |
| C        | 0.330927  | 0.309162  | 0.680325 |
| C        | 0.239767  | 1.813800  | 0.732531 |
| C        | 1.599593  | -0.367750 | 1.015762 |
| O        | -0.805196 | -1.725257 | 0.205148 |
| O        | -1.896903 | 0.265195  | 0.022322 |
| C        | -3.053144 | -0.477848 | -0.313654 |
| C        | -4.173788 | 0.504561  | -0.576142 |
| H        | 0.132147  | 2.290569  | -0.249445 |
| H        | -0.605265 | 2.163686  | 1.333022 |
| H        | 1.146061  | 2.228601  | 1.180440 |
| H        | 1.435415  | -1.366886 | 1.418973 |
| H        | 2.189249  | 0.205459  | 1.734191 |
| H        | -2.863346 | -1.094224 | -1.195075 |
| H        | -3.316925 | -1.155522 | 0.501645 |
| H        | -5.087423 | -0.027603 | -0.840713 |
| H        | -4.371840 | 1.108645  | 0.309363 |
| H        | -3.915312 | 1.173222  | -1.397303 |
| C        | 2.991922  | 0.968128  | -1.004859 |
| H        | 2.035829  | 1.362786  | -1.342599 |
| H        | 3.686347  | 0.943276  | -1.841727 |
| H        | 3.394769  | 1.615467  | -0.226125 |
| S        | 2.787073  | -0.713734 | -0.391575 |

8_ethylmethacrylate_HEI_6

| Datum                                           | Value      |
|-------------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -823.302694|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.147184|
| Number of Imaginary Frequencies                  | 0          |
| Frequencies (Top 3 out of 63)                    |            |
| 1. 29.2893 cm⁻¹                                   |            |
| 2. 41.5547 cm⁻¹                                   |            |
| 3. 74.5564 cm⁻¹                                   |            |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |    |    |    |
|----|----|----|----|
| C  | -0.832912 | 0.594089 | 0.340951 |
| C  | 0.338636  | 0.999909 | -0.262949 |
| C  | 0.910799  | 2.350856 | 0.054522  |
| C  | 1.145104  | 0.109492 | -1.119882 |
| O  | -1.591956 | 1.252839 | 1.096386  |
| O  | -1.194830 | -0.739884 | 0.067400 |
| C  | -2.560441 | -1.063930 | 0.250214 |
| C  | -3.425940 | -0.508587 | -0.86433 |
| H  | 0.169981  | 2.975523 | 0.551373  |
| H  | 1.790267  | 2.297623 | 0.709955  |
| H  | 1.239085  | 2.873157 | -0.851903 |
| H  | 1.572194  | 0.635931 | -1.978487 |
| H  | 0.578543  | -0.743426 | -1.482807 |
| H  | -2.602675 | -2.153723 | 0.258404 |
| H  | -2.907277 | -0.698056 | 1.216360 |
| H  | -4.467819 | -0.798778 | -0.725339 |
| H  | -3.091587 | -0.885469 | -1.833536 |
| H  | -3.368016 | 0.579450 | -0.875700 |
| C  | 1.930672  | -1.453305 | 1.067877 |
| H  | 1.405701  | -2.348232 | 0.738759 |
| H  | 1.225212  | -0.781665 | 1.556177 |
| H  | 2.716580  | -1.730452 | 1.766833 |
| S  | 2.687412  | -0.593542 | -0.321636 |

8_ethylmethacrylate_HEI_7_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.300484 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.145279 |

Number of Imaginary Frequencies
0

Frequencies (Top 3 out of 63)

1. 43.1518 cm⁻¹
2. 66.3112 cm⁻¹
3. 73.5543 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
8_ethylmethacrylate_HEI_8

Datum Value
M06-2X/def2tzvpp-IEFPCM(water) Energy -823.301403
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) -823.146944

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 63)

1. 42.4194 cm⁻¹
2. 52.4373 cm⁻¹
3. 62.7799 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     |     |     |
|-----|-----|-----|
| C   | -0.383712 | -0.322257 | 0.311205 |
| C   | 0.177715  | 0.603077  | 0.436546 |
| C   | 0.021918  | 2.075240  | 0.178280 |
C   1.534665  0.110011  0.760489
O  -0.778866 -1.569810  0.461714
O  -2.085286  0.228023 -0.018049
C  -3.165759 -0.680149 -0.110118
C  -4.406568  0.114206 -0.456079
H   0.550532  2.407929 -0.724947
H  -1.023670  2.351079  0.058911
H   0.428820  2.674161  1.002418
H   1.506856 -0.865299  1.243713
H   2.087456  0.805746  1.395764
H  -2.962904 -1.433541 -0.874577
H  -3.296538 -1.210202  0.836100
H  -5.267727 -0.548634 -0.539618
H  -4.617771  0.855736  0.314795
H  -4.278895  0.633397 -1.406066
C   4.165501 -0.511852  0.009318
H   4.503299  0.296468  0.656550
H   4.899541 -0.663429 -0.778976
H   4.077917 -1.427512  0.592499
S   2.585200 -0.092130 -0.756483

8_ethylmethacrylate_HEI_9_reopt2

| Datum                                                                 | Value         |
|-----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -823.300163   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -823.145506   |

Number of Imaginary Frequencies                                      0

Frequencies (Top 3 out of 63)

1.  9.3964 cm⁻¹
2.  39.8771 cm⁻¹
3.  62.1654 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian
Coordinates

C   0.872471 -0.001726 -0.624169
C  -0.316292  0.692562 -0.562534
C  -0.399532  2.078290  0.028557
C  -1.529859  0.047014 -1.103127
O   1.091523 -1.155018 -1.072059
O   1.964261  0.730819 -0.126630
C   3.183888  0.028358  0.025969
### 8_ethylmethacrylate_TS_10_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.296238  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140805 |
| Number of Imaginary Frequencies | 1 |

**Frequencies (Top 3 out of 63)**

1. -224.8647 cm⁻¹
2. 51.4355 cm⁻¹
3. 66.4367 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.755269 | -0.017236 | 0.305071  |
|-------|----------|-----------|-----------|
| C     | -0.293924| 0.949489  | 0.317833  |
| C     | -0.335706| 2.059681  | -0.697215 |
| C     | -1.359744| 0.738821  | 1.182746  |
| O     | 0.859842 | -1.017110 | 1.017099  |
| O     | 1.722770 | 0.265696  | -0.625898 |
| C     | 2.859060 | -0.592948 | -0.661896 |
| C     | 3.875138 | -0.215456 | 0.397304  |
| H     | -1.085519| 2.797606  | -0.408283 |
| H     | 0.621595 | 2.573286  | -0.796145 |
| H     | -0.603669| 1.704001  | -1.698874 |
8_ethylmethacrylate_TS_11

| Datum                                                  | Value       |
|--------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -823.291891 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.138658 |
| Number of Imaginary Frequencies                        | 1           |

Frequencies (Top 3 out of 63)

1. -258.2122 cm⁻¹  
2. 26.7295 cm⁻¹     
3. 48.7110 cm⁻¹     

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C          | -1.193619 | 0.910841 | 0.013757  |
|------------|-----------|----------|-----------|
| C          | 0.116088  | 1.325157 | 0.394083  |
| C          | 0.490654  | 2.750735 | 0.099852  |
| C          | 1.065384  | 0.410341 | 0.824832  |
| O          | -2.077818 | 1.641658 | -0.434572 |
| O          | -1.439330 | -0.423885| 0.184257  |
| C          | -2.748853 | -0.873613| -0.147121 |
| C          | -2.798920 | -2.362025| 0.108630  |
| H          | -0.277378 | 3.450519 | 0.432689  |
| H          | 1.424496  | 3.008870 | 0.600925  |
| H          | 0.635486  | 2.930399 | -0.972028 |
| H          | 0.737923  | -0.560757| 1.167172  |
| H          | 1.949976  | 0.790330 | 1.321570  |
| H          | -3.482400 | -0.341905| 0.461071  |
| H          | -2.959835 | -0.643818| -1.192454 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | -2.062387 | -2.881827 | -0.503478 |
| H       | -3.787097 | -2.748958 | -0.137538 |
| H       | -2.594496 | -2.580245 | 1.156416  |
| C       | 3.304229  | -1.529931 | 0.436279  |
| H       | 3.620801  | -0.897386 | 1.268214  |
| H       | 4.193122  | -1.986510 | 0.003957  |
| H       | 2.672470  | -2.323816 | 0.835998  |
| S       | 2.416045  | -0.546632 | -0.801366 |

8_ethylmethacrylate_TS_12_reopt

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.2968   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.142245 |
| Number of Imaginary Frequencies            | 1           |

Frequencies (Top 3 out of 63)

1. -234.6241 cm⁻¹
2. 31.9289 cm⁻¹
3. 32.3961 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 0.849516  | 0.931878  | -0.063083 |
| C       | -0.516754 | 1.268994  | -0.287967 |
| C       | -1.147119 | 2.257549  | 0.652805  |
| C       | -1.295326 | 0.577832  | -1.208894 |
| O       | 1.593395  | 1.453702  | 0.769524  |
| O       | 1.330874  | -0.051364 | -0.890396 |
| C       | 2.650808  | -0.520125 | -0.632891 |
| C       | 2.665741  | -1.531146 | 0.496393  |
| H       | -1.395253 | 1.807055  | 1.621913  |
| H       | -0.488029 | 3.102127  | 0.856547  |
| H       | -2.076014 | 2.644325  | 0.231210  |
| H       | -0.801085 | -0.017532 | -1.960298 |
| H       | -2.222685 | 1.032813  | -1.530509 |
| H       | 3.303424  | 0.322112  | -0.409464 |
| H       | 2.977084  | -0.978082 | -1.565426 |
| H       | 2.014220  | -2.372709 | 0.260872  |
| H       | 3.676609  | -1.909202 | 0.650860  |
| H       | 2.321723  | -1.070088 | 1.421330  |
| C       | -1.332994 | -1.397096 | 1.181496  |
### 8_ethylmethacrylate_TS_1

| Datum                                                                 | Value                  |
|-----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -823.296732            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -823.14183             |
| Number of Imaginary Frequencies                                       | 1                      |

#### Frequencies (Top 3 out of 63)

1. -227.1755 cm⁻¹  
2. 42.8545 cm⁻¹  
3. 56.0946 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C          | -0.648057 | -0.093216 | 0.669581 |
| C          | 0.381458  | -1.019357 | 0.326308 |
| C          | 0.220257  | -1.955994 | -0.840377|
| C          | 1.599354  | -0.908125 | 0.984499 |
| O          | -0.611263 | 0.780987  | 1.537058 |
| O          | -1.782254 | -0.254957 | -0.081525|
| C          | -2.865410 | 0.622664  | 0.207703 |
| C          | -3.991959 | 0.288623  | -0.742413|
| H          | 1.006844  | -2.711713 | -0.820364|
| H          | -0.740349 | -2.471803 | -0.828741|
| H          | 0.292801  | -1.441719 | -1.805874|
| H          | 2.286155  | -1.742430 | 0.940849 |
| H          | 1.626142  | -0.341281 | 1.902956 |
| H          | -3.171963 | 0.494032  | 1.246970 |
| H          | -2.538085 | 1.656334  | 0.086937 |
| H          | -4.843780 | 0.941034  | -0.553655|
| H          | -3.676165 | 0.424583  | 1.776374 |
| H          | -4.313206 | -0.744294 | -0.611448|
| C          | 1.853207  | 1.352931  | -1.126231|
| H          | 0.886130  | 0.849088  | -1.008413|
| H          | 2.112539  | 1.343835  | -2.184070|
| H          | 1.740417  | 2.386581  | -0.801200|
| S          | 3.074223  | 0.464022  | -0.144142|
8_ethylmethacrylate_TS_2

| Datum                                                                 | Value                  |
|-----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -823.296957            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -823.142367            |
| Number of Imaginary Frequencies                                       | 1                      |

**Frequencies (Top 3 out of 63)**

1. -237.7302 cm\(^{-1}\)  
2. 37.5853 cm\(^{-1}\)  
3. 45.6897 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

```plaintext
C    0.689195  1.039675  0.045855
C   -0.618736  1.147366 -0.509179
C   -1.485099  2.272794 -0.016605
C   -1.140268  0.155248 -1.331537
O    1.221886  1.848843  0.808323
O    1.377056 -0.079037 -0.341997
C    2.687884 -0.232452  0.190448
C    3.242000 -1.537959 -0.331213
H   -0.934329  3.212495  0.040067
H   -2.335913  2.417159  0.683956
H   -1.888886  2.080893  0.985078
H   -0.459330 -0.540837 -1.795317
H   -2.012112  0.397422 -1.924815
H    3.308832  0.611625 -0.114067
H    2.641186 -0.230337  1.280585
H    4.247701 -1.697228  0.056178
H    3.289121 -1.529353 -1.419767
H    2.615503 -2.372974 -0.018395
C   -1.489619 -1.173512  1.440899
H   -0.921647 -0.237751  1.377859
H   -0.798286 -1.974970  1.699315
H   -2.222973 -1.071373  2.239604
S   -2.289534 -1.453136 -0.149061
```

---
8_ethylmethacrylate_TS_3

| Datum                                             | Value     |
|---------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy             | -823.296624 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.141276 |
| Number of Imaginary Frequencies                   | 1         |

**Frequencies** (Top 3 out of 63)

1. -226.8481 cm⁻¹  
2. 44.4419 cm⁻¹  
3. 55.3320 cm⁻¹  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | C           | C           | C           | O           | O           | C           | C           | C           | H           | H           | H           | H           | H           | H           | H           | C           | H           | H           | S           |     |
|---|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|     |
|   | 0.755426    | -0.524470   | -0.551609   | 0.868086    | 0.141602    | -0.684209   | 0.3015932   | 1.477557    | 2.502931    | 0.445432    | 2.536251    | 1.746823    | -0.697390   | 0.486343    | 0.010776    | 2.002255    | 1.990802    | 1.517274    |     |
|   | -0.408079   | -1.205821   | -0.085931   | -1.888886   | 1.254938    | -1.055106   | 0.386665    | 1.477557    | -1.748943   | 2.089443    | 0.398943    | 2.089443    | 1.349725    | 1.398943    | 2.089443    | 0.398943    | 0.398943    |     |
|   | -0.420145   | -1.888886   | 1.254938    | -1.055106   | -0.816213   | 0.141602    | 0.3015932   | 1.477557    | 0.398943    | 2.089443    | 0.398943    | 2.089443    | 1.349725    | 1.398943    | 2.089443    | 0.398943    | 0.398943    |     |
|   | -1.579765   | -1.055106   | -0.816213   | 0.141602    | -1.581640   | 0.282673    | 0.3015932   | 1.477557    | 0.398943    | 2.089443    | 0.398943    | 2.089443    | 1.349725    | 1.398943    | 2.089443    | 0.398943    | 0.398943    |     |
|   | 0.868086    | 0.141602    | -1.581640   | 0.282673    | 0.3015932   | 0.420852    | 1.477557    | 0.398943    | 0.398943    | 2.089443    | 0.398943    | 2.089443    | 1.349725    | 1.398943    | 2.089443    | 0.398943    | 0.398943    |     |
|   | 1.833510    | -0.684209   | 0.282673    | 0.3015932   | 1.477557    | 0.398943    | 0.398943    | 0.398943    | 2.089443    | 0.398943    | 2.089443    | 0.398943    | 1.349725    | 1.398943    | 2.089443    | 0.398943    | 0.398943    | 0.398943    |

8_ethylmethacrylate_TS_4

| Datum | Value |
|-------|-------|

| Datum | Value |
## SI_esters.md

### Datum Value

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -823.296238   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -823.140804   |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 63)

1. -224.8127 cm⁻¹
2. 51.4406 cm⁻¹
3. 66.4346 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| C     | 0.755276  | -0.017351 | 0.305015  |
| C     | -0.293895 | 0.949410  | 0.317851  |
| C     | -0.335555 | 2.059728  | -0.697069 |
| C     | -1.359691 | 0.738737  | 1.182776  |
| O     | 0.858996  | -1.017304 | 1.016932  |
| O     | 1.722802  | 0.265667  | -0.625895 |
| C     | 2.859158  | -0.592891 | 0.397377  |
| C     | 3.875154  | -0.215453 | -0.408276 |
| H     | -1.085596 | 2.797474  | 0.305015  |
| H     | 0.621682  | 2.573527  | -0.789615 |
| H     | -0.603117 | 1.704139  | -1.698863 |
| H     | -2.012525 | 1.571061  | 1.407757  |
| H     | -1.223617 | 0.033252  | 1.988587  |
| H     | 2.539239  | -1.626672 | -0.542565 |
| H     | 3.277728  | -0.468018 | -1.659425 |
| H     | 4.756410  | -0.852089 | 0.316032  |
| H     | 4.187542  | 0.821325  | 0.273028  |
| H     | 3.448658  | -0.338100 | 1.391494  |
| C     | -2.107598 | -1.157766 | -1.157951 |
| H     | -1.11734  | -0.685367 | -1.157070 |
| H     | -2.568021 | -0.976985 | -2.128367 |
| H     | -1.972849 | -2.230950 | -1.027771 |
| S     | -3.078704 | -0.430999 | 0.174395  |

## 8_ethylmethacrylate_TS_5_reopt

### Datum Value

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -823.296732   |
| Datum | Value             |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.141832 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** *(Top 3 out of 63)*

1. -227.1311 cm\(^{-1}\)
2. 42.8469 cm\(^{-1}\)
3. 56.0697 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.647998 | 0.093444 | 0.669596 |
|-------|-----------|----------|----------|
| C     | 0.381499  | 1.019547 | 0.326184 |
| C     | 0.220383  | 1.955874 | -0.840758|
| C     | 1.599375  | 0.908364 | 0.984408 |
| O     | -0.611235 | -0.780542| 1.537285 |
| O     | -1.782155 | 0.254950 | -0.081622|
| C     | -2.865250 | -0.622693| 0.207765 |
| C     | -3.991888 | -0.288790| -0.742289|
| H     | 0.293740  | 1.441439 |-1.806119 |
| H     | -0.740538 | 2.471094 |-0.829710 |
| H     | 1.066505  | 2.712069 |-0.820504 |
| H     | 1.626077  | 0.341691 | 1.902971 |
| H     | 2.286262  | 1.742587 | 0.940581 |
| H     | -2.537881 | -1.656358| 0.087057 |
| H     | -3.171715 | -0.493987| 1.247047 |
| H     | -4.843679 | -0.941196| -0.553378|
| H     | -4.313143 | 0.744136 | -0.611413|
| H     | -3.676188 | -0.424863| -1.776263|
| C     | 1.852953  | -1.353064| -1.126122|
| H     | 0.885890  | -0.849230| -1.008158|
| H     | 1.740201  | -2.386753| -0.801203|
| H     | 2.112176  | -1.343851| -2.183987|
| S     | 3.074061  | -0.464259| -0.144058|

**8_ethylmethacrylate_TS_6**

| Datum | Value             |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296363 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.141501 |
### Datum | Value
--- | ---
Number of Imaginary Frequencies | 1

#### Frequencies (Top 3 out of 63)

1. -229.4294 cm⁻¹
2. 35.3037 cm⁻¹
3. 55.1186 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | -0.842406 | 0.595473 | 0.172133 |
| C    | 0.357153  | 1.066446 | -0.437191 |
| C    | 0.923976  | 2.363232 | 0.069435 |
| C    | 1.072220  | 0.286406 | -1.337977 |
| O    | -1.515518 | 1.205724 | 1.004713 |
| O    | -1.237599 | -0.648710 | -0.248475 |
| C    | -2.473270 | -1.139797 | 0.262539 |
| C    | -3.656840 | -0.579096 | -0.500245 |
| H    | 0.145404  | 3.110648 | 0.224818 |
| H    | 1.446293  | 2.244224 | 1.026736 |
| H    | 1.646327  | 2.765851 | -0.642102 |
| H    | 1.801131  | 0.779979 | -1.966908 |
| H    | 0.580051  | -0.557834 | -1.794535 |
| H    | -2.417454 | -2.221099 | 0.146277 |
| H    | -2.549101 | -0.904931 | 1.323050 |
| H    | -4.584404 | -1.009752 | -0.122300 |
| H    | -3.574671 | -0.817737 | -1.560536 |
| H    | -3.703780 | 0.502378 | -0.384860 |
| C    | 2.000888  | -0.949944 | 1.350394 |
| H    | 1.622431  | -1.929240 | 1.640996 |
| H    | 1.162647  | -0.242790 | 1.354743 |
| H    | 2.726538  | -0.619856 | 2.092532 |
| S    | 2.714576  | -0.963267 | -0.303896 |

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#### 8_ethylmethacrylate_TS_7_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296958 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.142366 |
| Number of Imaginary Frequencies | 1 |
Frequencies (Top 3 out of 63)

1.  -237.7303 cm⁻¹
2.   37.5553 cm⁻¹
3.   45.5261 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     |     |     |     |
|-----|-----|-----|-----|
| C   | -0.689340 | 1.039735 | 0.045878 |
| C   | 0.618640  | 1.147468 | -0.509066 |
| C   | 1.484863  | 2.273024 | -0.016537 |
| C   | 1.140258  | 0.155386 | -1.331443 |
| O   | -1.222060 | 1.848754 | 0.808448  |
| O   | -1.377201 | -0.078879| -0.342248 |
| C   | -2.687877 | -0.232642| 0.190456  |
| C   | -3.241769 | -1.538251| -0.331197 |
| H   | 2.335217  | 2.418026 | -0.684336 |
| H   | 0.933725  | 3.212463 | 0.040833  |
| H   | 1.889335  | 2.080901 | 0.984829  |
| H   | 2.012045  | 0.397686 | -1.924756 |
| H   | 0.459369  | -0.540757| -1.795202 |
| H   | -2.640947 | -0.230604| 1.280585  |
| H   | -3.309102 | 0.611303 | -0.113859 |
| H   | -4.247382 | -1.697779| 0.056312  |
| H   | -3.289026 | -1.529596| -1.419745 |
| H   | -2.615028 | -2.373133| -0.018505 |
| C   | 1.489782  | -1.173474| 1.440881  |
| H   | 2.223143  | -1.071139| 2.239520  |
| H   | 0.798921  | -1.975571| 1.699418  |
| H   | 0.921259  | -0.238323| 1.377812  |
| S   | 2.289702  | -1.453020| -0.149146 |

8_ethylmethacrylate_TS_8

| Datum                                              | Value         |
|----------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy              | -823.291618   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.138217   |
| Number of Imaginary Frequencies                    | 1             |

Frequencies (Top 3 out of 63)
1. -257.9744 cm⁻¹
2.  31.2376 cm⁻¹
3.  41.0854 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | -0.881701    | -0.284614    | 0.412432     |
| C       | 0.099659     | 0.745660     | 0.523856     |
| C       | -0.216277    | 2.150132     | 0.086880     |
| C       | 1.394819     | 0.369399     | 0.842590     |
| O       | -0.732685    | -1.487345    | 0.629138     |
| O       | -2.103423    | 0.186535     | 0.015669     |
| C       | -3.143658    | -0.777158    | -0.116223    |
| C       | -4.385496    | -0.050399    | -0.577579    |
| H       | -3.30505     | 2.236646     | -0.999607    |
| H       | -1.140525    | 2.523761     | 0.529422     |
| H       | 0.591139     | 2.821849     | 0.381631     |
| H       | 1.549122     | -0.601606    | 1.292430     |
| H       | 2.094801     | 1.134553     | 1.154800     |
| H       | -2.841881    | -1.541431    | -0.833749    |
| H       | -3.306243    | -1.271920    | 0.842496     |
| H       | -5.207260    | -0.755846    | -0.695260    |
| H       | -4.681805    | 0.706060     | 0.148483     |
| H       | -4.211177    | 0.438419     | -1.535689    |
| C       | 4.156642     | -0.579903    | 0.190739     |
| H       | 4.242845     | 0.179222     | 0.971442     |
| H       | 5.183693     | -0.618817    | -0.345080    |
| H       | 3.996832     | -1.544191    | 0.673678     |
| S       | 2.792868     | -0.171183    | -0.932476    |

8_ethylmethacrylate_TS_9_reopt2

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296624 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.141276 |
| Number of Imaginary Frequencies | 1 |

Frequencies (Top 3 out of 63)

1. -226.8158 cm⁻¹
2.  44.4284 cm⁻¹
3.  55.3154 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C    -0.755354  0.524530  0.551704
C     0.408123  1.205904  0.085987
C     0.420128  1.888974 -1.254880
C     1.579840  1.055104  0.816150
O    -0.867964 -0.141514  1.581767
O    -1.833456 -0.141514 -0.282558
C    -3.015886 -0.038663  0.047978
C    -2.929791 -1.477581 -0.420651
H     0.427608  1.178016 -2.089376
H    -0.445703  2.535960 -1.399017
H     1.316597  2.503401 -1.349538
H     1.499202  0.697290  1.831382
H     2.391845  1.746771  0.637136
H    -3.187521  0.010845  1.121948
H    -3.822658  0.486311 -0.461112
H    -3.859364 -2.002229 -0.198902
H    -2.760238 -1.517347 -1.496692
H    -2.112006 -1.990840  0.083189
C     1.498656 -1.624145 -0.748183
H     0.625828  0.961587  0.799212
H     1.209370 -2.524910 -0.207610
H     1.774800 -1.898206 -1.765536
S     2.832456 -0.738105  0.076940

ethylcrotonate_1

| Datum                                    | Value         |
|------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -385.096208   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.974384 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 48)

1.  62.3410 cm⁻¹
2.  89.9852 cm⁻¹
3.  120.9564 cm⁻¹
## M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -0.005849  | 0.380346   | -0.000001  |
| C       | 1.228916   | -0.430574  | -0.000002  |
| C       | 2.424209   | 0.150112   | 0.000004   |
| C       | 3.723952   | -0.574926  | 0.000003   |
| O       | -0.056631  | 1.588425   | 0.000013   |
| O       | -1.094641  | -0.394330  | -0.000019  |
| C       | -2.361818  | 0.282173   | -0.000023  |
| C       | -3.440869  | -0.771633  | 0.000024   |
| H       | 1.111378   | -1.506289  | -0.000010  |
| H       | 2.458753   | 1.235305   | 0.000008   |
| H       | 4.312208   | -0.293002  | 0.875035   |
| H       | 3.583743   | -1.653843  | 0.000001   |
| H       | 4.312208   | -0.293000  | -0.875029  |
| H       | -2.415690  | 0.919728   | 0.882068   |
| H       | -2.415713  | 0.919672   | -0.882152  |
| H       | -4.418596  | -0.292256  | 0.000019   |
| H       | -3.364684  | -1.401061  | -0.885397  |
| H       | -3.364664  | -1.401005  | 0.885482   |

## ethylcrotonate_2

| Datum                                         | Value   |
|-----------------------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy         | -385.095703 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.973593 |
| Number of Imaginary Frequencies               | 0       |

### Frequencies (Top 3 out of 48)

1. 57.9966 cm⁻¹
2. 90.3543 cm⁻¹
3. 128.1822 cm⁻¹

## M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 0.103620   | 0.146018   | -0.231043  |
| C       | -1.227323  | -0.465125  | -0.035237  |
| C       | -2.315458  | 0.291258   | 0.064474   |
| C       | -3.697361  | -0.225497  | 0.261317   |
### ethylcrotonate_3

| Datum                                                   | Value                      |
|---------------------------------------------------------|----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -385.095551                |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.973823                |
| Number of Imaginary Frequencies                        | 0                          |
| **Frequencies** (Top 3 out of 48)                       |                            |
| 1. 75.1575 cm$^{-1}$                                   |                            |
| 2. 86.7729 cm$^{-1}$                                   |                            |
| 3. 116.7384 cm$^{-1}$                                  |                            |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C  | 0.040576 | 0.898475 | -0.000000 |
|----|---------|---------|-----------|
| C  | -1.410827 | 0.632417 | -0.000001 |
| C  | -1.944138 | -0.585765 | 0.000001  |
| C  | -3.406939 | -0.865248 | 0.000000  |
| O  | 0.508672  | 2.014909 | -0.000001 |
| O  | 0.793492  | -0.203223 | 0.000002  |
| C  | 2.216138  | -0.004415 | 0.000003  |
| C  | 2.865173  | -1.365943 | -0.000003 |
| H  | -2.026988 | 1.522581 | -0.000003 |
| H  | -1.279549 | -1.442877 | 0.000002  |
| H  | -3.676715 | -1.459000 | 0.875119  |
| H  | -3.992539 | 0.051714 | -0.000002 |
| H  | -3.676714 | -1.459003 | -0.875118 |
**ethylcrotonate_4**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.095037   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.972999 |
| Number of Imaginary Frequencies            | 0             |

**Frequencies (Top 3 out of 48)**

1. 56.5065 cm⁻¹
2. 108.5598 cm⁻¹
3. 113.0448 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Datum | 0.151746 | 0.683455 | -0.105173 |
| C     | -1.311470| 0.639027 | 0.082298  |
| C     | -2.043215| -0.466339| -0.022715 |
| C     | -3.519350| -0.520060| 0.167220  |
| O     | 0.799001 | 1.700398 | 0.005118  |
| O     | 0.691175 | -0.498897| -0.412728 |
| C     | 2.117466 | -0.541731| -0.587284 |
| C     | 2.826839 | -0.639468| 0.745288  |
| H     | -1.759092| 1.595598 | 0.320300  |
| H     | -1.543367| -1.398591| -0.261882 |
| H     | -4.001397| -0.901777| -0.734484 |
| H     | -3.770388| -1.212809| 0.972363  |
| H     | -3.931172| 0.459400 | 0.401467  |
| H     | 2.291653 | -1.426259| -1.194441 |
| H     | 2.430675 | 0.340019 | -1.142506 |
| H     | 2.491363 | -1.519693| 1.292127  |
| H     | 3.900738 | -0.723845| 0.581810  |
| H     | 2.637483 | 0.246643 | 1.348327  |
**ethylcrotonate_5**

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -385.096208         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -384.974382         |
| Number of Imaginary Frequencies                                       | 0                   |

**Frequencies** (Top 3 out of 48)

1. 62.6219 cm⁻¹  
2. 90.2648 cm⁻¹  
3. 121.0773 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|       |       |       |       |
|-------|-------|-------|-------|
| C     | 0.005940 | 0.380069 | 0.000008 |
| C     | -1.229080 | -0.430568 | 0.000041 |
| C     | -2.424312 | 0.150313  | 0.000022 |
| C     | -3.724213 | -0.574642 | -0.000042 |
| O     | 0.057028  | 1.588103  | -0.000115 |
| O     | 1.094624  | -0.394736 | 0.000141 |
| C     | 2.361687  | 0.282223  | 0.000165 |
| C     | 3.441119  | -0.771291 | -0.000174 |
| H     | -1.111714 | -1.506299 | 0.000054 |
| H     | -2.458861 | 1.235505  | 0.000001 |
| H     | -4.312583 | -0.292644 | 0.874885 |
| H     | -4.312249 | -0.292883 | -0.875269 |
| H     | -3.584103 | -1.653592 | 0.000158 |
| H     | 2.415122  | 0.919979  | -0.881820 |
| H     | 2.415290  | 0.919575  | 0.882433 |
| H     | 4.418762  | -0.291727 | -0.000132 |
| H     | 3.365207  | -1.400954 | 0.885107 |
| H     | 3.365070  | -1.400523 | -0.885750 |

**ethylcrotonate_6**

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -385.087261         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -384.965131         |
**Datum** | **Value**
--- | ---
Number of Imaginary Frequencies | 0

**Frequencies** *(Top 3 out of 48)*

1. 42.2302 cm⁻¹
2. 88.2279 cm⁻¹
3. 137.4599 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C | -0.187096 | 0.970841 | -0.004797 |
| C | 0.757037 | -0.160441 | -0.170066 |
| C | 2.053508 | 0.020038 | 0.069987 |
| C | 3.094108 | -1.035055 | -0.059568 |
| O | 0.160070 | 2.081063 | 0.324520 |
| O | -1.491626 | 0.771046 | -0.237133 |
| C | -2.036563 | -0.511111 | -0.587120 |
| C | -2.195784 | -1.398682 | 0.627417 |
| H | 0.394667 | -1.128714 | -0.480836 |
| H | 2.380335 | 1.005718 | 0.384472 |
| H | 3.855410 | -0.723826 | -0.777140 |
| H | 3.605471 | -1.176141 | 0.894355 |
| H | 2.671356 | -1.984862 | -0.379967 |
| H | -3.005779 | -0.276119 | -1.019732 |
| H | -1.432787 | -0.974069 | -1.365726 |
| H | -2.820402 | -0.907010 | 1.371778 |
| H | -2.673645 | -2.333425 | 0.336603 |
| H | -1.233448 | -1.631964 | 1.081982 |

**ethylcrotonate_7**

**Datum** | **Value**
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -385.088063
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.966662
Number of Imaginary Frequencies | 0

**Frequencies** *(Top 3 out of 48)*
| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.305967            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy | -823.150045            |
| Number of Imaginary Frequencies            | 0                      |

**Frequencies (Top 3 out of 63)**

1. 33.3109 cm⁻¹  
2. 53.4500 cm⁻¹  
3. 71.7888 cm⁻¹
### ethylcrotonate_HEI_11

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.305113 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.148734 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

1. 39.6797 cm\(^{-1}\)
2. 52.3751 cm\(^{-1}\)
3. 64.2216 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.928666 | -0.908769 | -0.145831 |
|-------|----------|-----------|-----------|
| C     | 0.027810 | -0.095538 | 0.509971  |
| O     | -1.168831| -0.892872 | 0.960901  |
| O     | -2.232331| -0.089782 | -0.887749 |
| C     | -3.454731| -0.540882 | -0.332269 |
| C     | -4.044811| 0.472178  | 0.631761  |
**ethylcrotonate_HEI_12_reopt**

| Datum                                           | Value         |
|-------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -823.306455   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.14988    |

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 63)

1. 42.2425 cm⁻¹
2. 70.5028 cm⁻¹
3. 90.4644 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.381885| -0.518169| 0.672021 |
| C | -2.021624| 0.039902 | 1.938101 |
| O | 0.709076 | -2.032122| -0.658534|
| O | 2.257469 | -0.501902| -0.282430|
| C | 4.142204 | 0.912801 | -0.052320|
| H | -1.446390| -1.607052| 0.671829 |
| H | -1.984753| 1.131003 | 1.937818 |
| H | -3.062714| -0.266455| 2.035437 |
| H | -1.469174| -0.305557| 2.813615 |
| H | 2.089187 | 1.552714 | -0.214155|
| H | 2.485567 | 0.775853 | 1.321008 |
| H | 4.498212 | 1.865780 | 0.338207 |
| H | 4.719543 | 0.112999 | 0.411057 |
| H | 4.322929 | 0.891122 | -1.126790|
| C | -2.302108| 1.670970 | -0.857690|
| H | -2.715373| 2.016749 | -1.802417|
| H | -1.243144| 1.926466 | -0.817086|
| H | -2.829957| 2.160985 | -0.041867|
| S | -2.485799| -0.120009| -0.796282|
| H | 0.310618 | 0.869596 | 0.899836 |
### ethylcrotonate_HEI_14_reopt

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.303614 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.148205 |
| Number of Imaginary Frequencies | 0 |

#### Frequencies (Top 3 out of 63)

1. 27.6040 cm⁻¹
2. 46.5268 cm⁻¹
3. 57.7844 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.948669 | 1.113304 | -0.246348 |
|-------|----------|----------|-----------|
| C     | -0.386129| 1.191057 | 0.102179  |
| C     | -1.129353| 0.141279 | 0.828508  |
| C     | -2.288193| 0.785768 | 1.642986  |
| O     | 1.645886 | 1.949058 | -0.866512 |
| O     | 1.569067 | -0.065632| 0.175193  |
| C     | 2.942189 | -0.285601| -0.140604 |
| C     | 3.399406 | -1.548507| 0.385423  |
| H     | -0.465652| -0.426800| 1.480301  |
| H     | -2.845118| -0.078260| 2.154987  |
ethylcrotonate_HEI_1

| Datum                                         | Value            |
|-----------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy         | -823.305634      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.14866       |
| Number of Imaginary Frequencies               | 0                |

**Frequencies** (Top 3 out of 63)

1. 65.0236 cm⁻¹
2. 80.0896 cm⁻¹
3. 82.9878 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | -0.879636 | -1.049409 | 0.397043 |
| C    | 0.491532  | -1.145731 | 0.528670 |
| C    | 1.484577  | -0.561220 | -0.391153|
| C    | 2.718143  | -1.436930 | -0.584384|
| O    | -1.765165 | -1.50778 | 1.160427 |
| O    | -1.295206 | -0.386165 | -0.767021|
| C    | -2.666053 | -0.038275 | -0.843298|
| C    | -2.978252 | 1.204290  | -0.029576|
| H    | 1.031898  | -0.341681 | -1.356314|
| H    | 3.467631  | -0.955399 | -1.214589|
| H    | 3.176490  | -1.661617 | 0.380702 |
| H    | 2.429596  | -2.381270 | -1.046756|
| H    | -2.862854 | 0.140641  | -1.900892|
| H    | -3.282877 | -0.873217 | -0.513175|
## ethylcrotonate_HEI_2_reopt

| Datum                                                      | Value               |
|------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -823.305476         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.150072         |
| Number of Imaginary Frequencies                           | 0                   |

### Frequencies (Top 3 out of 63)

1. 30.0474 cm⁻¹
2. 51.5710 cm⁻¹
3. 60.5105 cm⁻¹

## M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C               | -0.788875 | -1.131876 | -0.487271 |
|-----------------|-----------|-----------|-----------|
| C               | 0.575301  | -1.267076 | -0.312869 |
| C               | 1.398633  | -0.439957 | 0.587050  |
| C               | 2.559055  | -1.202126 | 1.217113  |
| O               | -1.541915 | -1.763372 | -1.264653 |
| O               | -1.373991 | -0.169254 | 0.341073  |
| C               | -2.738351 | 0.122367  | 0.104006  |
| C               | -3.143619 | 1.224185  | 1.058814  |
| H               | 0.784293  | 0.008939  | 1.365334  |
| H               | 3.195585  | -0.553279 | 1.821037  |
| H               | 2.172719  | -1.999277 | 1.852817  |
| H               | 3.175820  | -1.659594 | 0.441148  |
| H               | -2.879065 | 0.436963  | -0.933308 |
| H               | -3.349975 | -0.769165 | 0.256605  |
| H               | -2.540166 | 2.116858  | 0.893602  |
| H               | -4.191723 | 1.484522  | 0.912156  |
| H               | -3.009774 | 0.905751  | 2.092716  |
| C               | 0.783342  | 1.830841  | -0.990897 |
| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.305034 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.148644 |

Number of Imaginary Frequencies

0

Frequencies (Top 3 out of 63)

1. 32.5518 cm⁻¹
2. 62.4814 cm⁻¹
3. 68.6626 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.954281 | -0.202177 | 0.832738 |
|-------|----------|-----------|----------|
| C     | -0.297217| -0.784737 | 0.829590 |
| C     | -1.242034| -0.775047 | -0.302116|
| C     | -2.024135| -2.076246 | -0.449610|
| O     | 1.793710 | -0.173629 | 1.762992 |
| O     | 1.293020 | 0.431579  | -0.372006|
| C     | 2.660958 | 0.751344  | -0.554897|
| C     | 3.475986 | -0.468373 | -0.944015|
| H     | -0.720086| -0.549028 | -1.230149|
| H     | -2.765693| -2.020111 | -1.248427|
| H     | -1.337679| -2.894305 | -0.669551|
| H     | -2.542496| -2.312927 | 0.481571 |
| H     | 2.681810 | 1.494009  | -1.353093|
| H     | 3.063352 | 1.204470  | 0.350277 |
| H     | 3.083712 | -0.915033 | -1.858085|
| H     | 4.517814 | -0.194449 | -1.114788|
| H     | 3.438875 | -1.210561 | -0.147349|
| C     | -1.556700| 2.016809  | 0.033250 |
| H     | -2.208969| 2.845070  | 0.301749 |
| H     | -1.015203| 2.261933  | -0.878279|
| H     | -0.843938| 1.834635  | 0.836538 |
**ethylcrotonate_HEI_4**

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.304432 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.148569 |

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 63)

1. 32.9298 cm$^{-1}$
2. 41.1005 cm$^{-1}$
3. 73.6421 cm$^{-1}$

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 1.229621 | 0.706873 | -0.513107 |
| C   | -0.017060 | 1.225520 | -0.227303 |
| C   | -1.107124 | 0.489875 | 0.458436 |
| C   | -2.015389 | 1.405585 | 1.268140 |
| O   | 2.189146  | 1.262265 | -1.096299 |
| O   | 1.399707  | -0.616272 | -0.082872 |
| C   | 2.721560  | -1.125963 | -0.099052 |
| C   | 3.526935  | -0.643718 | 1.093312 |
| H   | -0.700754 | -0.292176 | 1.100524 |
| H   | -1.440224 | 1.879334 | 2.065931 |
| H   | -2.422907 | 2.191098 | 0.629186 |
| H   | -2.847692 | 0.868608 | 1.723370 |
| H   | 2.614865  | -2.210867 | -0.072330 |
| H   | 3.216716  | -0.849853 | -1.029116 |
| H   | 3.036972  | -0.927262 | 2.025286 |
| H   | 4.525392  | -1.082700 | 1.082915 |
| H   | 3.624337  | 0.440858 | 1.063604 |
| C   | -3.290111 | -1.355626 | 0.210146 |
| H   | -4.074998 | -0.715713 | 0.607442 |
| H   | -2.767517 | -1.842510 | 1.033306 |
| H   | -3.744252 | -2.121442 | -0.415436 |
| S   | -2.112127 | -0.434004 | -0.808327 |
| H   | -0.227327 | 2.223467 | -0.591522 |
ethylcrotonate_HEI_5_reopt

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.306753    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.150531 |
| Number of Imaginary Frequencies            | 0              |

**Frequencies** (Top 3 out of 63)

1. 43.8838 cm⁻¹
2. 57.4572 cm⁻¹
3. 75.8027 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | -0.880384 | -0.653758 | 0.261636 |
| C   | 0.296865  | -0.898316 | -0.412076 |
| C   | 1.611412  | -0.695674 | 0.222122  |
| C   | 2.637962  | -1.769344 | -0.122601 |
| O   | -1.052322 | -0.242944 | 1.431463  |
| O   | -2.022143 | -0.957159 | -0.503253 |
| C   | -3.236697 | -0.370520 | -0.070919 |
| C   | -3.301649 | 1.105606  | -0.418991 |
| H   | 1.488393  | -0.629422 | 1.303064  |
| H   | 3.616203  | -1.555308 | 0.311448  |
| H   | 2.297307  | -2.735982 | 0.249234  |
| H   | 2.754440  | -1.847160 | -1.205245 |
| H   | -4.025400 | -0.919044 | -0.586700 |
| H   | -3.362873 | -0.513436 | 1.002041  |
| H   | -4.259013 | 1.530397  | -0.114842 |
| H   | -2.505190 | 1.644685  | 0.093934  |
| H   | -3.186635 | 1.250534  | -1.493676 |
| C   | 1.147730  | 2.090259  | 0.165720  |
| H   | 1.048727  | 2.204902  | 1.243517  |
| H   | 0.206922  | 1.726964  | -0.247401 |
| H   | 1.398602  | 3.051217  | -0.278161 |
| S   | 2.450998  | 0.922230  | -0.250312 |
| H   | 0.256831  | -1.212723 | -1.447251 |

ethylcrotonate_HEI_6
| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.306617 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.151889 |

Number of Imaginary Frequencies

0

**Frequencies** (Top 3 out of 63)

1. 30.8699 cm⁻¹
2. 43.3354 cm⁻¹
3. 57.3077 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

```
C       0.823678  -0.205695  0.359394
C      -0.256282  -0.757949 -0.299698
C      -1.611335  -0.750394  0.275389
C      -2.392504  -2.037274  0.031195
O       0.872757   0.336714  1.486566
O       2.015639  -0.302344 -0.372281
C       3.179860   0.212379  0.245840
C       4.339917  -0.008645 -0.700333
H      -1.556049  -0.543354  1.344198
H      -1.889406  -2.871249  0.521063
H      -3.413900  -1.975565  0.410921
H      -2.438369  -2.253434 -1.037923
H       3.054585   1.275977  0.461508
H       3.356012  -0.291616  1.198734
H       4.168914   0.505887 -1.645956
H       5.261670   0.374080 -0.262492
H       4.471987  -1.070871 -0.906121
C      -1.707722   2.050834 -0.099584
H      -1.680571   2.302774  0.958854
H      -0.697086   1.841381 -0.448944
H      -2.123280   2.886756 -0.658081
S       2.735153   0.605616 -0.401907
H      -0.112902  -1.165117  1.292740
```

**ethylcrotonate_HEI_7**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.306541 |
Datum | Value
---|---
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.149716

Number of Imaginary Frequencies | 0

**Frequencies (Top 3 out of 63)**

1. 42.0942 cm⁻¹
2. 72.5037 cm⁻¹
3. 81.2184 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C  | 0.905540 | 0.081508 | 0.039042 |
| C  | -0.169801 | -0.599580 | -0.490426 |
| C  | -1.412432 | -0.808878 | 0.273166 |
| C  | -2.030701 | -2.189220 | 0.078382 |
| O  | 1.051609 | 0.561871 | 1.185758 |
| O  | 1.958024 | 0.241778 | -0.880324 |
| C  | 3.223170 | 0.570661 | -0.335006 |
| C  | 3.900861 | -0.638784 | 0.282783 |
| H  | -1.224436 | -0.629901 | 1.331836 |
| H  | -2.980817 | -2.290771 | 0.605818 |
| H  | -2.207042 | -2.377636 | -0.982376 |
| H  | -1.345657 | -2.953475 | 0.446169 |
| H  | 3.811362 | 0.952054 | -1.170222 |
| H  | 3.117321 | 1.364237 | 0.404092 |
| H  | 4.887918 | -0.372586 | 0.662803 |
| H  | 3.302784 | -1.019462 | 1.110332 |
| H  | 4.019254 | -1.430966 | -0.457084 |
| C  | -1.949645 | 1.957022 | 0.062476 |
| H  | -1.807193 | 2.181487 | 1.117961 |
| H  | -0.980477 | 1.904573 | -0.432582 |
| H  | -2.552619 | 2.739222 | -0.393488 |
| S  | -2.799653 | 0.387714 | -0.164409 |
| H  | -0.124965 | -0.935831 | -1.518691 |

**ethylcrotonate_HEI_8**

Datum | Value
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.305817
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.15029
### Number of Imaginary Frequencies

| Datum                  | Value |
|------------------------|-------|
| Number of Imaginary Frequencies | 0     |

### Frequencies (Top 3 out of 63)

| Rank | Frequency   |
|------|-------------|
| 1    | 28.1445 cm$^{-1}$ |
| 2    | 46.9717 cm$^{-1}$ |
| 3    | 55.4236 cm$^{-1}$ |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -1.135004 | -0.472706 | 0.319501  |
| C    | -0.021000 | -0.888428 | -0.375305 |
| C    | 1.347565  | -0.675866 | 0.152261  |
| C    | 2.313216  | -1.792693 | -0.219380 |
| O    | -1.200108 | 0.131211  | 1.414137  |
| O    | -2.341620 | -0.828168 | -0.309888 |
| C    | -3.491463 | -0.104349 | 0.090847  |
| C    | -3.512307 | 1.290621  | -0.507227 |
| H    | 1.314793  | -0.553578 | 1.236599  |
| H    | 2.342781  | -1.917795 | -1.303248 |
| H    | 3.327372  | -1.598948 | 0.130474  |
| H    | 1.975113  | -2.731690 | 0.228877  |
| H    | -4.342013 | -0.685482 | -0.266580 |
| H    | -3.542302 | -0.052532 | 1.177994  |
| H    | -3.481456 | 1.240892  | -1.595995 |
| H    | -4.418468 | 1.821098  | -0.212359 |
| H    | -2.649968 | 1.858819  | -0.158998 |
| C    | 3.570293  | 1.114051  | 0.393814  |
| H    | 3.901167  | 2.146034  | 0.296146  |
| H    | 3.436407  | 0.889122  | 1.451718  |
| H    | 4.333190  | 0.459542  | -0.022060 |
| S    | 1.990701  | 0.953206  | -0.473933 |
| H    | -0.141809 | -1.374902 | -1.333914 |

### ethylcrotonate_HEI_9_reopt

| Datum                          | Value     |
|--------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.306125 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.150664 |
| Number of Imaginary Frequencies | 0         |
**Frequencies** (Top 3 out of 63)

1. 44.4110 cm⁻¹
2. 48.1958 cm⁻¹
3. 64.6996 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          |       |       |       |
|----------|-------|-------|-------|
| C        | 1.023152 | -0.004562 | 0.306510 |
| C        | -0.008208 | 0.773791 | -0.176525 |
| C        | -1.398108 | 0.600561 | 0.303849 |
| C        | -2.205596 | 1.890552 | 0.267037 |
| O        | 0.985312 | -0.910438 | 1.169346 |
| O        | 2.263212 | 0.302852 | -0.266955 |
| C        | 3.376858 | -0.428545 | 0.211074 |
| C        | 4.600689 | 0.055558 | -0.535568 |
| H        | -1.400101 | 0.187000 | 1.314668 |
| H        | -2.204015 | 2.305025 | -0.742694 |
| H        | -3.240989 | 1.741223 | 0.573706 |
| H        | -1.754862 | 2.624891 | 0.937385 |
| H        | 3.494208 | -0.277500 | 1.286809 |
| H        | 3.223230 | -1.497955 | 0.051092 |
| H        | 5.485918 | -0.483060 | -0.197874 |
| H        | 4.487142 | -0.107452 | -1.607354 |
| H        | 4.760054 | 1.120234 | -0.364933 |
| C        | -3.829137 | -0.903886 | 0.133816 |
| H        | -3.661881 | -0.990741 | 1.207314 |
| H        | -4.288618 | -1.823647 | -0.222416 |
| H        | -4.505797 | -0.074643 | -0.060923 |
| S        | -2.245836 | -0.704411 | -0.719316 |
| H        | 0.192997 | 1.507076 | -0.946003 |

**ethylcrotonate_TS_10_UNCON_m062x**

| Datum                              | Value       |
|------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.295752 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139981 |
| Number of Imaginary Frequencies    | 1           |

**Frequencies** (Top 3 out of 63)
1. -175.0856 cm\(^{-1}\)
2. 36.8416 cm\(^{-1}\)
3. 62.3980 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|       |          |          |          |
|-------|----------|----------|----------|
| C     | 0.820003 | 0.204286 | 0.900024 |
| C     | -0.005793| 0.866258 | -0.068900|
| C     | -1.313028| 1.159377 | 0.233330 |
| C     | -2.107029| 2.120710 | -0.599619|
| O     | 0.472796 | -0.113708| 2.031230 |
| O     | 2.107889 | -0.107369| 0.573120 |
| C     | 2.624683 | 0.179513 | -0.724468|
| C     | 4.056627 | -0.30311 | -0.760970|
| H     | -1.603485| 1.070484 | 1.270330 |
| H     | -1.835681| 3.144347 | -0.324473|
| H     | -1.893516| 1.989499 | -1.659942|
| H     | -3.176638| 2.000887 | -0.442722|
| H     | 2.570581 | 1.253339 | -0.913524|
| H     | 2.024600 | -0.333674| -1.479028|
| H     | 4.488667 | -0.101557| -1.740893|
| H     | 4.652561 | 0.214918 | -0.008705|
| H     | 4.106079 | -1.371829| -0.571482|
| C     | -1.360815| -2.022611| -0.441838|
| H     | -1.485003| -2.618465| -1.345475|
| H     | -1.260768| -2.699303| 0.406914 |
| H     | -0.422742| -1.460676| -0.539955|
| S     | -2.716644| -0.851919| -0.228139|
| H     | 0.368276 | 1.068037 | -1.060978|

**ethylcrotonate_TS_11_UNCON_m062x_reopt**

| Datum                                           | Value       |
|-------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -823.295752 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139982 |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 63)

1. -175.1679 cm\(^{-1}\)
2. 36.8576 cm\(^{-1}\)
3. 62.4158 cm\(^{-1}\)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.820027 | 0.204374 | 0.899973 |
| C | -0.005811| 0.866153 | -0.069013|
| C | -1.313092| 1.159233 | 0.233248 |
| C | -2.107047| 2.120701 | -0.599599|
| O | 0.472869 | -0.113459| 2.031251 |
| O | 2.107929 | -0.107287| 0.573104 |
| C | 2.624702 | 0.179437 | -0.724521|
| C | 4.056655 | -0.300365| -0.760967|
| H | -1.603416| 1.070454 | 1.270297 |
| H | -1.835595| 3.144292 | -0.324384|
| H | -1.893595| 1.989555 | -1.659942|
| H | -3.176664| 2.000970 | -0.442666|
| H | 2.570573 | 1.253237 | -0.913718|
| H | 2.024624 | -0.333859| -1.479014|
| H | 4.488693 | -0.101737| -1.740916|
| H | 4.652582 | 0.214972 | -0.008770|
| H | 4.106123 | -1.371857| -0.571331|
| C | -1.360934| -2.022763| -0.441525|
| H | -1.484885| -2.618452| -1.345304|
| H | -1.261359| -2.699592| 0.407169 |
| H | -0.422733| -1.460964| -0.539179|
| S | -2.716622| -0.851847| -0.228222|
| H | 0.368221 | 1.067885 | -1.061114|

ethylecrotonate_TS_12_UNCON_m062x_reopt

| Datum                                                                 | Value          |
|-----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -823.294376    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -823.138582    |
| Number of Imaginary Frequencies                                       | 1              |
| **Frequencies** (Top 3 out of 63)                                     |                |
| 1. -182.5303 cm⁻¹                                                     |                |
| 2. 38.0472 cm⁻¹                                                       |                |
| 3. 48.3092 cm⁻¹                                                       |                |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C   0.901368   -0.374582    0.844322
C   0.223690    0.638598    0.089497
C  -0.999934    1.104353    0.512344
C  -1.570969    2.380784   -0.031310
O   0.504458   -0.853166    1.901127
O   2.088268   -0.878382    0.391710
C   2.669261   -0.453010   -0.839454
C   3.434955     0.846297   -0.691946
H  -1.295544    0.840858    1.517728
H  -1.085282    3.229906    0.458744
H  -1.393668    2.464308   -1.103099
H  -2.641186    2.452637    0.150166
H   1.903878   -0.389172   -1.613391
H   3.347941   -1.258153   -1.116230
H   3.905413    1.108596   -1.639458
H   2.777074    1.661681   -0.395120
H   4.214833    0.737878    0.061198
C  -1.708036   -1.747879   -0.846020
H  -0.669546   -1.391728   -0.854053
H  -1.951237   -2.081971   -1.854006
H  -1.766124   -2.604198   -0.174091
S  -2.776261   -0.392584   -0.322582
H   0.629818    0.995722   -0.844367

ethylcrotonate_TS_1_UNCON_m062x

| Datum                                         | Value          |
|-----------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy         | -823.298556    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.142803    |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 63)

1. -208.4252 cm⁻¹
2.  35.0037 cm⁻¹
3.  52.7533 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### ethylcrotonate_TS_2_UNCON_m062x

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.298791
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.143494

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 63)

1. -209.7581 cm⁻¹
2. 46.8149 cm⁻¹
3. 59.3251 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.921355 | -1.010606 | 0.433737 |
|-------|-----------|-----------|----------|
| C     | 0.479507  | -1.248238 | 0.544244 |
| C     | 1.407937  | -0.906711 | -0.424753|
| C     | 2.766347  | -1.552458 | -0.420401|
| O     | -1.771656 | -1.305846 | 1.272043 |
| O     | -1.288390 | -0.415510 | -0.740743|
| C     | -2.667170 | -0.086914 | -0.895884|
| C     | -3.006269 | 1.217416  | -0.203435|
| H     | 1.016942  | -0.668083 | -1.403324|
| H     | 3.473013  | -1.010644 | -1.046779|
| H     | 3.168475  | -1.602803 | 0.591190 |
| H     | 2.684820  | -2.573481 | -0.803609|
| H     | -3.281328 | -0.901260 | -0.515490|
| H     | -2.819625 | -0.005477 | -1.970825|
| H     | -4.057005 | 1.462647  | -0.359686|
| H     | -2.823231 | 1.135840  | 0.866963 |
| H     | -2.399171 | 2.029627  | -0.602532|
| C     | 0.758204  | 1.946892  | 0.801144 |
| H     | 0.189934  | 1.086394  | 1.175203 |
| H     | 0.088416  | 2.566665  | 0.205951 |
| H     | 1.905219  | 2.525000  | 1.660643 |
| S     | 2.152253  | 1.327417  | -0.158992|
| H     | 0.804661  | -1.668541 | 1.487852 |
ethylcrotonate_TS_3_UNCON_m062x_reopt

| Datum                                                                 | Value          |
|-----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -823.298097    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -823.142494    |
| Number of Imaginary Frequencies                                       | 1              |

**Frequencies (Top 3 out of 63)**

1. -209.3744 cm\(^{-1}\)
2. 38.5523 cm\(^{-1}\)
3. 56.2011 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 0.977688 | 0.355824 | 0.738795 |
| C   | -0.296065 | 0.994541 | 0.757329 |
| C   | -1.151942 | 1.059736 | -0.329865 |
| C   | -2.252920 | 2.084339 | -0.353356 |
| O   | 1.762869  | 0.282339 | 1.682680 |
| O   | 1.296169  | -0.202482 | -0.467379 |
| C   | 2.582971  | -0.805882 | -0.582680 |
ethylcrotonate_TS_4_UNCON_m062x

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.29963 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.144172 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 63)

1. -207.8675 cm⁻¹
2.  34.4622 cm⁻¹
3.  50.7735 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   |  0.218718 |
|-----|-----------|
| C   | -0.381000 |
| C   | -0.436898 |
| C   |  0.232321 |
| C   | -0.308623 |
| O   |  1.387969 |
| O   | -0.609977 |
| C   | -0.084229 |
| C   | -0.150375 |
| H   |  1.310924 |
| H   | -0.118311 |
| H   | -1.386553 |
### ethylcrotonate_TS_5_UNCON_m062x

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -823.299725    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -823.144422    |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 63)

1. -200.9380 cm⁻¹
2. 45.8099 cm⁻¹
3. 67.8415 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | -0.827004 | -0.389511 | 0.379558 |
| C   | 0.263275  | -0.936306 | -0.356068|
| C   | 1.514302  | -1.065205 | 0.221478 |
| C   | 2.536470  | -1.988580 | -0.380786|
| O   | -0.819275 | 0.000682  | 1.544292 |
| O   | -1.979272 | -0.329951 | -0.355606|
| C   | -3.125209 | 0.199431  | 0.304918 |
| C   | -4.271490 | 0.179908  | -0.679069|
| H   | 1.541761  | -0.982745 | 1.299709 |
| H   | 2.559934  | -1.885915 | -1.465419|
| H   | 3.535271  | -1.793903 | 0.005889 |
| H   | 2.275304  | -3.023894 | -0.143997|
| H   | -2.911501 | 1.213687  | 0.645472 |
| H   | -3.348082 | -0.404002 | 1.186128 |
| H   | -5.170598 | 0.577803  | -0.210003|
ethylcrotonate_TS_6_UNCON_m062x

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.299209|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -823.143711|

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 63)

1. -202.2296 cm⁻¹
2. 35.9166 cm⁻¹
3. 50.0899 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C                  | 0.920147 | 0.159769 | 0.064137 |
|-------------------|---------|---------|---------|
| C                  | -0.196744 | 0.831469 | -0.511285 |
| C                  | -1.325021 | 1.106066 | 0.241279 |
| C                  | -2.307370 | 2.147561 | -0.217347 |
| O                  | 1.034007 | -0.235945 | 1.220895 |
| O                  | 1.936648 | -0.025721 | -0.835670 |
| C                  | 3.130166 | -0.634367 | -0.347541 |
| C                  | 4.026007 | 0.371711 | 0.346666 |
| H                  | -1.204798 | 1.021053 | 1.312977 |
| H                  | -2.502323 | 2.052990 | -1.285278 |
| H                  | -3.254282 | 2.072530 | 0.314223 |
| H                  | -1.892629 | 3.143154 | -0.035601 |
| H                  | 3.620323 | -1.043906 | -1.229246 |
| H                  | 2.873429 | -1.453259 | 0.322483 |
| H                  | 4.951539 | -0.108605 | 0.664762 |
| H                  | 4.277827 | 1.188330 | -0.329706 |
| C                  | 3.528285 | 0.781330 | 1.224003 |
| C                  | -1.684542 | -1.989964 | -0.385498 |
| H                  | -0.798186 | -1.478091 | -0.781137 |
|        | Value 1 | Value 2 | Value 3 |
|--------|---------|---------|---------|
| H      | -2.134649 | -2.557576 | -1.198809 |
| H      | -1.361293 | -2.686624 | 0.387549 |
| S      | -2.817599 | -0.740552 | 0.248653 |
| H      | -0.162759 | 1.057362  | -1.568995 |

**ethylcrotonate_TS_7_UNCON_m062x**

| Datum                                              | Value     |
|----------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy              | -823.294503 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139634 |
| Number of Imaginary Frequencies                    | 1         |

**Frequencies** (Top 3 out of 63)

1. -244.7558 cm⁻¹
2.  41.5160 cm⁻¹
3.  57.9074 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        | Value 1   | Value 2   | Value 3   |
|--------|-----------|-----------|-----------|
| C      | 1.190146  | 0.437151  | 0.292141  |
| C      | 0.076968  | 1.113936  | -0.282241 |
| C      | -1.203757 | 0.920649  | 0.200965  |
| C      | -2.290482 | 1.890499  | -0.169844 |
| O      | 1.179361  | -0.340534 | 1.241864  |
| O      | 2.366870  | 0.750570  | -0.334902 |
| C      | 3.546785  | 0.108777  | 0.143604  |
| C      | 3.700952  | -1.280316 | -0.442083 |
| H      | -1.286067 | 0.470646  | 1.183738  |
| H      | -2.137488 | 2.825321  | 0.377766  |
| H      | -2.256091 | 2.117647  | -1.235034 |
| H      | -3.280585 | 1.513458  | 0.075084  |
| H      | 3.525285  | 0.071988  | 1.231590  |
| H      | 4.366766  | 0.753148  | -0.169188 |
| H      | 3.723455  | -1.234264 | -1.530704 |
| H      | 4.632234  | -1.730482 | -0.097831 |
| H      | 2.872563  | -1.915689 | -0.133611 |
| C      | -3.609178 | -1.094446 | 0.555893  |
| H      | -3.334335 | -0.510805 | 1.441827  |
| H      | -3.825589 | -2.108551 | 0.884812  |
| H      | -4.509918 | -0.663828 | 0.133742  |
| S      | -2.226423 | -1.072950 | -0.627995 |
| H      | 0.250892  | 1.720823  | -1.160590 |
ethylocrotonate_TS_8_UNCON_m062x

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.294976 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140441 |
| Number of Imaginary Frequencies | 1 |

**Frequencies (Top 3 out of 63)**

1. -244.0623 cm⁻¹
2. 27.8887 cm⁻¹
3. 65.6806 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C     | C     | C     | O     | O     | C     | C     | O     | O     | C     | C     | C     | H     | H     | H     | H     | H     | H     | H     | S     | H     | H     | H     | S     | H     | H     | H     | H     | H     | H     | H     | H     |
|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|   | 1.101814 | 0.054690 | 0.337928 | 0.089042 | 0.941408 | -0.126156 | -1.213634 | 0.836682 | 0.324864 | -2.167023 | 1.977677 | 0.105373 | 0.981933 | -0.851565 | 2.318817 | 0.305503 | -0.233365 | 3.401835 | -0.514164 | 0.197256 | 4.639964 | -0.064389 | -0.542558 | -1.367100 | 0.259257 | 1.229445 | -1.913287 | 2.791534 | 0.791239 | -2.082374 | 2.359440 | -0.911756 | -3.200554 | 1.692928 | 0.287189 | 3.526003 | -0.413996 | 1.276608 | 3.172148 | -1.559812 | -0.012250 | 5.494138 | -0.668328 | -0.238620 | 4.506535 | -0.172993 | -1.618423 | 4.861065 | 0.979907 | -0.324164 | -3.859728 | -0.885398 | 0.353060 | -3.548326 | -0.485704 | 1.322736 | -4.228156 | -1.897385 | 0.516632 | -4.686736 | -0.275284 | -0.010166 | -2.452691 | -0.872950 | -0.793521 | 0.350083 | 1.647083 | -0.903298 |
# ethylcrotonate_TS_9_UNCON_m062x

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.294536   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139461   |

Number of Imaginary Frequencies

1

**Frequencies** (Top 3 out of 63)

1. -249.3636 cm\(^{-1}\)
2. 49.4722 cm\(^{-1}\)
3. 57.4567 cm\(^{-1}\)

# M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C         | 1.172701 | 0.024252 | -0.029577 |
|-----------|----------|----------|-----------|
| C         | 0.115476 | 0.920727 | -0.353435 |
| C         | -1.115164| 0.830125 | 0.271335  |
| C         | -2.073538| 1.985329 | 0.193060  |
| O         | 1.157400 | -0.874350| 0.806867  |
| O         | 2.295990 | 0.254899 | -0.779194 |
| C         | 3.443071 | -0.540828| -0.489578 |
| C         | 4.213038 | 0.002793 | 0.697093  |
| H         | -1.148613| 0.250176 | 1.186500  |
| H         | -1.716714| 2.789360 | 0.843831  |
| H         | -2.124021| 2.375764 | -0.823027 |
| H         | -3.076223| 1.711789 | 0.512866  |
| H         | 4.049307 | -0.503432| -1.393140 |
| H         | 3.136696 | -1.571036| -0.315688 |
| H         | 3.598929 | -0.030450| 1.595373  |
| H         | 5.109417 | -0.593996| 0.866786  |
| H         | 4.515996 | 1.033799 | 0.514998  |
| C         | -3.739957| -0.870870| 0.674416  |
| H         | -3.281176| -0.490696| 1.591949  |
| H         | -4.090527| -1.882451| 0.875218  |
| H         | -4.605544| -0.247558| 0.450134  |
| S         | -2.522719| -0.851098| -0.671653 |
| H         | 0.275090 | 1.622834 | -1.160606 |

# n-propylacrylate_10

| Datum | Value |
|-------|-------|
|       |       |
| Datum                                      | Value      |
|--------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.087549|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.964642|
| Number of Imaginary Frequencies            | 0          |

**Frequencies (Top 3 out of 48)**

1. 40.4598 cm⁻¹
2. 82.5976 cm⁻¹
3. 109.8485 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -0.845880 | 0.537374 | -0.243512 |
| C | -2.192323 | 0.218306 | 0.290927  |
| C | -2.638915 | -1.014935 | 0.480115 |
| O | -0.450649 | 1.671718 | -0.373987 |
| O | -0.136692 | -0.545876 | -0.559278 |
| C | 1.205605  | -0.373423 | -1.048135 |
| C | 2.206149  | -0.662527 | 0.052879 |
| C | 2.103631  | 0.305497 | 1.224095 |
| H | -2.790025 | 1.088540 | 0.525629 |
| H | -3.628547 | -1.192013 | 0.878165 |
| H | -2.028897 | -1.875888 | 0.243824 |
| H | 1.305874  | -1.083067 | -1.866258 |
| H | 1.316677  | 0.638805 | -1.431139 |
| H | 2.064834  | -1.688816 | 0.397138 |
| H | 3.201489  | -0.611797 | -0.393001 |
| H | 2.251687  | 1.333801 | 0.893272 |
| H | 2.852540  | 0.077369 | 1.981263 |
| H | 1.123493  | 0.244586 | 1.699012 |

**n-propylacrylate_11**

| Datum                                      | Value      |
|--------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.079724|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.956632|
| Number of Imaginary Frequencies            | 0          |

**Frequencies (Top 3 out of 48)**
1. 38.0769 cm\(^{-1}\)
2. 75.8175 cm\(^{-1}\)
3. 103.1965 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 0.961983  | -0.615594 | 0.084011  |
| C       | 1.450336  | 0.788797  | 0.188927  |
| C       | 2.599476  | 1.124848  | -0.380141 |
| O       | 1.619971  | -1.498690 | -0.410062 |
| O       | -0.246117 | -0.924630 | 0.565897  |
| C       | -1.160555 | 0.059159  | 1.079769  |
| C       | -1.829655 | 0.847889  | -0.029001 |
| C       | -2.602221 | -0.041899 | -0.994507 |
| H       | 0.867620  | 1.522432  | 0.723651  |
| H       | 2.978367  | 2.135351  | -0.319291 |
| H       | 3.182502  | 0.391746  | -0.921572 |
| H       | -1.898267 | -0.530367 | 1.621042  |
| H       | -0.654559 | 0.700068  | 1.799539  |
| H       | -1.081675 | 1.430343  | -0.571279 |
| H       | -2.501836 | 1.565184  | 0.445703  |
| H       | -3.091789 | 0.553771  | -1.763241 |
| H       | -1.938551 | -0.750585 | -1.489177 |
| H       | -3.368825 | -0.610589 | -0.466402 |

**n-propylacrylate\_12**

| Datum                                           | Value         |
|------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -385.080544   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.958206   |
| Number of Imaginary Frequencies                 | 0             |

**Frequencies** (Top 3 out of 48)

1. 21.0228 cm\(^{-1}\)
2. 81.4392 cm\(^{-1}\)
3. 110.4477 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
### n-propylacrylate_13

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -385.079839 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.956947 |

Number of Imaginary Frequencies: 0

**Frequencies (Top 3 out of 48)**

1. 40.8245 cm⁻¹
2. 69.3681 cm⁻¹
3. 81.9272 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | X       | Y       | Z       |
|-------|---------|---------|---------|
| 1.222904 | -0.549258 | -0.015991 |
| 1.245744 | 0.922285 | 0.222640 |
| 2.367374 | 1.599321 | 0.020238 |
| 2.191828 | -1.163774 | -0.390193 |
| 0.090861 | -1.227692 | 0.198411 |
| -1.132445 | -0.596058 | 0.604984 |
| -1.850653 | 0.053608 | -0.560364 |
n-propylacrylate_14

| Datum                                      | Value   |
|--------------------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.080361 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.958587 |
| Number of Imaginary Frequencies            | 0       |

**Frequencies (Top 3 out of 48)**

1. 10.9342 cm⁻¹
2. 79.7609 cm⁻¹
3. 127.4168 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 1.266279 | -0.531540 | 0.000003 |
| C   | 1.705502 | 0.891795  | 0.000007 |
| C   | 3.000161 | 1.177090  | -0.000008 |
| O   | 2.039039 | -1.458490 | -0.000002 |
| O   | -0.043571 | -0.798380 | 0.000005 |
| C   | -1.039355 | 0.237007  | 0.000005 |
| C   | -2.393824 | -0.434287 | -0.000005 |
| C   | -3.512798 | 0.599060  | -0.000004 |
| H   | 0.967036 | 1.678376  | 0.000024 |
| H   | 3.347031 | 2.200852  | -0.000005 |
| H   | 3.739151 | 0.386797  | -0.000024 |
| H   | -0.919603 | 0.858490  | -0.888988 |
| H   | -0.919611 | 0.858480  | 0.889007 |
| H   | -2.468110 | -1.076391 | -0.878868 |
| H   | -2.468117 | -1.076402 | 0.878850 |
| H   | -4.487294 | 0.114240  | -0.000010 |
### n-propylacrylate_15

| Datum                                                      | Value               |
|------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -385.078628         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -384.955611         |
| Number of Imaginary Frequencies                            | 0                   |

#### Frequencies (Top 3 out of 48)

1. 31.0134 cm⁻¹  
2. 66.5485 cm⁻¹  
3. 124.7589 cm⁻¹  

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C     | -0.97709 | -0.58951 | -0.16372 |       |       |       |       |       |       |       |
| C     | -1.245325 | 0.801965 | 0.297730 |       |       |       |       |       |       |       |
| C     | -2.491586 | 1.252525 | 0.325256 |       |       |       |       |       |       |       |
| O     | -1.793280 | -1.239041 | -0.771356 |       |       |       |       |       |       |       |
| O     | 0.210143 | -1.148199 | 0.086520 |       |       |       |       |       |       |       |
| C     | 1.231560 | -0.570877 | 0.917466 |       |       |       |       |       |       |       |
| C     | 2.364931 | -0.032724 | 0.067593 |       |       |       |       |       |       |       |
| C     | 1.978875 | 1.167051 | -0.786589 |       |       |       |       |       |       |       |
| H     | -0.424579 | 1.436806 | 0.591256 |       |       |       |       |       |       |       |
| H     | -2.713792 | 2.261019 | 0.644626 |       |       |       |       |       |       |       |
| H     | -3.316142 | 0.616995 | 0.030752 |       |       |       |       |       |       |       |
| H     | 1.579256 | -1.392420 | 1.540388 |       |       |       |       |       |       |       |
| H     | 0.811380 | 0.188424 | 1.574002 |       |       |       |       |       |       |       |
| H     | 3.180597 | 0.233221 | 0.742392 |       |       |       |       |       |       |       |
| H     | 2.729342 | -0.844165 | -0.565005 |       |       |       |       |       |       |       |
| H     | 2.811186 | 1.472744 | -1.418604 |       |       |       |       |       |       |       |
| H     | 1.137499 | 0.934361 | -1.441652 |       |       |       |       |       |       |       |
| H     | 1.702160 | 2.020366 | -0.165838 |       |       |       |       |       |       |
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -0.908008 | -0.263968 | 0.108678 |
| C | -2.044021 | 0.674965 | 0.287464 |
| C | -3.184052 | 0.484614 | -0.359113 |
| O | -0.921081 | -1.242771 | -0.597781 |
| O | 0.142149 | 0.110992 | 0.841345 |
| C | 1.330272 | -0.695549 | 0.747979 |
| C | 2.154874 | -0.326202 | -0.469950 |
| C | 2.609635 | 1.127488 | -0.454427 |
| H | -1.888105 | 1.506218 | 0.960895 |
| H | -4.019445 | 1.159856 | -0.239275 |
| H | -3.302141 | -0.359450 | -1.026422 |
| H | 1.875363 | -0.483917 | 1.665925 |
| H | 1.041687 | -1.744485 | 0.731355 |
| H | 3.020125 | -0.991787 | -0.488064 |
| H | 1.573811 | -0.536726 | -1.368834 |
| H | 1.755089 | 1.803826 | -0.448651 |
| H | 3.212965 | 1.356397 | -1.331722 |
| H | 3.209909 | 1.336206 | 0.432498 |
1. 52.5424 cm⁻¹
2. 71.0189 cm⁻¹
3. 107.4987 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       |        |        |        |
|-------|--------|--------|--------|
| C     | 1.053463 | 0.267226 | 0.009646 |
| C     | 2.037396 | -0.826592 | -0.187264 |
| C     | 3.326182 | -0.624048 | 0.040564 |
| O     | 1.319618 | 1.387292 | 0.373660 |
| O     | -0.184214 | -0.140734 | -0.268551 |
| C     | -1.230917 | 0.833060 | -0.116331 |
| C     | -2.543061 | 0.160360 | -0.447986 |
| C     | -2.888977 | -0.968070 | 0.514899 |
| H     | 1.647718 | -1.778546 | -0.520147 |
| H     | 4.053442 | -1.411483 | -0.098105 |
| H     | 3.679692 | 0.343314 | 0.373565 |
| H     | -1.216964 | 1.198041 | 0.911920 |
| H     | -1.022701 | 1.671143 | -0.780988 |
| H     | -2.500739 | -0.211677 | -1.473346 |
| H     | -3.317634 | 0.928650 | -0.421294 |
| H     | -3.848767 | -1.416262 | 0.262087 |
| H     | -2.132476 | -1.751489 | 0.485514 |
| H     | -2.949315 | -0.595763 | 1.538745 |

n-propylacrylate_3

| Datum                                           | Value     |
|------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -385.08853|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.965702|
| Number of Imaginary Frequencies                 | 0         |

Frequencies (Top 3 out of 48)

1. 58.9574 cm⁻¹
2. 73.3697 cm⁻¹
3. 98.4617 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### n-propylacrylate_4

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -385.088906 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.96649 |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 48)

1. 53.4974 cm⁻¹  
2. 80.7653 cm⁻¹  
3. 105.3513 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 1.161988 | 0.199749 | 0.000002 |
|-------|----------|----------|----------|
| C     | 2.327519 | -0.718988| 0.000001 |
| C     | 3.562610 | -0.241129| -0.000005|
| O     | 1.224169 | 1.405438 | -0.000002|
| O     | 0.013326 | -0.476915| 0.000007 |
| C     | -1.190790| 0.305012 | 0.000008 |
| C     | -2.366335| -0.643938| -0.000005|
### n-propylacrylate_5

| Datum                                           | Value       |
|-------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -385.088173 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.965056 |
| Number of Imaginary Frequencies                 | 0           |

**Frequencies (Top 3 out of 48)**

1. 56.1421 cm⁻¹  
2. 70.2291 cm⁻¹  
3. 105.4688 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 1.123411 | -0.000004 |
|-------|----------|-----------|
| H     | 2.113030 | -0.000005 |
| H     | 4.420988 | -0.000006 |
| H     | 3.737946 | -0.000009 |
| H     | -1.193175| 0.883074  |
| H     | -1.193167| -0.883047 |
| H     | -2.303040| 0.878713  |
| H     | -2.303033| -0.878733 |
| H     | -4.530008| -0.000013 |
| H     | -3.762930| 0.881940  |
| H     | -3.762923| -0.881938 |
n-propylacrylate_6

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -385.087967 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.965037 |

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 48)

1. 49.0213 cm⁻¹
2. 62.2427 cm⁻¹
3. 123.5831 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -0.952743 | -0.598466 | -0.068811 |
| C     | -2.235620 | 0.103973  | 0.311777  |
| C     | -2.494669 | 1.332542  | 0.112169  |
| O     | -0.719410 | -1.702720 | -0.501791 |
| O     | -0.095811 | 0.103388  | 0.671188  |
| C     | 1.194578  | -0.483684 | 0.916947  |
| C     | 2.134025  | -0.262460 | -0.252465 |
| C     | 2.355568  | 1.213627  | -0.556797 |
| H     | -2.953272 | -0.471892 | -0.880140 |
| H     | -3.445096 | 1.803714  | -0.097142 |
| H     | -1.765138 | 1.897513  | 0.676144  |
| H     | 1.557414  | 0.023593  | 1.808905  |
| H     | 1.064610  | -1.542602 | 1.130569  |
| H     | 1.739000  | -0.779258 | -1.128213 |
| H     | 3.081777  | -0.742682 | -0.001039 |
| H     | 3.049456  | 1.340895  | -1.386458 |
| H     | 1.418405  | 1.701528  | -0.824548 |
| H     | 2.767771  | 1.730656  | 0.311158  |

n-propylacrylate_7
| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -385.08856    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -384.966042   |

Number of Imaginary Frequencies

0

**Frequencies** (Top 3 out of 48)

1. 49.4234 cm⁻¹
2. 71.1791 cm⁻¹
3. 111.8923 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |       |       |       |
|-----|-------|-------|-------|
| C   | 1.189306 | -0.572939 | 0.071623 |
| C   | 2.315637 | 0.390670  | 0.055736 |
| C   | 2.170142 | 1.688041  | -0.172079 |
| O   | 1.333410 | -1.749568 | 0.309414 |
| O   | 0.010125 | -0.019365 | -0.198606 |
| C   | -1.129716 | -0.894825 | -0.188242 |
| C   | -2.353851 | -0.061715 | -0.491012 |
| C   | -2.620762 | 1.001804  | 0.566385 |
| H   | 3.281071 | -0.054646 | 0.253874 |
| H   | 3.023460 | 2.352078  | -0.168833 |
| H   | 1.197037 | 2.118387  | -0.366261 |
| H   | -0.974539 | -1.676235 | -0.931638 |
| H   | -1.197771 | -1.363292 | 0.794961 |
| H   | -3.202242 | -0.744510 | -0.561727 |
| H   | -2.234363 | 0.398744  | -1.473504 |
| H   | -3.521688 | 1.567079  | 0.332334 |
| H   | -2.754312 | 0.544427  | 1.547982 |
| H   | -1.789468 | 1.703210  | 0.631884 |

**n-propylacrylate_8**

| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -385.087927   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -384.965053   |

Number of Imaginary Frequencies

0

**Frequencies** (Top 3 out of 48)
1. 56.7943 cm⁻¹  
2. 76.5565 cm⁻¹  
3. 107.6175 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -1.034349 | 0.533367 | 0.090749 |
| C | -2.451013 | 0.234256 | -0.227549 |
| C | -2.963997 | -0.987617 | -0.231868 |
| O | -0.583984 | 1.655015 | 0.077950 |
| O | -0.318148 | -0.548390 | 0.394949 |
| C | 1.072215 | -0.349370 | 0.697064 |
| C | 1.908259 | -0.258067 | -0.563525 |
| C | 3.383991 | -0.097121 | -0.220829 |
| H | -3.043509 | 1.107935 | -0.462663 |
| H | -4.005165 | -1.152025 | -0.472855 |
| H | -2.358601 | -1.852003 | 0.004017 |
| H | 1.355060 | -1.217097 | 1.289685 |
| H | 1.179071 | 0.548468 | 1.304767 |
| H | 1.752118 | -1.161584 | -1.155236 |
| H | 1.563237 | 0.588043 | -1.158907 |
| H | 3.553174 | 0.814118 | 0.354174 |
| H | 3.741003 | -0.939611 | 0.373051 |
| H | 3.990032 | -0.041943 | -1.123474 |

n-propylacrylate_9

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -385.088297 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -384.966106 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 48)

1. 55.6198 cm⁻¹  
2. 71.0846 cm⁻¹  
3. 111.5755 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### n-propylacrylate_HEI_10_reopt

#### Datum

|                | Value         |
|----------------|---------------|
| M06-2X/def2tzvpp-IEFP CM(water) Energy | -823.302968   |
| M06-2X/def2tzvpp-IEFP CM(water) Free Energy (Quasiharmonic) | -823.147333   |

| Number of Imaginary Frequencies | 0 |

#### Frequencies (Top 3 out of 63)

1. 26.2349 cm\(^{-1}\)
2. 40.6139 cm\(^{-1}\)
3. 52.3465 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFP CM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 1.247984 | 0.591030 | -0.00002  |
| C | 2.556125 | -0.105558 | -0.00011  |
| C | 2.689170 | -1.424019 | 0.00004   |
| O | 1.144938 | 1.795548 | -0.00006  |
| O | 0.202370 | -0.232993 | 0.00011   |
| C | -1.095715 | 0.380185 | 0.00023   |
| C | -2.132429 | -0.718794 | -0.00015  |
| C | -3.539649 | -0.135426 | -0.00006  |
| H | 3.409360 | 0.559006 | -0.00029  |
| H | 3.667952 | -1.883452 | -0.00003  |
| H | 1.826428 | -2.076032 | 0.00022   |
| H | -1.185327 | 1.014304 | -0.883215 |
| H | -1.185335 | 1.014249 | 0.883300  |
| H | -1.983070 | -1.348162 | -0.878777 |
| H | -1.983081 | -1.348213 | 0.878713  |
| H | -4.288035 | -0.925874 | -0.00035  |
| H | -3.705143 | 0.484584 | 0.881892  |
| H | -3.705131 | 0.484637 | -0.881870 |
n-propylacrylate_HEI_11

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.30297 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.145789 |

Number of Imaginary Frequencies

0

Frequencies (Top 3 out of 63)

1. 35.6856 cm⁻¹
2. 55.8024 cm⁻¹
3. 72.6429 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -0.418929 | -0.733407 | 0.679414 |
|-------|-----------|-----------|----------|
| C     | 0.676265  | -1.342126 | 0.096788 |
| C     | 1.491866  | -0.753356 | -0.981632|
| O     | -1.139452 | -1.164140 | 1.608352 |
| O     | -0.722162 | 0.522747  | 0.132009 |
| C     | -1.962946 | 1.119425  | 0.463335 |
| C     | -2.972270 | 0.940907  | -0.660153|
| C     | -3.318159 | -0.521297 | -0.910063|
| H     | 1.857697  | -1.497001 | -1.691504|
| H     | 0.942255  | 0.002522  | -1.538637|
| H     | -2.340651 | 0.688991  | 1.389945 |
n-propylacrylate_HEI_12

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.305326|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -823.148069|
| Number of Imaginary Frequencies                                      | 0           |

**Frequencies** (Top 3 out of 63)

1. 30.8490 cm⁻¹
2. 50.0767 cm⁻¹
3. 76.7432 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |        |        |        |
|-----|--------|--------|--------|
| C   | -0.385781 | -1.096610 | 0.065437 |
| C   | 0.685745  | -1.049878 | -0.799334 |
| C   | 2.072774  | -1.081433 | -0.302025 |
| O   | -0.394333 | -1.199779 | 1.313979 |
| O   | -1.626309 | -1.059584 | -0.597664 |
| C   | -2.719802 | -0.585356 | 0.167690 |
| C   | -2.612695 | 0.902404  | 0.468589 |
| C   | -2.477743 | 1.747144  | -0.791770 |
| H   | 2.750939  | -1.666298 | -0.925628 |
| H   | 2.112914  | -1.478525 | 0.711589 |
| H   | -3.603595 | -0.779389 | -0.443797 |
| H   | -2.808435 | -1.152718 | 1.094641 |
| H   | -3.500354 | 1.200956  | 1.031952 |
| H   | -1.750945 | 1.060599  | 1.119894 |
| H   | -1.575699 | 1.472064  | -1.338711 |
n-propylacrylate_HEI_13

| Datum                                      | Value           |
|--------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.304846     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.14802 |
| Number of Imaginary Frequencies            | 0               |

**Frequencies** (Top 3 out of 63)

1. 36.6770 cm⁻¹
2. 48.4137 cm⁻¹
3. 78.1101 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| H | -2.419079 | 2.809180 | -0.553493 |
| H | -3.331551 | 1.597424 | -1.455796 |
| S | 2.939243  | 0.571382 | -0.242989 |
| C | 1.787684  | 1.466789 | 0.811783  |
| H | 1.841056  | 1.112256 | 1.839534  |
| H | 2.045888  | 2.522841 | 0.778626  |
| H | 0.776456  | 1.321918 | 0.430822  |
| H | 0.498558  | -0.985880 | -1.854535 |
n-propylacrylate_HEI_14

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.304755 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.14879  |
| Number of Imaginary Frequencies | 0             |

**Frequencies** (Top 3 out of 63)

1. 29.2539 cm⁻¹
2. 41.9626 cm⁻¹
3. 69.4278 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |         |         |         |
|---|---------|---------|---------|
| C | 0.184943 | -0.744058 | 0.058877 |
| C | -0.782679 | -0.621263 | -0.918618 |
| C | -2.191724 | -0.943677 | -0.636767 |
| O | 0.069578  | -1.149620 | 1.237648  |
| O | 1.459775  | -0.364789 | -0.379550 |
| C | 2.515359  | -0.500990 | 0.552244  |
| C | 3.789930  | -0.004908 | -0.102373 |
| C | 3.737226  | 1.476979  | -0.451845 |
| H | -2.699012 | -1.450137 | -1.459560 |
| H | -2.273582 | -1.569176 | 0.251434  |
| H | 2.301015  | 0.080703  | 1.453606  |
| H | 2.619074  | -1.545548 | 0.856096  |
| H | 3.980408  | -0.596448 | -1.000949 |
| H | 4.617351  | -0.196665 | 0.584327  |
| H | 4.672329  | 1.812795  | -0.899505 |
| H | 2.931603  | 1.679650  | -1.156460 |
| H | 3.558401  | 2.076223  | 0.443002  |
| S | -3.325323 | 0.514816  | -0.339256 |
| C | -2.474773 | 1.262547  | 1.060137  |
| H | -2.628426 | 0.684419  | 1.969702  |
| H | -2.864160 | 2.268176  | 1.201635  |
| H | -1.409686 | 1.309782  | 0.834817  |
| H | -0.504668 | -0.223341 | -1.884777 |
**n-propylacrylate_HEI_15**

| Datum                                                                 | Value               |
|-----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -823.304838         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -823.147063         |
| Number of Imaginary Frequencies                                       | 0                   |

**Frequencies (Top 3 out of 63)**

1. 49.3756 cm⁻¹  
2. 65.8180 cm⁻¹  
3. 88.5353 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 0.403403 | -0.941866 | 0.218284 |
| C | -0.706690 | -1.185870 | -0.563593 |
| C | -2.066486 | -1.152496 | 0.004484  |
| O | 0.461897  | -0.656880 | 1.434532  |
| O | 1.608349  | -1.083477 | -0.495246 |
| C | 2.807092  | -0.650694 | 0.121730  |
| C | 3.245777  | 0.699692  | -0.423515 |
| C | 2.234710  | 1.800879  | -0.133234 |
| H | -2.717774 | -1.938225 | -0.382233 |
| H | -2.035516 | -1.241131 | 1.090127  |
| H | 2.665325  | -0.599202 | 1.200828  |
| H | 3.565846  | -1.405637 | -0.095077 |
| H | 4.215734  | 0.949417  | 0.014289  |
| H | 3.398475  | 0.610954  | -1.502002 |
| H | 1.262877  | 1.544967  | -0.558148 |
| H | 2.550747  | 2.753519  | -0.558364 |
| H | 2.101013  | 1.932703  | 0.941312  |
| S | -3.071778 | 0.380700  | -0.350655 |
| C | -2.001296 | 1.606102  | 0.419687  |
| H | -0.974543 | 1.411333  | 0.111585  |
| H | -2.306089 | 2.593660  | 0.081002  |
| H | -2.068227 | 1.559130  | 1.505407  |
| H | -0.570441 | -1.394319 | -1.615592 |
# n-propylacrylate_HEI_16_reopt

| Datum                                             | Value         |
|---------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy             | -823.305058   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.148299   |

Number of Imaginary Frequencies

0

**Frequencies** (Top 3 out of 63)

1. 30.7961 cm⁻¹
2. 49.3253 cm⁻¹
3. 78.2586 cm⁻¹

# M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C         |  0.184504 | -0.996457 |  0.225922 |
|-----------|-----------|-----------|-----------|
| C         | -0.988638 | -1.219416 | -0.461953 |
| C         | -2.300894 | -0.986131 |  0.167884 |
| O         |  0.350290 | -0.598766 |  1.401306 |
| O         |  1.330169 | -1.309825 | -0.530166 |
| C         |  2.545340 | -0.738816 | -0.085491 |
| C         |  2.648384 |  0.737090 | -0.432897 |
| C         |  3.973891 |  1.328518 |  0.028571 |
| H         | -3.051953 | -1.732268 | -0.096910 |
| H         | -2.211584 | -0.963432 |  1.253380 |
| H         |  2.659417 | -0.875515 |  0.991186 |
| H         |  3.338290 | -1.296451 | -0.588272 |
| H         |  2.536680 |  0.854348 | -1.513317 |
| H         |  1.814132 |  1.260685 |  0.038674 |
| H         |  4.083096 |  1.239187 |  1.110678 |
| H         |  4.051861 |  2.384076 | -0.229174 |
| H         |  4.814975 |  0.808557 | -0.433680 |
| S         | -3.158742 |  0.602151 | -0.308833 |
| C         | -1.904229 |  1.779467 |  0.221607 |
| H         | -2.139573 |  2.749250 | -0.210966 |
| H         | -0.933410 |  1.440722 | -0.140084 |
| H         | -1.878042 |  1.864163 |  1.306614 |
| H         | -0.937844 | -1.524544 | -1.497780 |

# n-propylacrylate_HEI_17_reopt

| Datum                              | Value |
|------------------------------------|-------|

**Datum** | **Value**
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.30476
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.148158

Number of Imaginary Frequencies | 0

**Frequencies** (Top 3 out of 63)

1. 39.1238 cm⁻¹
2. 48.0679 cm⁻¹
3. 79.3053 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Element | X Coordinate | Y Coordinate | Z Coordinate |
|---------|--------------|--------------|--------------|
| C       | -0.192830    | -0.043859    | 0.480773     |
| C       | 0.709375     | -1.005726    | 0.072148     |
| C       | 2.074372     | -1.054142    | 0.623422     |
| O       | -0.054799    | 0.853624     | 1.342595     |
| O       | -1.424292    | -0.130360    | -0.181525    |
| C       | -2.430893    | 0.772545     | 0.233611     |
| C       | -3.679851    | 0.495732     | -0.580321    |
| C       | -4.249411    | -0.896075    | -0.336783    |
| H       | 2.447970     | -2.068169    | 0.774254     |
| H       | 2.128576     | -0.525933    | 1.574969     |
| H       | -2.097509    | 1.802909     | 0.090575     |
| H       | -2.639069    | 0.642181     | 1.300079     |
| H       | -3.448688    | 0.627295     | -1.639984    |
| H       | -4.423561    | 1.252905     | -0.322248    |
| H       | -3.527569    | -1.663703    | -0.613279    |
| H       | -5.157857    | -1.059969    | -0.915997    |
| H       | -4.494431    | -1.031023    | 0.718481     |
| S       | 3.417515     | -0.310359    | -0.444516    |
| C       | 2.772251     | 1.364236     | -0.585976    |
| H       | 3.326816     | 1.880895     | -1.366083    |
| H       | 1.718429     | 1.311581     | -0.857104    |
| H       | 2.877656     | 1.905524     | 0.352592     |
| H       | 0.423649     | -1.691071    | -0.713805    |

**n-propylacrylate_HEI_18**

**Datum** | **Value**
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.304797
### M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)

| Datum | Value    |
|-------|----------|
|       | -823.148557 |

### Number of Imaginary Frequencies

| Datum | Value |
|-------|-------|
|       | 0     |

### Frequencies (Top 3 out of 63)

1. 36.6580 cm\(^{-1}\)
2. 63.5029 cm\(^{-1}\)
3. 74.7329 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | -0.090500 | -0.443199 | 0.370556 |
| C    | 0.954265   | -1.093834 | -0.254676 |
| C    | 2.308502   | -1.088453 | 0.324182 |
| O    | -0.097371  | 0.180569  | 1.455993 |
| O    | -1.295382  | -0.532779 | -0.340344 |
| C    | -2.418458  | 0.101372  | 0.237560 |
| C    | -3.611603  | -0.121790 | -0.669336 |
| C    | -4.865621  | 0.537495  | -0.109617 |
| H    | 2.840744   | -2.032748 | 0.198873 |
| H    | 2.274303   | -0.854763 | 1.387712 |
| H    | -2.617810  | -0.305489 | 1.233045 |
| H    | -2.232195  | 1.172605  | 0.359437 |
| H    | -3.385227  | 0.278810  | -1.659759 |
| H    | -3.771400  | -1.195473 | -0.788891 |
| H    | -4.724074  | 1.613881  | -0.000201 |
| H    | -5.722770  | 0.377516  | -0.762318 |
| H    | -5.112669  | 0.133102  | 0.873232 |
| S    | 3.517755   | 0.127589  | -0.423170 |
| C    | 2.602504   | 1.652777  | -0.145652 |
| H    | 1.579352   | 1.517188  | -0.494429 |
| H    | 3.081630   | 2.446753  | -0.714055 |
| H    | 2.591932   | 1.917758  | 0.909996  |
| H    | 0.781605   | -1.559107 | -1.215206 |

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### n-propylacrylate_HEI_19_reopt

| Datum | Value    |
|-------|----------|
|       | -823.304782 |

| Datum | Value    |
|-------|----------|
|       | -823.149138 |
### Number of Imaginary Frequencies

**Value**: 0

### Frequencies (Top 3 out of 63)

1. 10.0902 cm⁻¹
2. 45.8621 cm⁻¹
3. 62.3465 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -0.224058 | -0.110744 | 0.051919 |
| C    | 0.805215  | -0.968736 | 0.376603 |
| C    | 1.984906  | -1.115632 | -0.495016 |
| O    | -0.376776 | 0.591037  | -0.973374 |
| O    | -1.214167 | -0.044336 | 1.050081 |
| C    | -2.459643 | 0.503927  | 0.665369 |
| C    | -3.311687 | -0.483806 | -0.114483 |
| C    | -4.651922 | 0.125453  | -0.505271 |
| H    | 2.356954  | -2.139773 | -0.552916 |
| H    | 1.765722  | -0.776276 | -1.506727 |
| H    | -2.964840 | 0.778324  | 1.593929 |
| H    | -2.308811 | 1.409387  | 0.075789 |
| H    | -2.759644 | -0.788986 | -1.005386 |
| H    | -3.465367 | -1.377617 | 0.494470 |
| H    | -5.210423 | 0.439037  | 0.378599 |
| H    | -5.268733 | -0.584287 | -1.055255 |
| H    | -4.509282 | 1.004323  | -1.136258 |
| S    | 3.515217  | -0.184356 | 0.033741 |
| C    | 2.846159  | 1.487058  | 0.036558 |
| H    | 3.560284  | 2.140573  | 0.532466 |
| H    | 2.673987  | 1.841841  | -0.978019 |
| H    | 1.904972  | 1.488322  | 0.585048 |
| H    | 0.775433  | -1.483890 | 1.326675 |

### n-propylacrylate_HEI_1_reopt

| Datum                                           | Value       |
|------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -823.30311  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.146099 |
| Number of Imaginary Frequencies                 | 0           |
**Frequencies** (Top 3 out of 63)

1. 44.4926 cm⁻¹
2. 61.0683 cm⁻¹
3. 75.2642 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 0.339511 | -1.392043 | -0.230036 |
| C | -1.034891 | -1.525844 | -0.190364 |
| C | -1.935091 | -0.793218 | 0.719190 |
| O | 1.152425  | -2.003627 | -0.962388 |
| O | 0.854109  | -0.467903 | 0.690745 |
| C | 2.266047  | -0.368968 | 0.771394 |
| C | 2.845836  | 0.586905  | -0.259437 |
| C | 2.388995  | 2.024615  | -0.050719 |
| H | -2.753546 | -1.409617 | 1.095270 |
| H | -1.401129 | -0.384852 | 1.575144 |
| H | 2.713579  | -1.356112 | 0.663837 |
| H | 2.475808  | 0.002756  | 1.777514 |
| H | 2.557424  | 0.233227  | -1.250423 |
| H | 3.936001  | 0.529989  | -0.201197 |
| H | 1.302374  | 2.090781  | -0.094842 |
| H | 2.799562  | 2.688779  | -0.811260 |
| H | 2.707924  | 2.394530  | 0.925806 |
| S | -2.865324 | 0.646346  | -0.028082 |
| C | -1.460663 | 1.671114  | -0.489133 |
| H | -0.991260 | 2.104032  | 0.392717 |
| H | -0.732514 | 1.054754  | -1.017079 |
| H | -1.810337 | 2.467683  | -1.142021 |
| H | -1.469435 | -2.206017 | -0.916370 |

**n-propylacrylate_HEI_20_reopt**

| Datum                                               | Value            |
|-----------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy               | -823.296058      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139571      |
| Number of Imaginary Frequencies                     | 0                |

**Frequencies** (Top 3 out of 63)
|   |   |   |
|---|---|---|
| 1. | 21.0489 cm⁻¹ |   |
| 2. | 52.1114 cm⁻¹ |   |
| 3. | 76.2079 cm⁻¹ |   |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 0.987887 | 1.418241 | -0.109080 |
| C | -0.353657 | 1.557836 | 0.171448 |
| C | -1.464401 | 0.806381 | -0.460409 |
| O | 1.931800 | 2.145299 | 0.278951 |
| O | 1.375738 | 0.383668 | -0.989221 |
| C | 1.058122 | -0.960972 | -0.659646 |
| C | 2.319008 | -1.732663 | -0.309084 |
| C | 2.976344 | -1.199234 | 0.956763 |
| H | -2.253605 | 1.464579 | -0.832758 |
| H | -1.120453 | 0.196673 | -1.295227 |
| H | 0.560710 | -1.417630 | -1.520452 |
| H | 0.359276 | -0.985669 | 0.179237 |
| H | 3.013603 | -1.671993 | -1.150336 |
| H | 2.055298 | -2.786559 | -0.189081 |
| H | 3.192222 | -0.135959 | 0.847469 |
| H | 3.905652 | -1.723328 | 1.179287 |
| H | 2.309067 | -1.316979 | 1.813401 |
| S | -2.316867 | -0.319596 | 0.728270 |
| C | -3.676769 | -0.896211 | -0.309683 |
| H | -4.283196 | -0.056114 | -0.645433 |
| H | -3.297394 | -1.437637 | -1.174912 |
| H | -4.296245 | -1.565087 | 0.283468 |
| H | -0.614575 | 2.357240 | 0.853316 |

**n-propylacrylate_HEI_22**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296867 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140117 |

**Number of Imaginary Frequencies**

0

**Frequencies (Top 3 out of 63)**

1. 30.0579 cm⁻¹
2. 44.6862 cm⁻¹
3. 87.5201 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| C     | -0.947143 | 1.317946  | 0.073572  |
| C     | 0.383686  | 1.509312  | -0.216832 |
| C     | 1.524330  | 0.830888  | 0.444765  |
| O     | -1.935842 | 1.933198  | -0.389904 |
| O     | -1.255478 | 0.345335  | 1.057761  |
| C     | -1.130639 | -1.006609 | 0.638973  |
| C     | -2.041336 | -1.361058 | -0.526079 |
| C     | -3.515340 | -1.152194 | -0.209517 |
| H     | 2.306898  | 1.529067  | 0.752386  |
| H     | 1.204525  | 0.275029  | 1.325410  |
| H     | -1.395520 | -1.608526 | 1.511764  |
| H     | -0.093371 | -1.228965 | 0.374548  |
| H     | -1.850530 | -2.404714 | -0.789225 |
| H     | -1.754789 | -0.759685 | -1.392782 |
| H     | -3.815218 | -1.750785 | 0.653214  |
| H     | -4.147388 | -1.436486 | -1.050974 |
| H     | -3.697582 | -0.103491 | 0.019652  |
| S     | 2.369879  | -0.359846 | -0.683536 |
| C     | 3.749612  | -0.860542 | 0.367567  |
| H     | 4.362528  | -1.565593 | -0.189408 |
| H     | 4.357458  | 0.002225  | 0.636474  |
| H     | 3.386514  | -1.344055 | 1.273216  |
| H     | 0.609937  | 2.258798  | -0.965241 |

n-propylacrylate_HEI_23

| Datum                                           | Value  |
|------------------------------------------------|--------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -823.297094 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140476 |
| Number of Imaginary Frequencies                 | 0      |

Frequencies (Top 3 out of 63)

1. 34.8166 cm⁻¹
2. 55.0050 cm⁻¹
3. 80.0592 cm⁻¹
# M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X        | Y        | Z        |
|---|----------|----------|----------|
| C | -1.034973| 1.572181 | -0.046648|
| C | 0.294852 | 1.632613 | -0.391153|
| C | 1.414693 | 0.985466 | 0.333872 |
| O | -1.998456| 2.174152 | -0.575717|
| O | -1.374444| 0.776286 | 1.077593 |
| C | -1.325580| -0.626372| 0.872610 |
| C | -2.237111| -1.111573| -0.242252|
| C | -2.143753| -2.624350| -0.396613|
| H | 2.251962 | 1.666528 | 0.505309 |
| H | 1.096829 | 0.594163 | 1.299627 |
| H | -1.629398| -1.076796| 1.820542 |
| H | -0.301814| -0.950936| 0.661349 |
| H | -1.947995| -0.620781| -1.174344|
| H | -3.263962| -0.809064| -0.026482|
| H | -1.122021| -2.925634| -0.635521|
| H | -2.793610| -2.985176| -1.192844|
| H | -2.431821| -3.130663| 0.526402 |
| S | 2.135421 | -0.418648| -0.622822|
| C | 3.527406 | -0.844125| 0.445167 |
| H | 4.073361 | -1.662517| -0.018632|
| H | 4.195552 | 0.008454 | 0.558435 |
| H | 3.176356 | -1.161993| 1.425721 |
| H | 0.539822 | 2.246248 | -1.249316|

## n-propylacrylate_HEI_24

| Datum | Value     |
|-------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.302987 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.146319 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 63)**

1. 30.7752 cm\(^{-1}\)
2. 44.5708 cm\(^{-1}\)
3. 55.7230 cm\(^{-1}\)
### n-propylacrylate_HEI_25

| Datum                              | Value     |
|------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.304482 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.146932 |
| Number of Imaginary Frequencies    | 0         |

**Frequencies** (Top 3 out of 63)

1. 45.5239 cm⁻¹
2. 50.8916 cm⁻¹
3. 79.2493 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C  | 0.466026 | 1.082777 | -0.150424 |
|----|----------|----------|-----------|
| C  | -0.660719| 0.719393 | -0.861211 |
| C  | -1.288266| -0.614541| -0.791742 |
| O  | 1.077863 | 2.175854 | -0.158560 |
| O  | 0.949451 | 0.067725 | 0.687370  |
| C  | 2.312652 | 0.161132 | 1.062466  |
| C  | 3.243356 | -0.201320| -0.084628 |
| C  | 2.986482 | -1.602577| -0.623845 |
| H  | -1.786293| -0.881103| -1.725142 |
| H  | -0.566453| -1.395258| -0.556164 |
| H  | 2.436055 | -0.549574| 1.882300  |
| H  | 2.534090 | 1.162302 | 1.431518  |
| H  | 4.273444 | -0.115064| 0.269882  |
| H  | 3.114944 | 0.536991 | -0.878538 |
| H  | 3.666701 | -1.846087| -1.439792 |
| H  | 1.965438 | -1.687044| -0.997092 |
| H  | 3.118911 | -2.351194| 0.159906  |
| S  | -2.599423| -0.868082| 0.517826  |
| C  | -3.765634| 0.393001 | -0.022679 |
| H  | -4.158761| 0.157603 | -1.011220 |
| H  | -4.587367| 0.427375 | 0.688843  |
| H  | -3.273242| 1.363977 | -0.049798 |
| H  | -1.128596| 1.490555 | -1.458030 |

C: Carbon, O: Oxygen, H: Hydrogen, S: Sulfur
n-propylacrylate_HEI_26

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296874 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139927 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 63)

1. 45.7248 cm⁻¹
2. 49.7497 cm⁻¹
3. 76.5644 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -0.910053 | -1.327867 | 0.076071 |
|-------|-----------|-----------|----------|
| C     | 0.429124  | -1.513584 | -0.176792|
| C     | 1.543434  | -0.789558 | 0.481895 |
| O     | -1.883057 | -1.967051 | -0.389028|
| O     | -1.242441 | -0.324400 | 1.021359 |
| C     | -1.155935 | 1.008701  | 0.538264 |
| C     | -2.153324 | 1.305700  | -0.570655|
n-propylacrylate_HEI_27_reopt

| Datum                              | Value          |
|------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296381   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139405   |

Number of Imaginary Frequencies

0

Frequencies (Top 3 out of 63)

1. 32.8653 cm⁻¹
2. 55.3591 cm⁻¹
3. 85.5520 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C        | -0.716524 | 1.300004 | -0.064584 |
|----------|-----------|----------|-----------|
| C        | 0.659055  | 1.289240 | -0.016124 |
| C        | 1.548409  | 0.526963 | -0.919409 |
| O        | -1.508887 | 2.009633 | 0.597818  |
| O        | -1.327116 | 0.446202 | -1.018004 |
| C        | -1.340563 | -0.931587| -0.673302 |
| C        | -2.122214 | -1.226005| 0.597485  |
| C        | -3.586173 | -0.821184| 0.500447  |
| H        | 2.363140  | 1.140647 | -1.310165 |
| H        | 1.004164  | 0.120230 | -1.770600 |
| H        | -1.804822 | -1.442152| -1.520648 |
### n-propylacrylate_HEI_2

| Datum                                              | Value           |
|----------------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy              | -823.303018     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.146391 |

**Number of Imaginary Frequencies**

0

**Frequencies (Top 3 out of 63)**

1. 47.5073 cm⁻¹  
2. 54.2514 cm⁻¹  
3. 64.6931 cm⁻¹ 

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C         | C         | O         | O         | C         | C         | H         | H         | H         |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| -0.837496 | -1.387925 | -0.076233 | -1.679795 | -0.930325 | -0.618774 | 0.506780  | -1.965231 | 0.479319  |
| 0.506780  | -1.679795 | -0.193907 | -0.930325 | -0.618774 | -0.193907 | 0.506780  | -1.965231 | -0.193907 |
| 1.590529  | -0.930325 | 0.479319  | -1.965231 | -0.193907 | -0.193907 | 0.506780  | -1.965231 | -0.193907 |
| -1.807527 | -1.965231 | 0.479319  | -1.965231 | -0.193907 | -0.193907 | 0.506780  | -1.965231 | -0.193907 |
| -1.109785 | -0.321811 | 0.793609  | 0.154016  | 0.821232  | 0.821232  | 0.154016  | 0.821232  | 0.821232  |
| -2.443868 | 0.154016  | 0.821232  | 0.154016  | 0.821232  | 0.821232  | 0.154016  | 0.821232  | 0.821232  |
| -2.745094 | 1.092009  | -0.337484 | 2.337469  | 3.337469  | 3.337469  | 2.337469  | 3.337469  | 3.337469  |
| -1.868151 | 2.337469  | -0.328092 | 2.337469  | 3.337469  | 3.337469  | 2.337469  | 3.337469  | 3.337469  |
| 2.429534  | -1.570746 | 0.758237  | -1.570746 | 0.758237  | 0.758237  | -1.570746 | 0.758237  | 0.758237  |
| 1.239130  | -0.416868 | 1.372739  | -0.416868 | 1.372739  | 1.372739  | -0.416868 | 1.372739  | 1.372739  |
| -2.541394 | 0.691000  | 1.767613  | 0.691000  | 1.767613  | 1.767613  | 0.691000  | 1.767613  | 1.767613  |
| -3.139841 | -0.683830 | 0.821155  | -0.683830 | 0.821155  | 0.821155  | -0.683830 | 0.821155  | 0.821155  |
| -2.611259 | 0.539207  | -1.269072 | 0.539207  | -1.269072 | -1.269072 | 0.539207  | -1.269072 | -1.269072 |
| -3.799272 | 1.375386  | -0.281348 | 1.375386  | -0.281348 | -0.281348 | 1.375386  | -0.281348 | -0.281348 |
| -2.094160 | 2.990605  | -1.170903 | 2.990605  | -1.170903 | -1.170903 | 2.990605  | -1.170903 | -1.170903 |
**n-propylacrylate_HEI_3**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.303798 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.147099 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

1. 34.0767 cm⁻¹
2. 61.5237 cm⁻¹
3. 62.3333 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C | 0.152483 | 1.578857 | 0.062461 |
| C | -1.151584 | 1.502414 | -0.387369 |
| C | -1.720481 | 0.339812 | -1.092653 |
| O | 0.690620 | 2.484074 | 0.742116 |
| O | 0.952915 | 0.501342 | -0.333729 |
| C | 2.233817 | 0.414851 | 0.259681 |
| C | 2.979229 | -0.741894 | -0.376295 |
| C | 2.284505 | -2.082694 | -0.178136 |
| H | -2.466236 | 0.614209 | -1.840220 |
| H | -0.952385 | -0.253869 | -1.583749 |
| H | 2.132185 | 0.250433 | 1.338857 |
| H | 2.780706 | 1.348202 | 0.121152 |
| H | 3.980880 | -0.771923 | 0.058426 |
| H | 3.103408 | -0.539504 | -1.442834 |
| H | 2.877578 | -2.900719 | -0.586616 |
| H | 1.312317 | -2.089372 | -0.669810 |
| H | 2.123237 | -2.279941 | 0.883847 |
| S | -2.685227 | -0.864205 | -0.028474 |
| C | -1.409689 | -1.285556 | 1.169960 |
### n-propylacrylate_HEI_4_reopt

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.303592    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -823.14754     |

**Number of Imaginary Frequencies**

0

#### Frequencies (Top 3 out of 63)

1. 20.2783 cm⁻¹
2. 44.1834 cm⁻¹
3. 61.4059 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C           | 0.154503 | 1.490006 | -0.037317 |
|-------------|----------|----------|-----------|
| C           | -1.089673| 1.371181 | -0.627310 |
| C           | -1.637756| 0.115206 | -1.171927 |
| O           | 0.682396 | 2.507622 | 0.469687  |
| O           | 0.896327 | 0.306200 | -0.037473 |
| C           | 2.189888 | 0.363946 | 0.530698  |
| C           | 2.795437 | -1.024374| 0.458473  |
| C           | 2.959924 | -1.524848| -0.971002 |
| H           | -2.255097| 0.269682 | -2.058289 |
| H           | -0.851712| -0.592792| -1.428239 |
| H           | 2.812058 | 1.078688 | -0.016932 |
| H           | 2.132931 | 0.707385 | 1.565905  |
| H           | 3.766094 | -0.994878| 0.958393  |
| H           | 2.166692 | -1.714169| 1.026772  |
| H           | 1.993532 | -1.590956| -1.469883 |
| H           | 3.423340 | -2.510889| -0.995249 |
| H           | 3.588767 | -0.843239| -1.547100 |
| S           | -2.814988| -0.824394| -0.058945 |
| C           | -1.725033| -1.108157| 1.345370  |
| H           | -1.250792| -0.166761| 1.621090  |
| H           | -2.326166| -1.472602| 2.175396  |
| H           | -0.956242| -1.840022| 1.103599  |
| H           | -1.717115| 2.252524 | -0.611964 |
n-propylacrylate_HEI_6_reopt

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.303628    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.147029 |
| Number of Imaginary Frequencies            | 0              |

**Frequencies (Top 3 out of 63)**

1. 19.5731 cm⁻¹
2. 44.5186 cm⁻¹
3. 64.6063 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| C | -0.41440 | 1.077059 | -0.388395 |
| C | 0.647093 | 0.671720 | -1.171015 |
| C | 1.360619 | -0.611176 | -1.020688 |
| O | -1.071749 | 2.142849 | -0.459116 |
| O | -0.769884 | 0.157559 | 0.611247 |
| C | -2.109496 | 0.219857 | 1.067584 |
| C | -3.086643 | -0.333352 | 0.041614 |
| C | -2.771998 | -1.772804 | -0.344612 |
| H | 1.664413 | -1.042024 | 1.973174 |
| H | -2.371966 | 1.244489 | 1.329965 |
| H | -4.095207 | -0.263752 | 0.456495 |
| H | -3.059480 | 0.307659 | -0.841872 |
| H | -3.483563 | -2.153640 | -1.077026 |
| H | -2.805997 | -2.426157 | 0.529599 |
| H | -1.772205 | -1.841365 | -0.774366 |
| S | 2.990346 | -0.541577 | -0.109993 |
| C | 2.417263 | 0.096583 | 1.472649 |
| H | 1.778816 | 0.961148 | 1.295495 |
| H | 3.286623 | 0.395497 | 2.053961 |
| H | 1.856367 | -0.658427 | 2.020250 |
| H | 1.014863 | 1.387930 | -1.894774 |
n-propylacrylate_HEI_8

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.30361             |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -823.147606            |
| Number of Imaginary Frequencies                                      | 0                      |

**Frequencies** (Top 3 out of 63)

1. 23.7525 cm⁻¹
2. 55.2818 cm⁻¹
3. 62.2719 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C           | 0.054534 | 1.475726 | 0.116495 |
| C           | 1.379934 | 1.433415 | -0.271457|
| C           | 1.989698 | 0.327936 | -1.033020|
| O           | -0.527284| 2.340304 | 0.812618 |
| O           | -0.712356| 0.410494 | -0.366823|
| C           | -2.032355| 0.308299 | 0.127244 |
| C           | -2.681021| -0.908814| -0.500397|
| C           | -4.115635| -1.085283| -0.019836|
| H           | 2.778510 | 0.661560 | -1.708716|
| H           | 1.253559 | -0.219004| -1.618555|
| H           | -2.603789| 1.209229 | -0.110721|
| H           | -2.022112| 0.212180 | 1.217962 |
| H           | -2.658051| -0.801174| -1.587021|
| H           | -2.089434| -1.793643| -0.255442|
| H           | -4.151285| -1.210559| 1.063503 |
| H           | -4.580598| -1.959776| -0.473074|
| H           | -4.721436| -0.214098| -0.273981|
| S           | 2.886112 | -0.969660| -0.021827|
| C           | 1.528178 | -1.510427| 1.028914 |
| H           | 0.781893 | -2.056621| 0.454844 |
| H           | 1.935442 | -2.154827| 1.804835 |
| H           | 1.060903 | -0.638177| 1.485186 |
| H           | 2.015735 | 2.227964 | -0.096407|

n-propylacrylate_HEI_9

| Datum | Value |
|-------|-------|
|       |       |
| Datum                                      | Value          |
|-------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -823.303315    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.146745 |
| Number of Imaginary Frequencies            | 0              |

Frequencies (Top 3 out of 63)

1. 21.7513 cm⁻¹  
2. 50.5084 cm⁻¹  
3. 68.9146 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C           | 0.228927 | 0.960356 | 0.372645 |
| C           | -0.973687| 1.367988 | -0.170399|
| C           | -1.803776| 0.550729 | -1.074820|
| O           | 0.975963 | 1.584398 | 1.161812 |
| O           | 0.631398 | -0.320137| -0.035323|
| C           | 1.947725 | -0.712010| 0.302243 |
| C           | 2.985166 | -0.142952| -0.650833|
| C           | 4.389731 | -0.602490| -0.281757|
| H           | -2.307728| 1.142069 |-1.841047 |
| H           | -1.218666| 0.219477 |-1.572955 |
| H           | 1.955298 | -1.803084| 0.251049 |
| H           | 2.180902 | -0.412863| 1.324985 |
| H           | 2.920131 | 0.945835 |-0.619402 |
| H           | 2.740065 | -0.455886| -1.668385|
| H           | 5.134002 | -0.206238| -0.971457|
| H           | 4.461845 | -1.691498| -0.301620|
| H           | 4.654937 | -0.271031| 0.723568 |
| S           | -3.248085| -0.342324| -0.287529|
| C           | -2.358363| -1.326452| 0.928929 |
| H           | -1.683694| -0.677259| 1.485654 |
| H           | -3.085539| -1.767237| 1.607180 |
| H           | -1.782285| 0.215657 | 0.449536 |
| H           | -1.353133| 2.324413 | 0.165387 |

n-propylacrylate_TS_10_UNCON_m062x_reopt

| Datum                                      | Value          |
|-------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -823.294629    |
### M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.138262 |

### Number of Imaginary Frequencies

| Datum | Value |
|-------|-------|
| Number of Imaginary Frequencies | 1 |

### Frequencies (Top 3 out of 63)

1. -193.9425 cm⁻¹
2. 34.3736 cm⁻¹
3. 39.7041 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | -0.460433 | 0.845650 | 0.416290 |
|--------|-----------|----------|----------|
| C      | 0.621387  | 1.392985 | -0.343796|
| C      | 1.287341  | 0.703731 | -1.335108|
| O      | -1.103298 | 1.440823 | 1.275010 |
| O      | -0.738673 | -0.451676| 0.099206 |
| C      | -1.889850 | -1.065966| 0.676393 |
| C      | -3.019370 | -1.129120| -0.33687 |
| C      | -3.497320 | 0.249095 | -0.773929|
| H      | 1.944242  | 1.248838 | -1.996074|
| H      | 0.828436  | -0.174060| -1.761259|
| H      | -1.581452 | -2.068690| 0.970738 |
| H      | -2.190912 | -0.511847| 1.563512 |
| H      | -2.682095 | -1.701440| -1.203073|
| H      | -3.842002 | -1.689664| 0.113627 |
| H      | -2.681348 | 0.817729 | -1.222585|
| H      | -3.871689 | 0.819147 | 0.076959 |
| H      | -4.295771 | 0.171037 | -1.511187|
| S      | 3.113866  | -0.596380| -0.505651|
| C      | 2.710857  | -0.422366| 1.242058 |
| H      | 1.900111  | 0.312342 | 1.337088 |
| H      | 2.370821  | -1.360769| 1.679152 |
| H      | 3.561832  | -0.059647| 1.817018 |
| H      | 0.938058  | 2.381872 | -0.042162|

### n-propylacrylate_TS_11_UNCON_m062x

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296727 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140393 |
## Frequency Data

**Frequencies** (Top 3 out of 63)

|   | Frequency (cm⁻¹) |
|---|------------------|
| 1 | -191.7471        |
| 2 | 41.1841          |
| 3 | 48.7538          |

## Molecular Geometry

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     | X          | Y          | Z          |
|-----|------------|------------|------------|
| C   | -0.333162  | -1.134016  | 0.032013   |
| C   | 0.780240   | -1.225104  | -0.861301  |
| C   | 2.057021   | -1.378750  | -0.370235  |
| O   | -0.304430  | -0.956662  | -0.631327  |
| C   | -2.667102  | -0.680622  | 0.162527   |
| C   | -2.712774  | 0.776628   | 0.589297   |
| H   | 2.862259   | -1.620930  | -1.046882  |
| H   | 2.178642   | -1.727661  | 0.643898   |
| H   | -3.515445  | -0.915359  | -0.480700  |
| H   | -2.683993  | -1.341632  | 1.027385   |
| H   | -1.851037  | 0.981025   | 1.227245   |
| H   | -3.605709  | 0.917860   | 1.202346   |
| H   | -1.833900  | 1.612643   | -1.203664  |
| H   | -2.775690  | 2.770290   | -0.264281  |
| H   | -3.596432  | 1.545620   | -1.234064  |
| S   | 3.074700   | 0.721317   | 0.184953   |
| C   | 1.579800   | 1.718502   | 0.052157   |
| H   | 0.786255   | 1.097855   | -0.387013  |
| H   | 1.234030   | 2.069873   | 1.024262   |
| H   | 1.727808   | 2.580385   | -0.597198  |
| H   | 0.592012   | -1.061737  | -1.912862  |

## Additional Data

**n-propylacrylate_TS_12_UNCON_m062x**

| Datum                                      | Value              |
|--------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.296536        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140925 |

Number of Imaginary Frequencies

|   | Value |
|---|-------|
|   | 1     |
Frequencies (Top 3 out of 63)

1. -190.1303 cm\(^{-1}\)
2.  28.0083 cm\(^{-1}\)
3.  49.0193 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|  |        |        |        |
|---|--------|--------|--------|
| C | 0.199249 | -0.897648 | 0.042587 |
| C | -0.779120 | -0.838550 | -0.998765 |
| C | -2.077403 | -1.229479 | -0.754977 |
| O | 0.027666   | -1.281149 | 1.194606  |
| O | 1.427744   | -0.471173 | -0.367465 |
| C | 2.468889   | -0.495067 | 0.606670  |
| C | 3.717121   | 0.077940  | -0.028227 |
| C | 3.560974   | 1.541325  | -0.421572 |
| H | -2.755216  | -1.364285 | -1.583887 |
| H | -2.271357  | -1.844554 | 0.110705  |
| H | 2.165149   | 0.096216  | 1.473847  |
| H | 2.627725   | -1.521276 | 0.941341  |
| H | 4.533459   | -0.032414 | 0.688170  |
| H | 3.978287   | -0.523486 | -0.901535 |
| H | 3.316930   | 2.149865  | 0.450960  |
| H | 2.760803   | 1.664127  | -1.150627 |
| H | 4.479496   | 1.932007  | -0.858009 |
| S | -3.415842  | 0.535637  | 0.144208  |
| C | -2.085478  | 1.734447  | 0.341789  |
| H | -1.168801  | 1.306926  | -0.087673 |
| H | -2.299460  | 2.665125  | -0.182041 |
| H | -1.893694  | 1.961524  | 1.390022  |
| H | -0.483718  | -0.399204 | -1.940756 |

n-propylacrylate_TS_13_UNCON_m062x

| Datum                                               | Value     |
|-----------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy               | -823.296048 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139897 |

Number of Imaginary Frequencies

1

Frequencies (Top 3 out of 63)
1. -185.1824 cm⁻¹
2. 35.3465 cm⁻¹
3. 44.3511 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X         | Y         | Z       |
|---------|-----------|-----------|---------|
| C       | 0.334230  | -0.161132 | 0.123142|
| C       | -0.600101 | -0.978203 | -0.588789|
| C       | -1.675857 | -1.537164 | 0.063308|
| O       | 0.308080  | 0.116821  | 1.316415|
| O       | 1.324209  | 0.319008  | -0.686306|
| C       | 2.349416  | 1.096249  | -0.069076|
| C       | 3.415975  | 0.223636  | 0.569010|
| C       | 4.103170  | -0.692329 | -0.435579|
| H       | -2.261156 | -2.296647 | -0.431967|
| H       | -1.649836 | -1.595425 | 1.140834|
| H       | 2.778623  | 1.688502  | -0.877673|
| H       | 1.905378  | 1.766653  | 0.664924|
| H       | 4.148793  | 0.884347  | 1.037769|
| H       | 2.957266  | -0.361881 | 1.367021|
| H       | 4.578868  | -0.111314 | -1.227715|
| H       | 3.384013  | -1.366415 | -0.900649|
| H       | 4.870774  | -1.298194 | 0.044658|
| S       | -3.565654 | -0.059682 | 0.152365|
| C       | -2.711422 | 1.401581  | -0.465931|
| H       | -2.593160 | 2.162806  | 0.304738|
| H       | -1.710669 | 1.100374  | -0.804190|
| H       | -3.232678 | 1.843528  | -1.314078|
| H       | -0.476524 | -1.063890 | -1.658892|

n-propylacrylate_TS_14_UNCON_m062x

| Datum                                           | Value        |
|------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -823.296497  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.1404   |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 63)

1. -187.6321 cm⁻¹
2. 36.6578 cm⁻¹
3. 61.9783 cm⁻¹
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X      | Y      | Z      |
|---|--------|--------|--------|
| C | 0.173921 | -1.063058 | 0.114872 |
| C | -1.050143 | -1.379478 | -0.554769 |
| C | -2.245029 | -1.339474 | 0.126346 |
| O | 0.311470 | -0.770823 | 1.296772 |
| O | 1.252950 | -1.122909 | -0.721909 |
| C | 2.505609 | -0.698172 | -0.192238 |
| C | 2.641161 | 0.813278 | -0.219577 |
| C | 4.001271 | 1.254772 | 0.304905 |
| H | -3.134932 | -1.738627 | -0.335911 |
| H | -2.224432 | -1.371755 | 1.204938 |
| H | 2.625422 | -1.075400 | 0.823481 |
| H | 3.260470 | -1.159801 | -0.828754 |
| H | 2.499990 | 1.159236 | -1.245637 |
| H | 1.841424 | 1.246751 | 0.383216 |
| H | 4.143982 | 0.931814 | 1.337159 |
| H | 4.102155 | 2.338719 | 0.276191 |
| H | 4.807710 | 0.827128 | -0.293018 |
| S | -3.183878 | 0.873623 | 0.178955 |
| C | -1.733775 | 1.725874 | -0.467110 |
| H | -1.985867 | 2.361881 | -1.314639 |
| H | -1.245055 | 2.335610 | 0.29269 |
| H | -1.012803 | 0.972664 | -0.813633 |
| H | -1.009479 | -1.538788 | -1.622758 |

### n-propylacrylate_TS_15_UNCON_m062x

| Datum                                             | Value          |
|---------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy              | -823.296181    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139947    |
| Number of Imaginary Frequencies                   | 1              |
| Frequencies (Top 3 out of 63)                     |                |
| 1. -189.5306 cm$^{-1}$                            |                |
| 2. 37.4187 cm$^{-1}$                              |                |
| 3. 50.8367 cm$^{-1}$                              |                |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.411492 | -1.032445| 0.130026 |
| C | -0.742747| -1.344155| -0.656768|
| C | -1.977469| -1.481960| -0.062174|
| O | 0.445152 | -0.851577| 1.340906 |
| O | 1.546110 | -0.965764| -0.629880|
| C | 2.782297 | -0.646972| 0.008143 |
| C | 3.187507 | 0.784436 | -0.293700|
| C | 2.225120 | 1.808291 | 0.292926 |
| H | -2.791867| -1.908586| -0.627310|
| H | -2.018921| -1.637576| 1.005081 |
| H | 2.688690 | -0.806460| 1.080925 |
| H | 3.517184 | -1.344896| -0.392535|
| H | 4.192610 | 0.938471 | 0.105463 |
| H | 3.254744 | 0.908589 | -1.376827|
| H | 2.187039 | 1.726266 | 1.379745 |
| H | 1.214499 | 1.653252 | -0.086868|
| H | 2.528302 | 2.823322 | 0.037503 |
| S | -3.137163| 0.601518 | 0.159917 |
| C | -1.789694| 1.646535 | -0.418177|
| H | -0.980045| 0.995018 | -0.776067|
| H | -2.098378| 2.284607 | -1.245287|
| H | -1.389084| 2.275641 | 0.376582 |
| H | -0.619287| -1.395584| -1.728950|

n-propylacrylate_TS_16_UNCON_m062x

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296181 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139947 |
| Number of Imaginary Frequencies | 1 |

Frequencies (Top 3 out of 63)

1. -189.5297 cm⁻¹
2. 37.4113 cm⁻¹
3. 50.8273 cm⁻¹
n-propylacrylate_TS_17_UNCON_m062x

| Datum | Value         |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296474 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140846 |

Number of Imaginary Frequencies
1

Frequencies (Top 3 out of 63)

1. -198.0046 cm⁻¹
2.  27.4894 cm⁻¹
3.  45.2616 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 0.218471 | -0.483343 | 0.372513 |
| C       | -0.691294 | -1.043991 | -0.578528 |
| C       | -1.923312 | -1.509633 | -0.175566 |
n-propylacrylate_TS_18_UNCON_m062x

| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296473 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140802 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 63)

1. -190.2879 cm⁻¹
2.  35.5518 cm⁻¹
3.  56.3993 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C    | 0.110711 | -0.712318 | 0.164784 |
|------|----------|-----------|----------|
| C    | -0.950505 | -1.079247 | -0.722276 |
| C    | -2.189540 | -1.417021 | -0.227802 |
| O    | 0.068007  | -0.661721 | 1.388849  |
| O    | 1.262329  | -0.407735 | -0.499578 |
| C    | 2.378818  | -0.032554 | 0.306000  |
| C    | 3.543380  | 0.255751  | -0.621323 |
n-propylacrylate_TS_19_UNCON_m062x

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296128
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.140015

Number of Imaginary Frequencies

Frequencies (Top 3 out of 63)

1. -189.7273 cm⁻¹
2. 42.3735 cm⁻¹
3. 52.5300 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 4.782494 | 0.660616 | 0.166520 |
| H | -2.915717 | -1.876330 | -0.880697 |
| H | -2.272964 | -1.672564 | 0.817706 |
| H | 2.124239 | 0.848040 | 0.894990 |
| H | 2.621003 | -0.840337 | 0.994777 |
| H | 3.750281 | -0.633213 | -1.220122 |
| H | 3.259453 | 1.050225 | -1.314041 |
| H | 4.592535 | 1.556354 | 0.759491 |
| H | 5.619015 | 0.870022 | -0.498339 |
| H | 5.087108 | -0.133651 | 0.849440 |
| S | -3.608472 | 0.495254 | 0.084571 |
| C | -2.324714 | 1.739482 | -0.142042 |
| H | -1.420364 | 1.240681 | -0.516255 |
| H | -2.618701 | 2.491779 | -0.872726 |
| H | -2.072228 | 2.241814 | 0.791505 |
| H | -0.764677 | -0.999489 | -1.783799 |

|   |   |   |
|---|---|---|
| C | -0.245252 | -0.366061 | 0.098606 |
| C | 0.851548 | -1.006696 | 0.757681 |
| C | 1.909080 | -1.503044 | 0.030354 |
| O | -0.378731 | -0.189195 | -1.106604 |
| O | -1.198436 | 0.062468 | 0.978610 |
| C | -2.365086 | 0.667791 | 0.428259 |
| C | -3.383610 | -0.363851 | -0.019891 |
| C | -4.645237 | 0.305485 | -0.549667 |
| H | 2.628955 | -2.147305 | 0.511150 |
| H | 1.774857 | -1.660317 | -1.028938 |
| H | -2.775781 | 1.282837 | 1.229156 |
n-propylacrylate_TS_1_UNCON_m062x

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.296286 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139308 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 63)

1. -202.1746 cm⁻¹
2. 48.0960 cm⁻¹
3. 57.9816 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C | 0.587763 | -1.480089 | 0.183356 |
| C | -0.792512 | -1.807984 | 0.018023 |
| C | -1.604022 | -1.232185 | -0.941083 |
| O | 1.327751 | -1.900521 | 1.069364 |
| O | 1.061766 | -0.627792 | -0.771860 |
| C | 2.350288 | -0.058020 | -0.554249 |
| C | 2.252103 | 1.171464 | 0.332345 |
| C | 1.438293 | 2.287370 | -0.311152 |
| H | -2.582017 | -1.655974 | -1.114127 |
| H | -1.147538 | -0.768686 | -1.801087 |
| H | 3.013963 | -0.804239 | -0.122579 |
| H | 2.716236 | 0.213711 | -1.544894 |
| H | 1.804198 | 0.874422 | 1.283774 |
| H | 3.264973 | 1.517952 | 0.549776 |
| H | 0.431219 | 1.941739 | -0.549601 |
n-propylacrylate_TS_20_UNCON_m062x

| Datum                                                | Value       |
|------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                | -823.280924 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.125582 |
| Number of Imaginary Frequencies                      | 1           |

**Frequencies** (Top 3 out of 63)

1.  -231.7627 cm⁻¹
2.   27.8383 cm⁻¹
3.   37.3630 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | 1.423935 | 1.281843 | -0.120285 |
| C          | -0.160134| 1.801755 | 0.306970  |
| C          | 1.071046 | 1.512718 | -0.239658 |
| O          | -2.501410| 1.775707 | 0.194731  |
| O          | -1.476077| 0.243291 | -1.013722 |
| C          | -0.686857| -0.938221| -0.831128 |
| C          | -1.548299| -2.054371| -0.270950 |
| C          | -2.049718| -1.732878| 1.131186  |
| H          | 1.876931 | 2.216391 | -0.095848 |
| H          | 1.133908 | 0.934565 | -1.153056 |
| H          | -0.293178| -1.204035| -1.813097 |
| H          | 0.148388 | -0.745839| -0.158029 |
| H          | -2.388591| -2.236154| -0.944344 |
| H          | -0.945377| -2.965656| -0.257485 |
| H          | -2.670482| -0.836270| 1.122618  |
| H          | -1.209480| -1.552668| 1.805508  |
| H          | -2.642518| -2.550323| 1.540260  |
| S          | 2.463483 | -0.135804| 0.836933  |
| C          | 3.111355 | -0.717494| -0.755036 |
n-propylacrylate_TS_21_UNCON_m062x

| Datum                                                   | Value         |
|---------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -823.286504   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.130025   |
| Number of Imaginary Frequencies                        | 1             |

**Frequencies** (Top 3 out of 63)

1.  -196.7059 cm⁻¹
2.   30.8511 cm⁻¹
3.   63.0580 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.934059 | 1.491399 | 0.197691 |
|-------|-----------|----------|----------|
| C     | 0.484815  | 1.699154 | 0.219895 |
| C     | 1.384707  | 1.345171 | -0.762291|
| O     | -1.717355 | 2.083408 | 0.931539 |
| O     | -1.498033 | 0.675918 | -0.746081|
| C     | -0.937633 | -0.602084| -1.063113|
| C     | -1.924037 | -1.685020| -0.669914|
| C     | -2.172139 | -1.708736| 0.832507 |
| H     | 2.315571  | 1.886467 | -0.822817|
| H     | 1.031203  | 0.946742 | -1.702227|
| H     | -0.741488 | -0.623498| -2.136759|
| H     | 0.007619  | -0.742967| -0.542569|
| H     | -2.861750 | -1.527571| -1.207093|
| H     | -1.520578 | -2.643405| -1.005053|
| H     | -2.572292 | -0.751795| 1.169197 |
| H     | -1.241220 | -1.890858| 1.373076 |
| H     | -2.881382 | -2.488697| 1.107265 |
| S     | 2.652671  | -0.636804| -0.241878|
| C     | 1.789642  | -1.041246| 1.287570 |
| H     | 1.002979  | -0.290040| 1.454487 |
| H     | 1.314662  | -2.021114| 1.238005 |
| H     | 2.458429  | -1.022682| 2.146824 |
| H     | 0.820844  | 2.291861 | 1.059982 |
n-propylacrylate_TS_22_UNCON_m062x

### Datum

| Description | Value         |
|-------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -823.280737   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.125298   |
| Number of Imaginary Frequencies          | 1             |

### Frequencies (Top 3 out of 63)

1. -223.1260 cm\(^{-1}\)
2. 26.1672 cm\(^{-1}\)
3. 42.5501 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C         | 1.250611 | 1.331741 | 0.098797 |
| C         | -0.029792 | 1.765899 | -0.367269 |
| C         | -1.238806 | 1.407351 | 0.181883  |
| O         | 2.313364  | 1.840134 | -0.234948 |
| O         | 1.308956  | 0.338569 | 1.052449  |
| C         | 0.784766  | -0.950441| 0.703152  |
| C         | 1.493970  | -1.543438| -0.500434 |
| C         | 2.994752  | -1.698297| -0.294971 |
| H         | -2.104257 | 2.022734 | -0.012277 |
| H         | -1.261886 | 0.870203 | 1.121011  |
| H         | 0.956550  | -1.564572| 1.587599  |
| H         | -0.285409 | -0.895706| 0.506673  |
| H         | 1.032912  | -2.512022| -0.707876 |
| H         | 1.293172  | -0.913733| -1.372562 |
| H         | 3.469524  | -2.142662| -1.169241 |
| H         | 3.202072  | -2.339176| 0.563996  |
| H         | 3.455416  | -0.728105| -0.111651 |
| S         | -2.515018 | -0.412939| -0.808431 |
| C         | -3.282247 | -0.752625| 0.800155  |
| H         | -2.568664 | -1.213137| 1.486819  |
| H         | -3.638883 | 0.173440 | 1.256014  |
| H         | -4.133430 | -1.423655| 0.695133  |
| H         | 0.005079  | 2.482647 | -1.176626 |
n-propylacrylate_TS_23_UNCON_m062x

| Datum                                                                 | Value     |
|----------------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.280607 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -823.124984 |

Number of Imaginary Frequencies

1

Frequencies (Top 3 out of 63)

1. -237.7369 cm⁻¹
2.  33.0504 cm⁻¹
3.  50.5078 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     |    |    |    |
|-----|----|----|----|
| C   | -2.001499 | -0.908009 | -0.017992 |
| C   | -0.941058 | -1.871085 | -0.034748 |
| C   |  0.293039 | -1.800093 |  0.580837 |
| O   | -3.152495 | -1.174244 | -0.352911 |
| O   | -1.814089 |  0.364645 |  0.443467 |
| C   | -0.565355 |  1.048693 |  0.332074 |
| C   | -0.813611 |  2.456776 | -0.167690 |
| C   |  0.497972 |  3.227357 | -0.257206 |
| H   |  0.814464 | -2.727456 |  0.765204 |
| H   |  0.508979 | -1.022459 |  1.299560 |
| H   | -0.093562 |  1.085528 |  1.318189 |
| H   |  0.101840 |  0.519115 | -0.348290 |
| H   | -1.291393 |  2.404519 | -1.147962 |
| H   | -1.508951 |  2.963630 |  0.504192 |
| H   |  0.340136 |  4.236998 | -0.633165 |
| H   |  1.197746 |  2.723171 | -0.926631 |
| H   |  0.971973 |  3.304331 |  0.722820 |
| S   |  2.174439 | -1.063354 | -0.698285 |
| C   |  2.872007 | -0.083458 |  0.660836 |
| H   |  2.827303 | -0.643361 |  1.597127 |
| H   |  3.915939 |  0.159954 |  0.468435 |
| H   |  2.323300 |  0.850526 |  0.795900 |
| H   | -1.215093 | -2.785133 | -0.543927 |

n-propylacrylate_TS_24_UNCON_m062x
| Datum                                           | Value          |
|------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -823.285149    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.128957    |

Number of Imaginary Frequencies 1

**Frequencies** (Top 3 out of 63)

1. -200.8378 cm⁻¹
2. 34.0236 cm⁻¹
3. 43.7972 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        |        |        |
|--------|--------|--------|
| C      | -0.480049 | 1.691898 | 0.135819 |
| C      | 0.890081  | 1.598848 | -0.278761|
| C      | 1.448978  | 0.760844 | -1.222967|
| O      | -0.925616 | 2.653237 | 0.755428 |
| O      | -1.402443 | 0.742886 | -0.200564|
| C      | -1.068789 | -0.637308| -0.366247 |
| C      | -2.109512 | -1.475802| 0.349392 |
| C      | -3.511695 | -1.296369| -0.217231 |
| H      | 2.375971  | 1.069729 | -1.680634 |
| H      | 0.825126  | 0.147527 | -1.853931 |
| H      | -1.070572 | -0.873996| -1.434178 |
| H      | -0.074933 | -0.835370| 0.026378 |
| H      | -1.802727 | -2.521073| 0.266535 |
| H      | -2.093159 | -1.221748| 1.411656 |
| H      | -4.232429 | -1.922690| 0.307302 |
| H      | -3.536675 | -1.567185| -1.274330|
| H      | -3.836200 | -0.260248| -0.128097|
| S      | 2.580630  | -1.124501| -0.282897 |
| C      | 2.068116  | -0.849372| 1.422408 |
| H      | 1.450254  | -1.664186| 1.799694 |
| H      | 2.922970  | -0.725991| 2.085451 |
| H      | 1.474055  | 0.076013 | 1.460878 |
| H      | 1.509932  | 2.365820 | 0.166246 |

**n-propylacrylate_TS_25_UNCON_m062x**

| Datum                                           | Value          |
|------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -823.291258    |
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| Datum | Value                        |
|-------|-----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.136363 |
| Number of Imaginary Frequencies | 1 |

**Frequencies (Top 3 out of 63)**

1.  -221.3390 cm\(^{-1}\)
2.  34.5866 cm\(^{-1}\)
3.  49.1308 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |               |               |               |
|-----|---------------|---------------|---------------|
| C   | 0.497808      | -0.789976     | 0.208781      |
| C   | -0.657176     | -1.353626     | -0.417844     |
| C   | -1.912433     | -1.103366     | 0.085436      |
| O   | 0.520828      | -0.074880     | 1.203637      |
| O   | 1.655017      | -1.142194     | -0.425948     |
| C   | 2.868519      | -0.604390     | 0.092902      |
| C   | 3.135793      | 0.796512      | -0.425463     |
| C   | 4.455515      | 1.336389      | 0.110460      |
| H   | -2.756434     | -1.674408     | -0.273948     |
| H   | -1.999535     | -0.734170     | 1.098038      |
| H   | 2.836671      | -0.608581     | 1.182541      |
| H   | 3.651720      | -1.286925     | -0.237346     |
| H   | 3.152158      | 0.770474      | -1.516852     |
| H   | 2.310682      | 1.444237      | -0.126632     |
| H   | 4.656245      | 2.336810      | -0.270009     |
| H   | 5.287627      | 0.693512      | -0.181152     |
| H   | 4.440519      | 1.388597      | 1.200105      |
| S   | -3.055023     | 0.882777      | -0.630411     |
| C   | -4.343185     | 0.631859      | 0.622890      |
| H   | -5.293057     | 1.057453      | 0.303695      |
| H   | -4.070863     | 1.082318      | 1.576699      |
| H   | -4.497469     | -0.438506     | 0.789145      |
| H   | -0.514492     | -1.894277     | -1.342191     |

### n-propylacrylate_TS_26_UNCON_m062x

| Datum | Value                        |
|-------|-----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.29573 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139636 |
**Datum** | **Value**
---|---
Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 63)

1. -190.4109 cm⁻¹
2. 33.0459 cm⁻¹
3. 40.3239 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 0.384173 | -0.111023 | 0.033183 |
|-----|----------|-----------|----------|
| C   | -0.580155| -0.693207 | 0.916837 |
| C   | -1.603952| -1.464577 | 0.416938 |
| O   | 0.417613 | -0.217724 | -1.186061|
| O   | 1.322169 | 0.618057  | 0.709050 |
| C   | 2.411105 | 1.176391  | -0.024724|
| C   | 3.666443 | 0.344707  | 0.169599 |
| C   | 3.529895 | -1.070505 | -0.376361|
| H   | -2.209372| -2.048392 | 1.093114 |
| H   | -1.509789| -1.855575 | -0.584609|
| H   | 2.144258 | 1.239060  | -1.078212|
| H   | 2.554012 | 2.183095  | 0.366862 |
| H   | 3.905735 | 0.314040  | 1.234891 |
| H   | 4.490869 | 0.862649  | -0.325648|
| H   | 4.441269 | -1.643944 | -0.209640|
| H   | 3.325321 | -1.055110 | -1.447248|
| H   | 2.708260 | -1.597283 | 0.111080 |
| S   | -3.508833| -0.149841 | -0.243338|
| C   | -2.723007| 1.459550  | -0.043056|
| H   | -2.577362| 1.964613  | -0.997549|
| H   | -3.301284| 2.111663  | 0.610235 |
| H   | -1.736865| 1.308967  | 0.416914 |
| H   | -0.518979| -0.437020 | 1.964794 |

**n-propylacrylate_TS_27_UNCON_m062x**

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.286476 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.129522 |
| Number of Imaginary Frequencies | 1 |
**Frequencies** (Top 3 out of 63)

1. \(-181.3012\) cm\(^{-1}\)
2. \(60.8337\) cm\(^{-1}\)
3. \(64.9417\) cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |         |         |         |
|-----|---------|---------|---------|
| C   | 0.799288| 1.434898| 0.195528|
| C   | -0.611953| 1.670001| 0.299670|
| C   | -1.532407| 1.376569| -0.675269|
| O   | 1.635042 | 1.893569| 0.960075 |
| O   | 1.256515 | 0.725865| -0.894379|
| C   | 0.925099 | -0.668589| 0.054503 |
| H   | -2.490574| 1.870480| -0.660738|
| H   | -1.196496| 1.036013| -1.643720|
| H   | -0.154766| -0.803483| -0.859974|
| H   | 1.248424 | -1.003201| -1.922555|
| H   | 1.302869 | -1.098584| 1.125763 |
| H   | 1.330980 | -2.492639| 0.066177 |
| H   | 3.649067 | -1.931778| 0.827956 |
| H   | 3.474058 | -0.302287| 0.171297 |
| H   | 3.515932 | -1.693010| -0.915429|
| S   | -2.753393| -0.725169| -0.245154|
| C   | -1.759628| -1.221964| 1.174824 |
| H   | -1.203893| -2.140368| 0.983587 |
| H   | -1.030489| -0.427398| 1.388270 |
| H   | -2.370683| -1.364582| 2.065082 |
| H   | -0.917856| 2.184077 | 1.201142 |

**n-propylacrylate_TS_28_UNCON_m062x**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.280737 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.125294 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 63)
1.  -223.1178 cm⁻¹
2.   26.4036 cm⁻¹
3.   42.4995 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| C | 1.250599| 1.331740| 0.098764|
| C | -0.029813| 1.765859| -0.367310|
| C | -1.238849| 1.407272| 0.181791|
| O | 2.313338| 1.840139| -0.235026|
| O | 1.308988| 0.338637| 1.052484|
| C | 0.784893| -0.950440| 0.703292|
| C | 1.494043| -1.543439| -0.500324|
| C | 2.994850| -1.698206| -0.294983|
| H | -2.104319| 2.022590| -0.012502|
| H | -1.261972| 0.870218| 1.120972|
| H | 0.956813| -1.564510| 1.587756|
| H | -0.285303| -0.895825| 0.506906|
| H | 1.033027| -2.512060| -0.707687|
| H | 1.293132| -0.913787| -1.372463|
| H | 3.202278| -2.338925| 0.564079|
| H | 3.455507| -0.727971| -0.111885|
| H | 3.469548| -2.142715| -1.169220|
| S | -2.514952| -0.413138| -0.808413|
| C | -3.282553| -0.752352| 0.800095|
| H | -4.134244| -1.422722| 0.694972|
| H | -2.569382| -1.213427| 1.486803|
| H | -3.638531| 0.173968| 1.255961|
| H | 0.005052| 2.482563| -1.176707|

**n-propylacrylate_TS_2_UNCON_m062x**

| Datum                                                   | Value         |
|---------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -823.290649   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.134391   |
| Number of Imaginary Frequencies                        | 1             |

**Frequencies** *(Top 3 out of 63)*

1.  -246.6090 cm⁻¹
2.   48.7749 cm⁻¹
3.   61.2303 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | -0.918703| -1.453437| 0.045137 |
| C       | 0.370059 | -2.059324| -1.155795|
| C       | 1.498848 | -1.547064| 0.450520 |
| O       | -1.952629| -1.852929| -0.573763|
| O       | -0.924292| -0.335293| 0.735493 |
| C       | -2.141658| 0.402938 | 0.813355 |
| C       | -2.324024| 1.314110 | -0.388218|
| C       | -1.175761| 2.301979 | -0.553776|
| H       | 2.404311 | -2.136202| 0.436373 |
| H       | 1.387989 | -0.897390| 1.307217 |
| H       | -2.981650| -0.282388| 0.914791 |
| H       | -2.053082| 0.993994 | 1.725511 |
| H       | -2.425833| 0.697802 | -1.282788|
| H       | -3.268059| 1.848647 | -0.258908|
| H       | -0.232614| 1.777483 | -0.714712|
| H       | -1.065849| 2.921170 | 0.339108 |
| H       | -1.346907| 2.963622 | -1.402692|
| S       | 2.540597 | 0.311577 | 0.620267 |
| C       | 2.209316 | 1.448457 | 0.758379 |
| H       | 1.182972 | 1.321408 | 1.106926 |
| H       | 2.885009 | 1.266724 | 1.594503 |
| H       | 2.334915 | 2.483338 | 0.441105 |
| H       | 0.436157 | -2.883612| -0.851954|

n-propylacrylate_TS_3_UNCON_m062x

| Datum                                                                 | Value       |
|-----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -823.296424|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -823.14028  |
| Number of Imaginary Frequencies                                       | 1           |

Frequencies (Top 3 out of 63)

1. -202.9832 cm\(^{-1}\)
2. 34.7653 cm\(^{-1}\)
3. 46.0316 cm\(^{-1}\)
**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | -0.281936 | 1.580021 | 0.090925 |
|------|-----------|----------|----------|
| C    | 1.047510  | 1.662135 | -0.428224|
| C    | 1.583942  | 0.727445 | -1.290714|
| O    | -0.810483 | 2.378816 | 0.860248 |
| O    | -0.972431 | 0.493484 | -0.350273|
| C    | -2.291793 | 0.322452 | 0.158728 |
| C    | -2.853791 | -0.955359| -0.427132|
| C    | -2.064863 | -2.191706| -0.014546|
| H    | 2.518377  | 0.950507 | -1.784011|
| H    | 0.917273  | 0.082251 | -1.840588|
| H    | -2.252533 | 0.266201 | 1.249446 |
| H    | -2.902161 | 1.185566 | -0.110463|
| H    | -3.890356 | -1.043734| -0.095903|
| H    | -2.875299 | -0.866339| -1.515423|
| H    | -2.510629 | -3.097395| -0.424370|
| H    | -2.042893 | -2.288605| 1.072555 |
| H    | -1.034770 | -2.131536| -0.366117|
| S    | 2.533243  | -1.138847| -0.165629|
| C    | 1.758013  | -0.823392| 1.430153 |
| H    | 0.927211  | -1.502013| 1.623926 |
| H    | 2.475814  | -0.907932| 2.244791 |
| H    | 1.367765  | 0.202480 | 1.427571 |
| H    | 1.651127  | 2.464115 | -0.026292|

**n-propylacrylate_TS_4_UNCON_m062x**

| Datum | Value     |
|-------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -823.295637 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139891 |

Number of Imaginary Frequencies 1

**Frequencies** (Top 3 out of 63)

1. -199.8551 cm⁻¹
2.  27.6314 cm⁻¹
3.  47.7665 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
### n-propylacrylate_TS_5_UNCON_m062x

| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -823.295437   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -823.139675   |
| Number of Imaginary Frequencies                                      | 1             |

#### Frequencies (Top 3 out of 63)

1. -198.9504 cm⁻¹  
2. 30.1126 cm⁻¹  
3. 43.5154 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C           | -0.226691 | 1.461752 | -0.130895 |
| C           | 0.992785  | 1.372390 | -0.872147 |
| O           | -0.667538 | 2.467998 | 0.418470  |
| O           | -0.915740 | 0.289891 | -0.071665 |
| C           | -2.145213 | 0.304567 | 0.648044  |
| C           | -2.728356 | -1.091509| 0.598231  |
| C           | -3.063911 | -1.540670| -0.818179 |
| H           | 2.244184  | 0.275127 | -2.189892 |
| H           | 0.714628  | -0.572617| -1.676251 |
| H           | -1.959968 | 0.620995 | 1.675494  |
| H           | -2.824998 | 1.027925 | 0.191319  |
| H           | -2.021431 | -1.785998| 1.057709  |
| H           | -3.627540 | -1.097957| 1.217349  |
| H           | -3.505089 | -2.536735| -0.821419 |
| H           | -2.168917 | -1.564388| -1.439139 |
| H           | -3.776031 | -0.854943| -1.280773 |
| S           | 2.688213  | -1.195977| -0.043754 |
| C           | 2.197336  | -0.399917| 1.496557  |
| H           | 1.714589  | 0.555374 | 1.252435  |
| H           | 1.488654  | -1.003646| 2.063024  |
| H           | 3.058309  | -0.188673| 2.129183  |
| H           | 1.607657  | 2.261578 | -0.855653 |
### n-propylacrylate_TS_6_UNCON_m062x

| Datum | Value            |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -823.295034 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.138743 |

Number of Imaginary Frequencies: 1

**Frequencies (Top 3 out of 63)**

1. -196.3583 cm⁻¹
2. 38.0449 cm⁻¹
3. 46.1265 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          | X         | Y         | Z         |
|----------|-----------|-----------|-----------|
| O        | -0.980837 | 1.767714  | 1.153414  |
| O        | -0.664265 | 0.648971  | -0.776143 |
| C        | -2.049012 | 0.314747  | -0.785356 |
| C        | -2.333074 | -0.921834 | 0.046894  |
| C        | -3.811844 | -1.284690 | 0.006747  |
| H        | 3.051962  | 1.470560  | -0.776249 |
| H        | 1.607266  | 0.811215  | -1.670749 |
| H        | -2.636024 | 1.160519  | -0.427742 |
| H        | -2.296015 | 0.133643  | -1.831537 |
| H        | -1.728479 | -1.747250 | -0.334810 |
| H        | -2.014745 | -0.733439 | 1.073526  |
| H        | -4.014489 | -2.180794 | 0.591426  |
| H        | -4.140515 | -1.470979 | -1.016998 |
| H        | -4.421937 | -0.475379 | 0.410614  |
| S        | 2.792096  | -1.119225 | -0.320855 |
| C        | 1.680507  | -1.472744 | 1.052289  |
| H        | 0.941210  | -2.230662 | 0.795068  |
| H        | 1.145869  | -0.548153 | 1.309497  |
| H        | 2.224589  | -1.802904 | 1.936177  |
| H        | 1.609735  | 2.078018  | 1.139440  |
n-propylacrylate_TS_7_UNCON_m062x_reopt

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.295147    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.138847    |

Number of Imaginary Frequencies
1

Frequencies (Top 3 out of 63)

1. -200.9284 cm⁻¹
2. 27.8511 cm⁻¹
3. 50.9087 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 0.500500 | -1.300919 | 0.353451 |
| C   | -0.890999 | -1.621721 | 0.445652 |
| C   | -1.811325 | -1.335925 | -0.541629 |
| O   | 1.360245  | -1.601430 | 1.175795 |
| O   | 0.819994  | -0.615225 | -0.781046 |
| C   | 2.184416  | -0.268636 | -1.015528 |
| C   | 2.432749  | 1.195005  | -0.699710 |
| C   | 2.320981  | 1.515419  | 0.784871 |
| H   | -2.785094 | -1.800833 | -0.493729 |
| H   | -1.458059 | -1.109494 | -1.535008 |
| H   | 2.831270  | -0.910844 | -0.420052 |
n-propylacrylate_TS_8_UNCON_m062x

| Datum | Value         |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy  | -823.295477 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139998 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 63)

1. -197.4896 cm⁻¹
2. 36.2689 cm⁻¹
3. 50.5428 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.048062 | 1.454952 | 0.091117 |
|-------|----------|----------|----------|
| C     | 1.281887 | 1.517457 | -0.431079 |
| C     | 1.807057 | 0.582081 | -1.297741 |
| O     | -0.565258 | 2.271097 | 0.848936 |
| O     | -0.754444 | 0.371613 | -0.334624 |
| C     | -2.090541 | 0.255073 | 0.143359 |
| C     | -2.690671 | -1.004776 | 1.235014 |
| C     | -4.127895 | -1.196610 | 0.025571 |
| H     | 2.356282 | 0.803064 | -1.002283 |
| H     | 1.135607 | -0.69318 | -1.34259 |
| H     | -2.086903 | 0.215248 | 1.235014 |
| H     | -2.665595 | 1.135207 | -0.152963 |
| H     | -2.652029 | -0.944083 | -1.530370 |
| H     | -4.560015 | -2.102850 | -0.395868 |
### n-propylacrylate_TS_9_UNCON_m062x

| Datum                                      | Value              |
|--------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -823.294998        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -823.139103        |

**Number of Imaginary Frequencies** 1

#### Frequencies (Top 3 out of 63)

1. -197.5854 cm\(^{-1}\)
2. 38.8321 cm\(^{-1}\)
3. 43.0094 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 0.266920 | 0.982587 | 0.304347 |
| C   | 0.958525 | 1.486860 | -0.234834|
| C   | 1.674979 | 0.853565 | -1.227722|
| O   | -0.946884| 1.523244 | 1.171556 |
| O   | -0.652187| -0.207173| -0.239437|
| C   | -1.899765| -0.744597| 0.190817 |
| C   | -3.068817| -0.144552| -0.567778|
| C   | -4.386775| -0.766225| -0.123942|
| H   | 2.474569 | 1.389891 | -1.716344|
| H   | 1.186133 | 0.104773 | -1.830293|
| H   | -1.833140| -1.815719| -0.000593|
| H   | -2.018053| -0.586399| 1.262784 |
| H   | -3.080993| 0.933044 | -0.398857|
| H   | -2.914666| -0.306088| -1.636544|
| H   | -4.384051| -1.845107| -0.287454|
| H   | -5.226762| -0.346354| -0.675311|
| H   | -4.561386| -0.590597| 0.938570 |
| S   | 3.213322 | -0.770619| -0.378778|
| C   | 2.533041 | -0.837045| 1.288541 |
|  |  |  |
|---|---|---|
| H | 1.827201 | -0.004392 | 1.407101 |
| H | 1.995898 | -1.766452 | 1.475876 |
| H | 3.311036 | -0.727195 | 2.042830 |
| H | 1.338017 | 2.378382 | 0.245161 |
**1_pentene-3-one_truncated_1**

| Datum                                                                 | Value            |
|-----------------------------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -231.227508      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -231.162782      |
| Number of Imaginary Frequencies                                        | 0                |

**Frequencies (Top 3 out of 27)**

1. 123.2502 cm⁻¹  
2. 159.7787 cm⁻¹  
3. 300.6150 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     | X   | Y   | Z   |
|-----|-----|-----|-----|
| C   | -0.826853 | 1.293812 | 0.000000 |
| H   | -0.384491 | 1.763114 | 0.878963 |
| H   | -1.900669 | 1.453387 | -0.000001 |
| C   | -0.542713 | -0.184126 | -0.000002 |
| H   | -0.384489 | 1.763116 | -0.878961 |
| C   | 0.866606  | -0.648954 | 0.000001  |
| O   | -1.440894 | -1.001993 | -0.000006 |
| C   | 1.916006  | 0.163733 | 0.000006  |
| H   | 2.925190  | -0.225188 | 0.000008  |
| H   | 1.806529  | 1.240522 | 0.000008  |
| H   | 0.986797  | -1.725800 | -0.000001 |
### 1_pentene-3-one_truncated_2

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -231.226386 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -231.162235 |

Number of Imaginary Frequencies

**Frequencies (Top 3 out of 27)**

1. 69.2637 cm⁻¹  
2. 141.8725 cm⁻¹  
3. 276.6380 cm⁻¹  

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**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 1.163030 | 1.423480 | 0.000000 |
| H | 1.785624 | 1.234348 | 0.876313 |
| H | 0.818211 | 2.452875 | 0.000000 |
| C | 0.000000 | 0.473637 | 0.000000 |
| H | 1.785624 | 1.234348 | -0.876313 |
| C | 0.342042 | -0.979598 | 0.000000 |
| O | -1.149435 | 0.859046 | 0.000000 |
| C | -0.601670 | -1.910979 | 0.000000 |
| H | -0.360685 | -2.964942 | 0.000000 |
| H | -1.647057 | -1.628325 | 0.000000 |
| H | 1.393353 | -1.239908 | 0.000000 |

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### 1_pentene-3-one_trunc_HEI_1

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -669.451211 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.351765 |

Number of Imaginary Frequencies

**Frequencies (Top 3 out of 42)**

1. 78.4530 cm⁻¹  
2. 97.4899 cm⁻¹  

3. 109.7831 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|      |         |         |         |
|------|---------|---------|---------|
| C    | -1.594231 | -0.023062 | 0.130894 |
| C    | -0.610517  | -0.929647  | -0.191544 |
| C    | 0.642447   | -1.045653  | 0.587993  |
| O    | -1.574597  | 0.800674   | 1.109540  |
| H    | -0.734764  | -1.562413  | -1.061618 |
| H    | 0.526936   | -0.580426  | 1.566424  |
| H    | 0.967820   | -2.077190  | 0.733976  |
| C    | 1.548936   | 1.430218   | -0.314502 |
| H    | 1.527528   | 1.909009   | 0.662677  |
| H    | 0.545070   | 1.422696   | -0.737351 |
| H    | 2.222877   | 1.976256   | -0.970762 |
| S    | 2.135787   | -0.267989  | -0.190811 |
| C    | -2.842004  | 0.013255   | -0.741619 |
| H    | -2.814542  | -0.710232  | -1.556016 |
| H    | -3.723149  | -0.180233  | -0.125727 |
| H    | -2.961375  | 1.014301   | -1.162277 |

1_pentene-3-one_trunc_HEI_2

| Datum                                    | Value         |
|------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -669.447746   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.34827    |

Number of Imaginary Frequencies

0

Frequencies (Top 3 out of 42)

1. 74.9024 cm⁻¹
2. 100.1561 cm⁻¹
3. 118.2623 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|      |         |         |         |
|------|---------|---------|---------|
| C    | -1.686191 | -0.160400 | -0.099270 |
| C    | -0.629063 | -1.042791 | -0.089567 |
| C    | 0.599687  | -0.969265 | 0.732702 |
### 1_pentene-3-one_trunc_HEI_3

| Datum                                    | Value            |
|------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -669.450513      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.351422      |
| Number of Imaginary Frequencies          | 0                |

#### Frequencies (Top 3 out of 42)

1. 60.3905 cm\(^{-1}\)
2. 87.2277 cm\(^{-1}\)
3. 101.0128 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | -1.722719 | -0.060916 | 0.002746 |
|--------|-----------|-----------|----------|
| C      | -0.601697 | 0.389393  | 0.662119 |
| C      | 0.536654  | -0.512517 | 0.946590 |
| O      | -1.907187 | -1.251517 | -0.424716|
| H      | -0.539071 | 1.425773  | 0.966591 |
| H      | 1.045705  | -0.272038 | 1.881248 |
| H      | 0.202268  | -1.549367 | 0.989129 |
| C      | 2.391805  | 1.162451  | -0.259742|
| H      | 2.792193  | 1.401440  | 0.724954 |
| H      | 1.545383  | 1.812468  | -0.475406|
| H      | 3.165688  | 1.320526  | -1.007327|
| S      | 1.877581  | -0.561970 | -0.336279|
| C      | -2.858009 | 0.922360  | -0.243363|
| H      | -2.649615 | 1.918308  | 0.146582 |
### 1_pentene-3-one_trunc_HEI_4

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.446335 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.347804 |

**Frequencies** (Top 3 out of 42)

1. 42.4781 cm⁻¹
2. 76.7734 cm⁻¹
3. 95.7518 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 1.757821 | 0.242688 | 0.013807 |
|-------|----------|----------|----------|
| C     | 0.606662 | 0.570038 | 0.695576 |
| C     | -0.496293 | -0.350136 | 1.064826 |
| O     | 2.688490 | 1.065590 | -0.291624 |
| H     | 0.475570 | 1.616171 | 0.954720 |
| H     | -0.166498 | -1.361263 | 1.300081 |
| H     | -1.040091 | 0.018571 | 1.935444 |
| C     | -2.327146 | 1.059017 | -0.485315 |
| H     | -1.470202 | 1.664228 | -0.776688 |
| H     | -2.771230 | 1.469740 | 0.420718 |
| H     | -3.066116 | 1.071686 | -1.282975 |
| S     | -1.808446 | -0.645424 | -0.226252 |
| C     | 1.995109 | -1.193783 | -0.437272 |
| H     | 2.926222 | -1.557450 | 0.002304 |
| H     | 1.193527 | -1.886415 | -0.189554 |
| H     | 2.129116 | -1.200156 | -1.520750 |

### 1_pentene-3-one_trunc_HEI_5

| Datum | Value |
|-------|-------|
### SI_ketones.md

| Datum                                                                 | Value             |
|----------------------------------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.450723       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.351983       |
| Number of Imaginary Frequencies                                      | 0                 |

#### Frequencies (Top 3 out of 42)

1. 60.0177 cm⁻¹  
2. 82.6555 cm⁻¹  
3. 88.1153 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.839392  | 0.161371  | 0.057582  |
| C | 0.837178  | -0.691971 | 0.458993  |
| C | -0.514698 | -0.194370 | 0.814903  |
| O | 1.744500  | 1.431484  | -0.055193 |
| H | 1.024194  | -1.757160 | 0.499193  |
| H | -0.982326 | -0.766771 | 1.617966  |
| H | -0.471022 | 0.855197  | 1.107174  |
| C | -3.177773 | 0.349517  | 0.154733  |
| H | -3.023931 | 1.367964  | 0.508321  |
| H | -3.478431 | -0.281438 | 0.989999  |
| H | -3.969114 | 0.349343  | -0.591586 |
| S | -1.674267 | -0.289029 | -0.614624 |
| C | 3.197099  | -0.439294 | -0.278061 |
| H | 3.223710  | -1.522382 | -0.161586 |
| H | 3.461403  | -0.188040 | -1.307668 |
| H | 3.960590  | 0.004364  | 0.364805  |

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**1_pentene-3-one_trunc_HEI_6**

| Datum                                                                 | Value             |
|----------------------------------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -669.447007       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -669.348535       |
| Number of Imaginary Frequencies                                      | 0                 |

#### Frequencies (Top 3 out of 42)

1. 60.0177 cm⁻¹  
2. 82.6555 cm⁻¹  
3. 88.1153 cm⁻¹  

---
1.  54.9921 cm\(^{-1}\)
2.  70.9232 cm\(^{-1}\)
3.  93.9559 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X Coordinate  | Y Coordinate  | Z Coordinate |
|---------|---------------|---------------|--------------|
| C       | -1.940682     | -0.094426     | 0.015405     |
| C       | -0.868079     | -0.903273     | 0.314278     |
| C       | 0.475207      | -0.453312     | 0.766411     |
| O       | -3.088507     | -0.508935     | -0.369362    |
| H       | -1.001294     | -1.971317     | 0.172064     |
| H       | 0.449971      | 0.450801      | 1.374671     |
| H       | 0.977788      | -1.225798     | 1.350268     |
| C       | 3.120241      | 0.307493      | 0.231727     |
| H       | 3.455235      | -0.545933     | 0.819449     |
| H       | 2.969622      | 1.162686      | 0.888985     |
| H       | 3.885164      | 0.554928      | -0.500957    |
| S       | 1.596600      | -0.089227     | -0.653596    |
| C       | -1.810860     | 1.419251      | 0.142248     |
| H       | -2.501450     | 1.777038      | 0.909135     |
| H       | -0.808390     | 1.769814      | 0.379773     |
| H       | -2.119151     | 1.872501      | -0.801362    |

### 1_pentene-3-one_trunc_TS_1

| Datum                                                                 | Value        |
|-----------------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -669.435969  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -669.339302  |

| Number of Imaginary Frequencies                                       | 1            |

#### Frequencies (Top 3 out of 42)

1.  -164.8676 cm\(^{-1}\)
2.   37.8484 cm\(^{-1}\)
3.   42.9396 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### 1_pentene-3-one_trunc_TS_2

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy       | -669.437096 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.339121 |
| Number of Imaginary Frequencies | 1 |

#### Frequencies (Top 3 out of 42)

1. -191.8724 cm⁻¹  
2. 68.2150 cm⁻¹  
3. 92.3069 cm⁻¹  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 1.705684 | 0.002919 | -0.092905 |
|-------|----------|----------|-----------|
| C     | -0.777795| -0.907357| -0.691104 |
| C     | 0.244610 | -1.511648| 0.006323  |
| O     | -2.645096| 0.517540 | -0.717424 |
| H     | 0.210335 | -1.558282| 1.083584  |
| H     | 0.810213 | -2.302405| -0.463600 |
| C     | 1.439205 | 1.394867 | -0.461241 |
| H     | 1.342290 | 2.160503 | 0.308369  |
| H     | 0.431811 | 1.140302 | -0.817378 |
### 1_pentene-3-one_trunc_TS_3_reopt

| Datum                                                      | Value          |
|------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -669.435981    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.339242    |
| Number of Imaginary Frequencies                            | 1              |

#### Frequencies (Top 3 out of 42)

1. -162.5073 cm⁻¹
2. 40.8243 cm⁻¹
3. 51.5580 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 1.644765 | -0.108756 | 0.163923 |
|-----|----------|-----------|----------|
| C   | 0.751163 | -0.773832 | -0.754900|
| C   | -0.281756| -1.541789 | -0.307523|
| O   | 1.541082 | -0.183479 | 1.390375 |
| H   | 0.889453 | -0.591637 | -1.812927|
| H   | -0.872728| -2.129833 | -0.992139|
| H   | -0.315100| -1.829012 | 0.732158 |
| C   | -1.482476| 1.482427  | -0.171534|
| H   | -1.979955| 2.068135  | -0.944208|
| H   | -0.464565| 1.262932  | -0.521481|
| H   | -1.400970| 2.096584  | 0.725422 |
| S   | -2.341940| -0.071946 | 0.151212 |
| C   | 2.745190 | 0.744554  | -0.432246|
| H   | 3.032788 | 0.407802  | -1.426362|
| H   | 2.382027 | 1.771445  | -0.516996|
| H   | 3.610129 | 0.746917  | 0.227813 |

### 1_pentene-3-one_trunc_TS_4
### M06-2X/def2tzvpp-IEFPCM(water) Energy

| Datum                                                                 | Value     |
|----------------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -669.437096 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -669.339121 |

### Frequencies (Top 3 out of 42)

1. -191.6744 cm⁻¹
2. 68.2909 cm⁻¹
3. 92.3051 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|          | 1.705667 | 0.002977 | 0.092882 |
|----------|----------|----------|----------|
| C        | 0.777803 | -0.907373| 0.691114 |
| C        | -0.244448| -1.511890| -0.006257|
| O        | 2.644996 | 0.517635 | 0.717445 |
| H        | 0.868700 | -1.050115| 1.761787 |
| H        | -0.210360| -1.558488| -1.083521|
| H        | -0.810060| -2.302577| 0.463782 |
| C        | -1.439021| 1.394779 | 0.461295 |
| H        | -0.431847| 1.139885 | 0.817835 |
| H        | -1.992225| 1.814789 | 1.300314 |
| H        | -1.341471| 2.160177 | -0.308480|
| S        | -2.219194| -0.102122| -0.168648|
| C        | 1.512570 | 0.353303 | -1.370656|
| H        | 1.711605 | -0.515050| -2.001253|
| H        | 0.481388 | 0.660414 | -1.558226|
| H        | 2.195974 | 1.153061 | -1.643706|

### 1_pentene-3-one_trunc_TS_5_reopt2

| Datum                                                                 | Value     |
|----------------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                               | -669.431086 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -669.335612 |

### Frequencies (Top 3 out of 42)


1. -195.1898 cm⁻¹
2. 17.8017 cm⁻¹
3. 43.6376 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C   1.966469  0.186865  0.060046
C   1.037753 -0.842938  0.442568
C  -0.218811 -0.531550  0.879482
O   1.690195  1.391013  0.059939
H   1.339271 -1.874280  0.317517
H  -0.864703 -1.290307  1.295789
H  -0.441714  0.490551  1.151009
C  -3.104427  0.446796  0.503037
H  -2.947093  1.516158  0.646199
H  -2.875488 -0.053122  1.448009
H  -4.160814  0.285758  0.291412
S  -2.056711 -0.211103 -0.827613
C   3.355258 -0.237109 -0.372009
H   3.523541 -1.305616 -0.260331
H   3.498066  0.037779 -1.418280
H   4.095043  0.310228  0.212234

1_pentene-3-one_trunc_TS_6_reopt

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -669.431731 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -669.335181 |

Number of Imaginary Frequencies | 1

Frequencies (Top 3 out of 42)

1. -224.1020 cm⁻¹
2. 41.4689 cm⁻¹
3. 63.7765 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
2_2-cyclopentene-1-one_1

| Datum                                                                 | Value         |
|-----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -269.343244   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -269.270219   |
| Number of Imaginary Frequencies                                       | 0             |
| **Frequencies** (Top 3 out of 30)                                     |               |
| 1. 95.3968 cm⁻¹                                                      |               |
| 2. 295.9541 cm⁻¹                                                      |               |
| 3. 471.7202 cm⁻¹                                                      |               |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C  -0.049004  -1.192797   0.000000  
C  -1.468512  -0.616104  -0.000000  
C  -1.257968  0.871505   0.000000  
C   0.028018   1.224371   0.000000  
C   0.872978   0.016502  -0.000000  
H   0.164467  -1.801338   0.877858  
H   0.164467  -1.801339  -0.877857  
H  -2.046271  -0.918386   0.874408  
H  -2.046270  -0.918385  -0.874409  
O   2.084282  -0.021394  -0.000001  

C          -2.086146       -0.055435       -0.004248  
C          -1.045632       -0.986959        0.295902  
C           0.188533       -0.618016        0.782486  
O          -3.189715       -0.402559       -0.450947  
H          -1.241795       -2.022057        0.041391  
H           0.329603        0.359155        1.222598  
H           0.862545       -1.378304        1.151112  
C           3.140840        0.228713        0.499499  
H           2.647370        0.261262        1.475617  
H           3.689822        1.161246        0.376397  
H           3.858687       -0.590566        0.516788  
S           1.899082        0.008891       -0.806509  
C          -1.822616        1.420383        0.232738  
H          -1.692508        1.621292        1.297348  
H          -0.906668        1.734454       -0.270582  
H          -2.664516        1.999628       -0.137210  

S           1.899082        0.008891       -0.806509  
C          -1.822616        1.420383        0.232738  
H          -1.692508        1.621292        1.297348  
H          -0.906668        1.734454       -0.270582  
H          -2.664516        1.999628       -0.137210  

C          -2.086146       -0.055435       -0.004248  
C          -1.045632       -0.986959        0.295902  
C           0.188533       -0.618016        0.782486  
O          -3.189715       -0.402559       -0.450947  
H          -1.241795       -2.022057        0.041391  
H           0.329603        0.359155        1.222598  
H           0.862545       -1.378304        1.151112  
C           3.140840        0.228713        0.499499  
H           2.647370        0.261262        1.475617  
H           3.689822        1.161246        0.376397  
H           3.858687       -0.590566        0.516788  
S           1.899082        0.008891       -0.806509  
C          -1.822616        1.420383        0.232738  
H          -1.692508        1.621292        1.297348  
H          -0.906668        1.734454       -0.270582  
H          -2.664516        1.999628       -0.137210  

C          -0.049804       -1.192797        0.000000  
C          -1.468512       -0.616104       -0.000000  
C          -1.257968        0.871505        0.000000  
C           0.028018        1.224371        0.000000  
C           0.872978        0.016502       -0.000000  
H           0.164467       -1.801338        0.877858  
H           0.164467       -1.801339       -0.877857  
H          -2.046271       -0.918386        0.874408  
H          -2.046270       -0.918385       -0.874409  
O           2.084282       -0.021394       -0.000001  

SI_ketones.md
6/7/2022
2_2cyclopentene1one_HEI_1

Datum | Value
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -707.560008
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -707.451882
Number of Imaginary Frequencies | 0

Frequencies (Top 3 out of 45)

|   |   |
|---|---|
| 1 | 90.4697 cm\(^{-1}\) |
| 2 | 116.9776 cm\(^{-1}\) |
| 3 | 163.3776 cm\(^{-1}\) |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 1.337131 | 0.627083 | 0.980639 |
| C | 0.180697 | 1.500371 | 0.486253 |
| C | -0.401709 | 0.757764 | -0.739318 |
| C | 0.685877 | -0.159908 | -1.152951 |
| C | 1.669749 | -0.293778 | -0.199973 |
| H | 2.214570 | 1.208385 | 1.269424 |
| H | 1.061895 | 0.012797 | 1.843000 |
| H | 0.563229 | 2.465567 | 0.150488 |
| H | -0.575477 | 1.697263 | 1.245981 |
| O | 2.709759 | -1.025590 | -0.179143 |
| H | 0.644392 | -0.743357 | -2.064572 |
| H | -0.733623 | 1.459233 | -1.507666 |
| C | -1.509903 | -1.150970 | 1.009142 |
| H | -1.348491 | -0.574797 | 1.918868 |
| H | -0.589782 | -1.666353 | 0.733726 |
| H | -2.295077 | -1.882478 | 1.185034 |
| S | -2.024422 | -0.090932 | -0.352743 |

2_2cyclopentene1one_HEI_2

Datum | Value
--- | ---
| Datum                                                | Value  |
|------------------------------------------------------|--------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                | -707.55707 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -707.449835 |
| Number of Imaginary Frequencies                      | 0      |

**Frequencies (Top 3 out of 45)**

1. 61.8777 cm⁻¹
2. 89.0043 cm⁻¹
3. 144.2390 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | -1.996467 | 0.971164 | 0.107697 |
| C | -0.562570 | 1.505519 | 0.109368 |
| C | 0.319157  | 0.293679 | 0.483511 |
| C | -0.531719 | -0.884896 | 0.156037 |
| C | -1.847411 | -0.547099 | -0.054807 |
| H | -2.511526 | 1.172872 | 1.051782 |
| H | -2.611606 | 1.391909 | -0.689499 |
| H | -0.402164 | 2.349493 | 0.779386 |
| H | -0.298832 | 1.834446 | -0.898453 |
| O | -2.864052 | -1.273261 | -0.298194 |
| H | -0.171597 | -1.905276 | 0.199607 |
| H | 0.627179  | 0.341834 | 1.534760 |
| C | 2.767331  | -1.002656 | 0.242993 |
| H | 2.838421  | -0.923485 | 1.327003 |
| H | 3.770496  | -1.023243 | -0.176821 |
| H | 2.251983  | -1.923648 | -0.022714 |
| S | 1.908133  | 0.428558  | -0.436768 |

**2_2cyclopentene1one_HEI_3**

| Datum                                                | Value  |
|------------------------------------------------------|--------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                | -707.557663 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -707.450409 |
| Number of Imaginary Frequencies                      | 0      |

**Frequencies (Top 3 out of 45)**

1.   |
2.   |
3.   |
1. 70.5385 cm⁻¹
2. 78.4695 cm⁻¹
3. 138.2238 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |        |        |        |
|---|--------|--------|--------|
| C | -1.679958 | 1.234260 | -0.090144 |
| C | -0.149286 | 1.282289 | -0.104711 |
| C | 0.302710 | -0.066390 | 0.499907 |
| C | -0.885375 | -0.953372 | 0.327055 |
| C | -2.026144 | -0.257017 | 0.005318 |
| H | -2.099899 | 1.744433 | 0.782120 |
| H | -2.134212 | 1.686269 | -0.973778 |
| H | 0.266977 | 2.133818 | 0.433532 |
| H | 0.209026 | 1.337075 | -1.134028 |
| O | -3.223446 | -0.655187 | -0.158644 |
| H | -0.864290 | -2.012045 | 0.554849 |
| H | 0.617515 | 0.061545 | 1.543437 |
| C | 3.010265 | 0.479215 | 0.134645 |
| H | 2.768133 | 1.445621 | -0.304128 |
| H | 3.978411 | 0.153106 | -0.238333 |
| H | 3.061722 | 0.574774 | 1.218560 |
| S | 1.784432 | -0.762313 | -0.327844 |

2_2cyclopentene1one_TS_1_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -707.549412 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -707.443019 |
| Number of Imaginary Frequencies | 1 |

Frequencies (Top 3 out of 45)

1. -205.8851 cm⁻¹
2. 57.7381 cm⁻¹
3. 86.6377 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
2_2cyclopentene1one_TS_2

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -707.549412 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -707.443018 |
| Number of Imaginary Frequencies                            | 1           |

**Frequencies** (Top 3 out of 45)

1. 205.9218 cm⁻¹
2. 57.8145 cm⁻¹
3. 86.6484 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -1.336086 | 0.561259  | -1.033107 |
| C | -0.504475 | 1.663028  | -0.376708 |
| C | 0.055954  | 0.972842  | 0.850468  |
| C | -0.757034 | -0.076736 | 2.093599  |
| C | 1.625754  | -1.510764 | -0.418550 |
| H | 0.636858  | -1.671785 | 0.028144  |
| H | 2.300271  | -2.269668 | -0.023804 |
| S | 2.180523  | 0.154808  | 0.001580  |
### 2_2cyclopentene1one_TS_3

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -707.546155
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -707.440464

**Number of Imaginary Frequencies** | **1**

**Frequencies** (Top 3 out of 45)

1. -240.3974 cm⁻¹
2. 65.5299 cm⁻¹
3. 86.6001 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | -1.424525 | 1.080435 | -0.601664 |
| C   | -0.221742 | 1.337753 | 0.305501  |
| C   | 0.042175  | -0.019608| 0.921248  |
| C   | -1.102650 | -0.792741| 0.839582  |
| C   | -2.041330 | -0.205741| -0.055255 |
| H   | -2.154220 | 1.888316 | -0.626734 |
| H   | -1.104616 | 0.886496 | -1.629272 |
| H   | -0.494306 | 2.027231 | 1.109900  |
| H   | 0.643690  | 1.750960 | -0.206210 |
| O   | -3.161180 | -0.616024| -0.384733 |
| H   | -1.253767 | -1.749340| 1.318688  |
| H   | 0.768502  | -0.117189| 1.715675  |
| C   | 3.019008  | 0.444515 | 0.070299  |
| H   | 3.110883  | 1.269582 | -0.635806 |
| H   | 4.009162  | 0.018810 | 0.227894  |
| H   | 2.681055  | 0.858968 | 1.025102  |
| S   | 1.841090  | -0.810832| -0.506228 |
3_3methyl3pentene2one_HEI_1

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.063725    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -747.911649    |
| Number of Imaginary Frequencies                                      | 0              |

**Frequencies** (Top 3 out of 60)

1.  66.3362 cm$^{-1}$  
2.  72.0385 cm$^{-1}$  
3.  107.1973 cm$^{-1}$

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | -1.630516 | -0.247313 | -0.325560 |
| C   | -0.600481 | 0.555849  | 0.112707  |
| C   | 0.692358  | 0.502380  | -0.626557 |
| O   | -1.562519 | -1.070521 | -1.313654 |
| H   | 0.537805  | -0.049345 | -1.551347 |
| C   | 1.201485  | -2.023450 | 0.517199  |
| H   | 1.192187  | -2.605977 | -0.401827 |
| H   | 1.735803  | -2.574126 | 1.288312  |
| H   | 0.177527  | -1.835139 | 0.838302  |
| S   | 2.026841  | -0.440157 | 0.282680  |
| C   | -2.994937 | -0.219073 | 0.353744  |
| H   | -3.109171 | 0.536598  | 1.133156  |
| H   | -3.753613 | -0.030717 | -0.410181 |
| H   | -3.207142 | -1.195541 | 0.780362  |
| C   | 1.311846  | 1.864193  | -0.927610 |
| H   | 2.228994  | 1.765451  | -1.510058 |
| H   | 0.604859  | 2.471101  | -1.495529 |
| H   | 1.551604  | 2.401785  | -0.008695 |
| C   | -0.643154 | 1.481489  | 1.301207  |
| H   | 0.275323  | 1.383617  | 1.891401  |
| H   | -0.713468 | 2.541205  | 1.025846  |
| H   | -1.469619 | 1.270330  | 1.975818  |

3_3methyl3pentene2one_HEI_2_reopt
### M06-2X/def2tzvpp-IEFPCM(water) Energy

| Datum                                                      | Value     |
|------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -748.063096 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.912213 |

### Number of Imaginary Frequencies

| Datum                                                      | Value     |
|------------------------------------------------------------|-----------|
| Number of Imaginary Frequencies                            | 0         |

### Frequencies (Top 3 out of 60)

1. 33.6500 cm⁻¹
2. 55.3677 cm⁻¹
3. 83.8813 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Datum                                                      | Value     |
|------------------------------------------------------------|-----------|
| C                                                          | -1.741808 0.024117 0.117984 |
| C                                                          | -0.557887 -0.624941 -0.158461 |
| C                                                          | 0.679406 -0.503771 0.656247 |
| O                                                          | -2.757568 0.012873 -0.670201 |
| H                                                          | 0.476622 0.013280 1.589696 |
| C                                                          | 0.990950 2.012458 -0.543407 |
| H                                                          | 1.617310 2.718969 -1.083861 |
| H                                                          | 0.136007 1.730467 -1.155845 |
| H                                                          | 0.634580 2.477662 0.374788 |
| S                                                          | 1.984409 0.557072 -0.177710 |
| C                                                          | -1.961648 0.830059 1.393377 |
| H                                                          | -2.901236 0.506991 1.845636 |
| H                                                          | -1.179134 0.761120 2.144289 |
| H                                                          | -2.085056 1.882685 1.125424 |
| C                                                          | 1.394963 -1.811979 0.990629 |
| H                                                          | 0.726390 -2.454355 1.564807 |
| H                                                          | 1.692487 -2.350144 0.090990 |
| H                                                          | 2.292669 -1.630373 1.584357 |
| C                                                          | -0.444402 -1.300294 -1.501473 |
| H                                                          | -1.343797 -1.873283 -1.731549 |
| H                                                          | -0.324071 -0.576504 -2.319631 |
| H                                                          | 0.409787 -1.976538 -1.553507 |

### 3_3methyl3pentene2one_HEI_3

| Datum                                                      | Value     |
|------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -748.06253 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910748 |
| Datum | Value |
|-------|-------|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 60)

1. 56.9238 cm⁻¹  
2. 65.2228 cm⁻¹  
3. 90.0391 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Element | x (Å) | y (Å) | z (Å) |
|---------|-------|-------|-------|
| C       | 1.813051 | -0.534569 | 0.188810 |
| C       | 0.862337  | 0.445426  | 0.012412  |
| C       | -0.513470 | 0.190679  | 0.547015  |
| O       | 1.602504  | -1.673118 | 0.752550  |
| H       | -0.460061 | -0.634872 | 1.255730  |
| C       | -3.148212 | -0.748314 | -0.026888 |
| H       | -3.758208 | -1.342185 | -0.704549 |
| H       | -2.992361 | -1.314341 | 0.891126  |
| H       | -3.674177 | 0.175985  | 0.201553  |
| S       | -1.563950 | -0.441179 | -0.842551 |
| C       | 3.249087  | -0.333456 | -0.280714 |
| H       | 3.914308  | -0.564407 | 0.553468  |
| H       | 3.474290  | -1.053202 | -1.071599 |
| H       | 3.486660  | 0.663288  | -0.642646 |
| C       | -1.169431 | 1.399980  | 1.202122  |
| H       | -0.525863 | 1.775323  | 2.001148  |
| H       | -1.322640 | 2.205705  | 0.483181  |
| H       | -2.135275 | 1.148536  | 1.640380  |
| C       | 1.057957  | 1.754326  | -0.709894 |
| H       | 1.062491  | 2.623213  | -0.040120 |
| H       | 1.982236  | 1.785156  | -1.281631 |
| H       | 0.243858  | 1.931166  | -1.422807 |

**3_3methyl3pentene2one_HEI_4**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.057756 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.905898 |
| Number of Imaginary Frequencies | 0 |
**Frequencies (Top 3 out of 60)**

1. 53.1761 cm\(^{-1}\)
2. 81.0240 cm\(^{-1}\)
3. 108.0376 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C   | C   | O   | H   | C   | S   | C   | H   | H   | H   | C   | H   | H   |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|   | 1.653974 | 0.079486 | -0.357499 | 2.790261 | -0.486444 | -0.573822 | -1.075759 | -0.328801 | 1.624586 | -1.938690 | -1.417532 | -0.926603 | -2.596511 | -1.538487 | -1.784255 | -0.931049 | -1.735357 | -1.191039 | -2.308590 | -2.026644 | -0.102549 | -1.916913 | 0.325600 | -0.480031 | 1.437977 | 1.369515 | -1.141456 | 1.812757 | 1.212819 | -2.154246 | 0.399494 | 1.684264 | -1.202140 | 2.027660 | 2.178933 | -0.702331 | -0.520456 | 1.701025 | 1.410711 | 0.144685 | 1.702043 | 2.275132 | -0.124411 | 2.408079 | 0.684946 | -1.501761 | 2.056573 | 1.731850 | 0.898754 | -1.726070 | 1.178587 | 0.033098 | -2.388715 | 1.064408 | 1.768699 | -2.228905 | 0.759523 | 1.064434 | -1.626632 | 2.259523 |

**3_3methyl3pentenone2one_HEI_5**

| Datum                                      | Value      |
|--------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.057952|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.905219|

Number of Imaginary Frequencies 0

**Frequencies (Top 3 out of 60)**
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |    |    |    |
|----|----|----|----|
| C  | 2.031464 | 0.069725 | -0.119648 |
| C  | 0.718367 | 0.356285 | 0.180638  |
| C  | -0.364129 | -0.665004 | 0.325571  |
| O  | 2.953152 | 0.955040 | -0.286942 |
| H  | 0.013767 | -1.654678 | 0.085411  |
| C  | -2.906051 | 0.615983 | -0.203032 |
| H  | -3.664972 | 0.813244 | -0.957679 |
| H  | -3.383561 | 0.162672 | 0.662896  |
| H  | -2.442409 | 1.556465 | 0.085135  |
| S  | -1.711346 | -0.505919 | -0.962051 |
| C  | 2.537874 | -1.361360 | -0.274549 |
| H  | 3.401794 | -1.487154 | 0.381121  |
| H  | 1.827508 | -2.153216 | -0.052391 |
| H  | 2.897626 | -1.499297 | -1.297038 |
| C  | -0.995439 | -0.739934 | 1.716031  |
| H  | -0.228969 | -1.035273 | 2.433845  |
| H  | -1.391716 | 0.224623 | 2.032112  |
| H  | -1.807337 | -1.468229 | 1.753549  |
| C  | 0.302538 | 1.798026 | 0.303191  |
| H  | -0.314686 | 1.987618 | 1.187772  |
| H  | 1.186516 | 2.429418 | 0.365056  |
| H  | -0.284971 | 2.135861 | -0.560668 |

3_3methyl3pentene2one_HEI_6

| Datum                                                                 | Value            |
|-----------------------------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -748.060302      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -747.907513      |
| Number of Imaginary Frequencies                                        | 0                |

Frequencies (Top 3 out of 60)

|    |    |
|----|----|
| 1. | 68.1181 cm-1 |
| 2. | 84.1947 cm-1 |
| 3. | 119.3058 cm-1 |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |    |    |    |
|---|----|----|----|
| C | 1.805886 | -0.197183 | -0.023541 |
| C | 0.652561  | 0.547838  | 0.092503  |
| C | -0.537675 | 0.109234  | 0.887138  |
| O | 2.866050  | 0.172426  | -0.651108 |
| H | -0.241276 | -0.527351 | 1.719000  |
| C | -1.842270 | -0.247572 | -1.618405 |
| H | -2.424841 | -0.900885 | -2.264298 |
| H | -2.345755 | 0.715016  | -1.542672 |
| H | -0.849032 | -1.10775  | -2.043082 |
| S | -1.707267 | -1.055901 | -0.014915 |
| C | 1.910631  | -1.579739 | 0.611963  |
| H | 2.693572  | -1.567497 | 1.374437  |
| H | 0.993702  | -1.960340 | 1.054950  |
| H | 2.230827  | -2.283954 | -0.158608 |
| C | -1.354734 | 1.266797  | 1.456786  |
| H | -0.708990 | 1.931911  | 2.034402  |
| H | -1.813882 | 1.858636  | 0.664186  |
| H | -2.147224 | 0.899097  | 2.107044  |
| C | 0.580742  | 1.887895  | -0.596594 |
| H | 0.629193  | 2.736568  | 0.097163  |
| H | 1.421203  | 1.979900  | -1.282465 |
| H | -0.340474 | 2.021077  | -1.171645 |

3_3methyl3pentene2one_HEI_7_reopt

| Datum | Value         |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.057172 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.906012 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 60)

1. 37.9088 cm⁻¹
2. 59.3419 cm⁻¹
3. 62.6720 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
3_3methyl3pentene2one_TS_1

| Datum                                      | Value       |
|-------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.054371 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903537 |
| Number of Imaginary Frequencies           | 1           |

**Frequencies (Top 3 out of 60)**

1.  -206.0842 cm⁻¹
2.   63.5762 cm⁻¹
3.   65.7839 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |         |         |         |
|---|---------|---------|---------|
| C | -1.624443 | -0.201746 | -0.476678 |
| C | -0.638576 | 0.690179  | 0.060681  |
| C | 0.510208  | 0.909529  | -0.681484 |
| O | -1.501191 | -0.792577 | -1.565257 |
### 3_3methyl3pentene2one_TS_2_reopt

| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.057292 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.906178 |

**Number of Imaginary Frequencies**
1

**Frequencies** (Top 3 out of 60)

1. -217.7724 cm⁻¹
2. 69.2213 cm⁻¹
3. 88.4286 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -1.724072 | -0.204748 | -0.199913 |
|-------|-----------|-----------|-----------|
| C     | -0.681056 | 0.724464  | 0.078062  |
| C     | 0.452074  | 0.790267  | -0.734591 |
| O     | -2.776806 | -0.288251 | 0.467169  |
| H     | 0.388198  | 0.390269  | -1.699739 |
| C     | 1.018288  | -1.779872 | 1.019362  |
| H     | 1.417834  | -1.888163 | 2.026973  |
| H     | 0.034490  | -1.299881 | 1.095223  |
| H     | 0.883325  | -2.771345 | 0.587775  |
3_3methyl3pentene2one_TS_3_reopt

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.048351 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.89856 |
| Number of Imaginary Frequencies | 1 |

Frequencies (Top 3 out of 60)

1.  -250.5005 cm⁻¹
2.   48.9800 cm⁻¹
3.   55.4228 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -1.802765 | -0.660850 | -0.252804 |
|-------|-----------|-----------|-----------|
| C     | -0.992333 | 0.508201  | -0.109532 |
| C     | 0.300306  | 0.472080  | -0.616970 |
| O     | -1.418300 | -1.707696 | -0.808540 |
| H     | 0.520146  | -0.351122 | -1.285172 |
| C     | 3.186909  | -0.735499 | -0.266237 |
| H     | 3.743147  | -1.652948 | -0.077324 |
| H     | 2.774035  | -0.799658 | -1.276886 |
| H     | 3.888010  | 0.098798  | -0.243183 |
| S     | 1.843881  | -0.527206 | 0.937901  |
| C     | -3.221535 | -0.641854 | 0.296594  |
| H     | -3.798931 | 0.188325  | -0.11692  |
| H     | -3.710304 | -1.578737 | 0.042441  |
| H     | -3.216081 | -0.526287 | 1.382068  |
3_3methyl3pentene2one_TS_4_reopt

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.049978
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.898667

Number of Imaginary Frequencies: 1

**Frequencies** (Top 3 out of 60)

1. -223.8345 cm⁻¹
2. 27.0791 cm⁻¹
3. 67.7120 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 1.645050 | 0.069623 | -0.322836 |
|-------|----------|----------|-----------|
| C     | 0.727112 | -0.108408| 0.749467  |
| C     | -0.422347| 0.654934 | 0.990326  |
| O     | 2.663068 | -0.646177| -0.444978 |
| H     | -0.888193| 0.407786 | 1.936895  |
| C     | -1.347346| -1.373862| -1.236431 |
| H     | -1.442418| -1.094559| -2.285228 |
| H     | -0.285319| -1.325890| -0.966212 |
| H     | -1.683725| -2.402924| -1.116143 |
| S     | -2.251259| -0.245768| -0.160985 |
| C     | 1.400447 | 1.118040 | -1.394317 |
| H     | 2.099716 | 0.945771 | -2.209344 |
| H     | 0.378343 | 1.059961 | -1.772620 |
| H     | 1.554302 | 2.125711 | -1.007535 |
| C     | -0.630391| 2.114392 | 0.651633  |
| H     | 0.143778 | 2.716332 | 1.141412  |
| H     | -0.610410| 2.328641 | -0.406088 |
| H     | -1.597763| 2.438368 | 1.037596  |
| C     | 0.958161 | -1.329641| 1.605941  |
3_3methyl3pentene2one_TS_5_reopt3

| Datum                                           | Value            |
|------------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -748.057292      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.906178      |
| Number of Imaginary Frequencies                 | 1                |

**Frequencies (Top 3 out of 60)**

1. -217.7642 cm⁻¹
2. 69.1951 cm⁻¹
3. 88.4098 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | O     | H     | S     | C     | H     | H     | H     |
|-------|-------|-------|-------|-------|-------|-------|-------|
| -1.724082 | -2.776805 | 0.388170 | 1.018472 | -1.554770 | 1.325506 | 0.788189 | -1.587998 |
| -0.681094  | 0.452022  | 0.058202  | 0.452022  | 0.582022  | 0.582022  | 0.582022  | 0.582022  |
| 0.724425   | 0.790287  | -0.288362 | 0.309275  | -1.779868 | -2.771374 | 1.417568  | 0.346236  |
| 0.078084   | -0.734572 | 0.467191  | -1.699714 | 1.019351  | 0.587768  | 2.026968  | 1.095184  |
| -0.199900  | -0.731708 | 0.004613  | 0.199900  | -1.371164 | -1.371164 | -1.371164 | -1.371164 |
| 0.194337   | 1.933651  | 1.933651  | 1.933651  | 1.933651  | 1.933651  | 1.933651  | 1.933651  |
3_3methyl3pentene2one_TS_6_reopt

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.057292      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.906178 |

Number of Imaginary Frequencies 1

**Frequencies (Top 3 out of 60)**

1. -217.7722 cm⁻¹
2. 69.2253 cm⁻¹
3. 88.4140 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -1.724106  | -0.204906  | -0.199917  |
| C    | -0.681133  | 0.724391   | 0.078055   |
| C    | 0.452003   | 0.790249   | -0.734619  |
| O    | -2.776833  | -0.288484  | 0.467160   |
| H    | 0.388133   | 0.309259   | -1.699770  |
| H    | 1.018634   | -1.779438  | 1.019848   |
| H    | 0.882847   | -2.770806  | 0.588272   |
| H    | 1.418361   | -1.880008  | 2.027178   |
| H    | 0.35198    | -1.298869  | 1.096360   |
| S    | 2.074531   | -0.731836  | 0.004378   |
| C    | -1.554749  | -1.163674  | -1.371164  |
| H    | -1.607376  | -0.634234  | -2.323912  |
| H    | -0.588656  | -1.670089  | -1.331391  |
| H    | -2.354333  | -1.899501  | -1.337854  |
| C    | 1.325487   | 2.016480   | -0.732116  |
| H    | 0.788119   | 2.845668   | -1.203307  |
| H    | 1.588102   | 2.319927   | 0.279558   |
| H    | 2.245650   | 1.847915   | -1.289499  |
| C    | -0.749797  | 1.547358   | 1.335526   |
| H    | -0.746665  | 2.623355   | 1.140950   |
| H    | -1.655606  | 1.308529   | 1.888637   |
| H    | 0.110357   | 1.342140   | 1.983766   |

3_3methyl3pentene2one_TS_7
### M06-2X/def2tzvpp-IEFPCM(water) Energy

-748.049803

### M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)

-747.898941

### Number of Imaginary Frequencies

1

### Frequencies (Top 3 out of 60)

1.  -224.7761 cm\(^{-1}\)
2.   57.7775 cm\(^{-1}\)
3.   72.7277 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |       |       |       |
|---|-------|-------|-------|
| C | -1.584744 | 0.244807 | 0.339204 |
| C | -0.649780 | 0.072012 | -0.724507 |
| C | 0.505471  | 0.847419 | -0.853699 |
| O | -1.524097 | 1.126292 | 1.220327  |
| H | 0.997523  | 0.751481 | -1.814508 |
| C | 1.316989  | -1.441245| 1.174113  |
| H | 1.539566  | -2.491855| 0.989555  |
| H | 1.477575  | -1.230259| 2.230812  |
| H | 0.997523  | -1.273634| 0.951211  |
| S | 2.296686  | -0.359686| 0.116092  |
| C | -2.763235 | -0.719890| 0.392248  |
| H | -3.405171 | -0.59685 | -0.482217 |
| H | -2.427280 | -1.758253| 0.951211  |
| H | -3.345274 | -0.523919| 1.289184  |
| C | 0.713847  | 2.194842 | -0.215684 |
| H | -0.044237 | 2.893032 | -0.583866 |
| H | 0.618134  | 2.152005 | 0.863397  |
| H | 1.696402  | 2.584745 | -0.477556 |
| C | -0.786065 | -1.111039| -1.654646 |
| H | -1.809536 | -1.268686| -1.997471 |
| H | -0.165961 | -0.966908| -2.540118 |
| H | -0.456700 | -2.047645| -1.186839 |

---

### 3_methyl-3-pentene-2-one_1

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy       | -309.853172 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.736065 |
| Datum                      | Value               |
|----------------------------|---------------------|
| Number of Imaginary Frequencies | 0                  |

**Frequencies** (Top 3 out of 45)

1. 69.5428 cm⁻¹
2. 104.7879 cm⁻¹
3. 138.1506 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | 2.628339 | -0.570494 | -0.000002 |
|------|----------|-----------|-----------|
| H    | 2.978382 | 0.456989  | -0.000039 |
| H    | 3.040586 | -1.078133 | -0.874262 |
| C    | 1.142087 | -0.692102 | -0.000001 |
| H    | 3.040581 | -1.078066 | 0.874299  |
| C    | 0.237318 | 0.292936  | -0.000011 |
| C    | -1.215551| -0.040346 | 0.000007  |
| C    | -1.670291| -1.480184 | 0.000005  |
| O    | -2.037247| 0.856923  | 0.000026  |
| H    | -2.755890| -1.501151 | -0.00019  |
| H    | -1.296468| -2.003460 | -0.879627 |
| H    | -1.296509| -2.003441 | 0.879666  |
| H    | 0.779000 | -1.713457 | 0.000014  |
| C    | 0.543945 | 1.761406  | -0.00024  |
| H    | 0.101022 | 2.239362  | -0.874245 |
| H    | 0.101171 | 2.239351  | 0.874279  |
| H    | 1.611024 | 1.959329  | -0.00112  |

**3_methyl-3-pentene-2-one_2**

| Datum                              | Value               |
|------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -309.85038          |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.732627          |
| Number of Imaginary Frequencies    | 1                   |

**Frequencies** (Top 3 out of 45)

1. -8.6017 cm⁻¹
2. 85.7224 cm⁻¹
3. 121.8236 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |        |        |        |
|---|--------|--------|--------|
| C | 2.732992 | -0.267869 | 0.000212 |
| H | 2.926606 | 0.800678  | -0.000001 |
| H | 3.217942 | -0.707951 | -0.873567 |
| C | 1.283784 | -0.613384 | 0.000135  |
| H | 3.217764 | -0.707575 | 0.874280  |
| C | 0.234211 | 0.213403  | -0.000072 |
| C | -1.128565 | -0.419639 | -0.000060 |
| C | -2.322726 | 0.498515  | 0.000241  |
| O | -1.281246 | -1.624838 | -0.000250 |
| H | -3.235006 | -0.089983 | 0.000067  |
| H | -2.299943 | 1.147303  | 0.876743  |
| H | -2.299982 | 1.147914  | -0.875804 |
| H | -1.128565 | -0.419639 | 0.000135  |
| C | -2.322726 | 0.498515  | -0.000241 |
| H | 1.314142  | 1.714049  | -0.000283 |
| H | -0.176775 | 2.135199  | -0.877680 |
| H | -0.179224 | 2.135481  | 0.876722  |
| H | 1.342754  | 2.061298  | -0.000074 |

4_4-methyl-3-pentene-2-one_1

| Datum                                      | Value           |
|--------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -309.85227      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.735792 |
| Number of Imaginary Frequencies            | 0               |

Frequencies (Top 3 out of 45)

1. 46.8412 cm⁻¹
2. 104.1799 cm⁻¹
3. 130.2159 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |        |        |        |
|---|--------|--------|--------|
| C | -2.402099 | -1.005957 | -0.038832 |
| H | -2.151541 | -2.053496 | -0.188385 |
### 4_4-methyl-3-pentene-2-one_2

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -309.849963      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.732399 |
| Number of Imaginary Frequencies            | 0                |
| **Frequencies (Top 3 out of 45)**          |                  |
| 1.  | 40.9809 cm⁻¹ |
| 2.  | 112.0935 cm⁻¹|
| 3.  | 159.2112 cm⁻¹|

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |       |       |       |
|-----|-------|-------|-------|
| C   | -2.458273 | -0.836351 | 0.059437 |
| H   | -2.308520  | -1.904489  | 0.195487 |
| H   | -3.036795  | -0.669299  | -0.851739 |
| C   | -1.163192  | -0.082859  | -0.014205 |
| H   | -3.061061  | -0.451199  | 0.885234  |
| C   | -0.007626  | -0.763178  | 0.011171  |
| C   | 1.386858   | -0.282842  | -0.004378 |
| C   | 1.733347   | 1.179014   | 0.107209  |
| O   | 2.282129   | -1.107822  | -0.086578 |
| H   | 2.793752   | 1.267476   | 0.326454  |
| H   | 1.528635   | 1.679563   | -0.840310 |
| H   | 1.146939   | 1.674052   | 0.878466  |
| Datum | Value     |
|-------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.066189 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.913331 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 60)

1. 74.6308 cm⁻¹  
2. 86.3018 cm⁻¹  
3. 105.8432 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | -1.335302 | 1.407977 | -0.099059 |
|------|-----------|---------|-----------|
| H    | -0.058382 | -1.845601 | 0.057038  |
| H    | -0.584735 | 1.896169 | -0.710734 |
| H    | -2.316736 | 1.639892 | -0.509837 |
| H    | -1.295005 | 1.845447 | 0.901515  |

| Datum | Value     |
|-------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.066189 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.913331 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 60)

1. 74.6308 cm⁻¹  
2. 86.3018 cm⁻¹  
3. 105.8432 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C    | -1.801872 | -0.052346 | 0.026782  |
|------|-----------|---------|-----------|
| C    | -0.670628 | -0.611036 | -0.527478 |
| C    | 0.693892  | -0.710207 | 0.069675  |
| O    | -1.931745 | 0.497771  | 1.172916  |
| C    | 0.824352  | 2.129648  | -0.036523 |
| H    | 1.244607  | 3.000094  | -0.536112 |
| H    | -0.202802 | 1.973712  | -0.363371 |
| H    | 0.841709  | 2.290981  | 1.039492  |
| S    | 1.805936  | 0.698261  | -0.510200 |
| C    | -3.072545 | -0.090902 | -0.819834 |
| H    | -2.936441 | -0.574370 | -1.786632 |
| H    | -3.856410 | -0.616059 | -0.269333 |
| H    | -3.427349 | 0.929606  | -0.981909 |
| C    | 0.726889  | -0.734087 | 1.595915  |
| H    | 0.099769  | -1.552571 | 1.957954  |
| H    | 1.748790  | -0.895676 | 1.944089  |
| H    | 0.334543  | 0.185813  | 2.017926  |
| H    | -0.750299 | -0.986794 | -1.541834 |
| C    | 1.416021  | -1.949732 | -0.462756 |
| H    | 2.454339  | -1.981416 | -0.125233 |
| H    | 0.908194  | -2.844028 | -0.096771 |
| H    | 1.403672  | -1.971671 | -1.553092 |
### 4_4methyl3pentene2one_HEI_2_reopt

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.066213 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.913977 |

Number of Imaginary Frequencies 0

**Frequencies** (Top 3 out of 60)

1. 53.6281 cm\(^{-1}\)
2. 62.3332 cm\(^{-1}\)
3. 102.8842 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C         | H         | S         |
|---|-----------|-----------|-----------|
|   | 1.849163  | -0.885987 | -0.056809 |
| C | 0.719226  | 0.091795  | 0.711684  |
| C | -0.577548 | 0.680612  | 0.266486  |
| O | 2.005290  | 0.212333  | -1.288785 |
| C | -1.644857 | -1.962213 | 0.176209  |
| H | -1.988032 | -2.780757 | -0.452841 |
| H | -0.647976 | -2.190484 | 0.552387  |
| H | -2.335225 | -1.844666 | 1.009456  |
| S | -1.564227 | -0.482980 | -0.845303 |
| C | 3.062848  | -0.711281 | 0.625231  |
| H | 2.890891  | -0.952856 | 1.673618  |
| H | 3.346087  | -1.623085 | 0.094403  |
| H | 3.910742  | -0.026116 | 0.555777  |
| C | -1.449410 | 1.008564  | 1.479394  |
| H | -0.937348 | 1.731983  | 2.109393  |
| H | -2.411476 | 1.413888  | 1.174785  |
| H | -1.627966 | 0.110580  | 2.084473  |
| H | 0.747121  | -0.271599 | 1.732209  |
| C | -0.427476 | 1.937412  | -0.591095 |
| H | -1.403015 | 2.304915  | -0.919108 |
| H | 0.048410  | 2.717415  | 0.007507  |
| H | 0.201418  | 1.734383  | -1.453537 |

### 4_4methyl3pentene2one_HEI_3
### 4-methyl3-pentene-2-one HEI 4

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.055956 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903669 |
**Datum** | **Value**
---|---
Number of Imaginary Frequencies | 0

**Frequencies** (Top 3 out of 60)

1. 46.2976 cm⁻¹  
2. 74.1079 cm⁻¹  
3. 117.9714 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -1.972311 | -0.555236 | -0.144727 |
| C     | -0.618582 | -0.529740 | -0.374827 |
| C     | 0.399616  | 0.550084  | -0.053096 |
| O     | -2.735790 | -1.545446 | -0.449065 |
| C     | 2.287636  | -1.481173 | 0.604768  |
| H     | 3.157727  | -2.035459 | 0.259364  |
| H     | 2.458617  | -1.159585 | 1.629589  |
| H     | 1.411940  | -2.126305 | 0.562075  |
| S     | 2.080017  | -0.079373 | -0.507817 |
| C     | -2.706175 | 0.612412  | 0.507416  |
| H     | -3.628878 | 0.783969  | -0.048420 |
| H     | -2.900645 | 0.340851  | 1.527212  |
| H     | -2.148936 | 1.543936  | 0.546420  |
| C     | 0.264670  | 1.802699  | -0.932552 |
| H     | -0.705076 | 2.270698  | -0.766634 |
| H     | 1.041575  | 2.536985  | -0.705901 |
| H     | 0.331122  | 1.535759  | -1.987757 |
| H     | -0.226170 | -1.411495 | -0.871112 |
| C     | 0.440061  | 0.961290  | 1.423428  |
| H     | -0.585946 | 1.408842  | 1.724613  |
| H     | 0.607269  | 0.094576  | 2.062051  |
| H     | 1.233964  | 1.688745  | 1.603637  |

**4_4methyl3pentene2one_HEI_5_reopt**

| Datum | Value |
---|---|
M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.0638 |
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.912165 |
Number of Imaginary Frequencies | 0 |
**Frequencies (Top 3 out of 60)**

1. 32.1574 cm⁻¹
2. 51.7066 cm⁻¹
3. 118.9265 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 2.137445 | -0.08007 | 0.000017 |
| C | 0.874037 | -0.615888 | 0.000003 |
| C | -0.386387 | 0.222661 | 0.000028 |
| O | 2.443433 | 1.165302 | 0.000055 |
| C | -3.239578 | -0.009553 | -0.000185 |
| H | -4.080030 | -0.700783 | -0.000057 |
| H | -3.301804 | 0.612689 | 0.889890 |
| H | -3.301787 | 0.612343 | -0.890502 |
| S | -1.747234 | -1.020672 | 0.000030 |
| C | 3.315231 | -1.048186 | -0.000020 |
| H | 3.011087 | -2.094620 | -0.000060 |
| H | 3.938248 | -0.861857 | -0.877841 |
| H | 3.938247 | -0.861925 | 0.877818 |
| C | -0.484162 | 1.103183 | 1.248782 |
| H | 0.394531 | 1.748183 | 1.274260 |
| H | -1.376407 | 1.733053 | 1.236241 |
| H | -0.498089 | 0.490928 | 2.150396 |
| H | 0.769984 | -1.694233 | -0.000045 |
| C | -0.484191 | 1.103194 | -1.248694 |
| H | -1.376404 | 1.733139 | -1.236080 |
| H | 0.394532 | 1.748183 | -1.274198 |
| H | -0.498201 | 0.491001 | -2.150329 |

**4_4methyl3pentene2one_HEI_6**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.059573 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.906263 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 60)**
1. 69.2260 cm⁻¹  
2. 95.5568 cm⁻¹  
3. 126.6959 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       | C          | C          | C           | O          | C          | H           | H           | H           | S           | C          | H           | H           | H           | C           | H           | H           | H           | C           | H           | H           | H           |
|-------|------------|------------|-------------|------------|------------|-------------|-------------|-------------|-------------|------------|-------------|-------------|-------------|------------|-------------|-------------|-------------|------------|-------------|-------------|-------------|
|       | -1.887292  | 0.126238   | -0.289003   | -2.903447  | 0.839183   | -2.135067   | -0.113088   | 0.647584    | 0.706106    | 0.647584   | 0.126238    | 0.706106    | 0.647584    | -0.289003  | 0.839183    | -2.135067   | -0.113088   | 0.647584   | 0.706106    | 0.647584   | 0.126238   |
|       | -0.652422  | 0.638370   | -0.630927   | 0.647584   | 0.706106   | 0.638370    | 0.630927    | 0.647584    | 0.706106    | 0.647584   | 0.638370    | 0.630927    | 0.647584    | 0.638370   | 0.630927   | 0.647584    | 0.706106    | 0.647584   | 0.706106    | 0.647584   | 0.638370   |
|       | 0.647584   | 0.706106   | 0.095247    | -2.903447  | 0.171893   | -2.135067   | -0.113088   | -2.903447   | 0.171893    | -2.135067  | -0.113088   | -2.903447   | 0.171893    | -2.135067  | -0.113088  | -2.903447   | 0.171893    | -2.135067  | -0.113088  | -2.903447  | 0.171893   |
|       | 0.171893   | -2.135067  | -0.113088   | 0.647584   | 0.706106   | 0.638370    | 0.630927    | 0.647584    | 0.706106    | 0.647584   | 0.638370    | 0.630927    | 0.647584    | 0.706106   | 0.647584   | 0.638370    | 0.630927   | 0.647584   | 0.706106   | 0.647584   |

Frequencies (Top 3 out of 60)

1. -192.0031 cm⁻¹  
2. 39.3684 cm⁻¹  
3. 72.4582 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -1.808205 | -0.088340 | 0.093059 |
| C | -0.694988 | -0.555196 | -0.666864 |
| C | 0.516191 | -1.024574 | -0.176483 |
| O | -1.874694 | -0.029864 | 1.332286 |
| C | 0.705338 | 2.264416 | -0.204278 |
| H | 1.077688 | 2.923439 | -0.988181 |
| H | -0.196578 | 1.765234 | -0.582085 |
| H | 0.416981 | 2.874825 | 0.651570 |
| S | 1.912246 | 1.000192 | 0.241844 |
| C | -3.018922 | 0.393853 | -0.691075 |
| H | -2.895173 | 0.307146 | -1.768141 |
| H | -3.892396 | -0.182245 | -0.382928 |
| H | -3.212204 | 1.436808 | -0.435561 |
| C | 0.652818 | -1.594864 | 1.211754 |
| H | 0.212813 | -2.599254 | 1.210865 |
| H | 1.703502 | -1.690513 | 1.482055 |
| H | 0.132843 | -0.998273 | 1.950476 |
| H | -0.777047 | -0.439051 | -1.741147 |
| C | 1.448089 | -1.666373 | -1.174634 |
| H | 2.473909 | -1.674219 | -0.810903 |
| H | 1.136119 | -2.705392 | -1.326972 |
| H | 1.419238 | -1.156195 | -2.135720 |

4_4methyl3pentene2one_TS_2_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.05414 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903702 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 60)

1. -191.9785 cm⁻¹
2. 39.1700 cm⁻¹
3. 72.4445 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
4_4methyl3pentene2one_TS_3_reopt

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.051624 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.900102 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 60)

1. -219.6187 cm⁻¹
2. 56.8082 cm⁻¹
3. 67.6907 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 1.875580 | -0.102654 | -0.174920 |
| C | 0.694841 | -0.685784 | -0.716015 |
| C | -0.514292 | -1.003815 | -0.935866 |
| O | 2.917053 | 0.018707 | -0.848685 |
4_4methyl3pentene2one_TS_4_reopt

Datum | Value
--- | ---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.051086
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.899231
Number of Imaginary Frequencies | 1

Frequencies (Top 3 out of 60)

1. -230.0830 cm⁻¹
2.  39.1090 cm⁻¹
3.  81.8258 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|  |   |   |   |
|---|---|---|---|
| C | -0.650821 | 2.195497 | -0.528460 |
| H | -0.271771 | 2.925685 | 0.186561 |
| H | 0.204093 | 1.633887 | -0.921647 |
| H | -1.119721 | 2.728344 | -1.354859 |
| S | -1.779083 | 1.022391 | 0.243690 |
| C | 1.885401 | 0.456747 | 1.235250 |
| H | 2.681547 | 1.195191 | 1.304352 |
| H | 0.927401 | 0.913391 | 1.486749 |
| H | 2.088151 | -0.333257 | 1.960231 |
| C | -1.505595 | -0.733463 | -0.975643 |
| H | -1.204240 | -2.783335 | -1.054063 |
| H | -2.508654 | -1.701767 | -0.554484 |
| H | -1.532562 | -1.310311 | -1.978167 |
| H | 0.737942 | -0.821335 | -1.792766 |
| C | -0.609647 | -1.475157 | 1.340224 |
| H | -1.651112 | -1.497414 | 1.659820 |
| H | -0.221089 | -2.498241 | 1.389432 |
| H | -0.053878 | -0.866987 | 2.042684 |
| Datum                                      | Value            |
|-------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -748.050048      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.900209      |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 60)

1. -238.0725 cm\(^{-1}\)
2. 63.3513 cm\(^{-1}\)
3. 68.2148 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| C | 2.184143 | 0.368472 | 1.152179 |
| H | 3.180761 | 0.798970 | 1.211373 |
| H | 1.458335 | 1.100481 | 1.506110 |
| H | 2.128070 | -0.496051 | 1.812284 |
| C | -1.349744 | -1.986686 | -0.655850 |
| H | -0.949797 | -2.98124 | -0.464481 |
| H | -2.361620 | -1.946967 | -0.254272 |
| H | -1.389341 | -1.836104 | -1.732980 |
| H | 0.661795 | -0.807567 | -1.774741 |
| C | -0.480152 | -1.079198 | 1.518447 |
| H | 0.201435 | -1.874296 | 1.838304 |
| H | -0.191419 | -0.160937 | 2.018790 |
| H | -1.484060 | -1.339142 | 1.847912 |
| C | -0.480152 | -1.079198 | 1.518447 |
| H | 0.201435 | -1.874296 | 1.838304 |
| H | -0.191419 | -0.160937 | 2.018790 |
| H | -1.484060 | -1.339142 | 1.847912 |
4_4methyl3pentene2one_TS_6

| Datum                                                      | Value           |
|------------------------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -748.051086     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.89923      |

Number of Imaginary Frequencies

- 1

Frequencies (Top 3 out of 60)

1. -230.1214 cm⁻¹
2. 39.1601 cm⁻¹
3. 81.7792 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates:

| C              | 0.563657 | 2.937495 | -0.178761 |
|----------------|----------|----------|-----------|
| C              | 1.974042 | 1.896306 | -0.373716 |
| C              | 0.758316 | 1.992717 | -1.662063 |
| C              | -1.324668| 0.970704 | -1.460523 |
| C              | 0.420962 | 0.719820 | 1.539864  |
| H              | 1.491020 | 0.802566 | 1.725645  |
| H              | -0.075235| 1.539742 | 2.072730  |
| H              | 0.041955 | -0.214556| 1.934537  |

| Datum                                                      | Value           |
|------------------------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -748.051086     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.89923      |

Number of Imaginary Frequencies

- 1

Frequencies (Top 3 out of 60)

1. -230.1214 cm⁻¹
2. 39.1601 cm⁻¹
3. 81.7792 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates:

| C              | -1.917914 | 0.016957 | -0.293519 |
|----------------|-----------|----------|-----------|
| C              | -0.697561 | 0.625770 | -0.704398 |
| C              | 0.450239  | 0.970023 | 0.010323  |
| O              | -2.831458 | -0.206094| -1.113370 |
| C              | 0.816283  | -2.165912| 0.045123  |
| H              | 1.112074  | -3.034232| -0.632648 |
| H              | 0.666741  | -2.487955| 0.987312  |
| H              | -0.140008 | -1.803494| -0.438577 |
| S              | 2.030521  | -0.840196| -0.181999 |
| C              | -2.184323 | -0.368369| 1.152123  |
| H              | -3.181038 | -0.798656| 1.211227  |
| H              | -1.458701 | -1.100522| 1.506127  |
| H              | -2.128118 | 0.496147 | 1.812227  |
| C              | 1.349688  | 1.986798 | -0.655633 |
| H              | 0.949663  | 2.988181 | -0.464139 |
| H              | 2.361562  | 1.947097 | -0.254049 |
| H              | 1.389306  | 1.836366 | -1.732783 |
| H              | -0.661745 | 0.807622 | -1.774709 |
| C              | 0.480172  | 1.078890 | 1.518518  |
### 4-hexene-3-one_1

| Datum                                                                 | Value               |
|------------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -309.849904         |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -309.732746         |
| Number of Imaginary Frequencies                                        | 0                   |
| **Frequencies** (Top 3 out of 45)                                      |                     |
| 1. 44.1323 cm⁻¹                                                       |                     |
| 2. 96.9275 cm⁻¹                                                       |                     |
| 3. 146.8401 cm⁻¹                                                      |                     |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 3.043151 | -0.116681 | 0.000001 |
|-------|----------|-----------|----------|
| C     | 1.685162 | -0.791352 | -0.000001|
| C     | 0.522605 | 0.170935  | 0.000000 |
| C     | -0.825990| -0.450014 | 0.000001 |
| C     | -1.935729| 0.283922  | -0.000001|
| C     | -3.322371| -0.257597 | 0.000000 |
| O     | 0.684996 | 1.374738  | 0.000000 |
| H     | 3.839136 | -0.859204 | 0.000000 |
| H     | 3.161851 | 0.514548 | -0.879496|
| H     | 3.161850 | 0.514546 | 0.879498 |
| H     | 1.560052 | -1.445398 | 0.868430 |
| H     | 1.560053 | -1.445396 | -0.868434|
| H     | -0.873631| -1.533387 | 0.0000002|
| H     | -1.824251| 1.364411 | -0.000002|
| H     | -3.867913| 0.101191 | -0.874806|
| H     | -3.330175| -1.345693| 0.000001 |
| H     | -3.867913| 0.101193 | 0.874806 |

### 4-hexene-3-one_2
| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -309.85036   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.73259   |

Number of Imaginary Frequencies

0

**Frequencies (Top 3 out of 45)**

1. 76.2755 cm⁻¹
2. 112.6474 cm⁻¹
3. 165.6365 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   | C          | C          | C          | C          | C          | O          | H          | H          | H          | H          | H          | H          | H          | H          | H          | H          | H          | H          | H          |
|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|   | -2.750722  | -0.747446  | -0.820958  | 0.540844   | 0.630537   | -0.417074  | -0.324930  | 1.561569   | -1.748740  | 0.000002   | 0.879388   | 0.879386   | 0.871019   | 0.871014   | 0.000001   | -0.832313  | 0.875176   | -0.000000  |
|   | -1.234314  | -0.820958  | 0.540844   | -0.324930  | 1.561569   | -1.748740  | -0.218098  | -1.370457  | -1.370460  | 0.000002   | 0.879388   | 0.879386   | 0.871019   | 0.871014   | 0.000001   | 0.875176   | 0.000000   | 0.000000   |
|   | -0.574456  | 0.540844   | -0.324930  | 1.561569   | -1.748740  | -0.218098  | -1.370457  | -1.370460  | 0.000002   | 0.879388   | 0.879386   | 0.871019   | 0.871014   | 0.000001   | 0.875176   | 0.000000   | 0.000000   |
|   | 0.901016   | 0.630537   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   |
|   | 1.723149   | -0.417074  | -0.000000  | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   |
|   | 3.210170   | -0.324930  | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   |
|   | -1.236558  | 1.561569   | -0.000000  | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   |
|   | -3.177887  | -1.748740  | 0.000002   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   |
|   | -3.114124  | -0.218098  | 0.879388   | 0.879386   | 0.871019   | 0.871014   | 0.000001   | 0.875176   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   |
|   | -3.114126  | -0.218098  | 0.879388   | 0.879386   | 0.871019   | 0.871014   | 0.000001   | 0.875176   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   | 0.000000   |
|   | -0.869182  | -1.370457  | -0.871019  | 0.871014   | 0.000001   | 0.875176   | 0.000000   |
|   | -0.869179  | -1.370460  | 0.871014   | 0.000001   | 0.875176   |
|   | 1.293322   | 1.642137   | 0.000001   |
|   | 1.306810   | -1.419428  | -0.000001   |
|   | 3.619991   | -0.832313  | -0.875176   |
|   | 3.547794   | 0.709382   | 0.000001   |
|   | 3.619990   | -0.832313  | 0.875177   |

**4-hexene-3-one_3**

| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -309.848044 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.730454 |

Number of Imaginary Frequencies

0

**Frequencies (Top 3 out of 45)**
1. 59.1809 cm⁻¹
2. 85.4025 cm⁻¹
3. 165.1824 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 2.328968 | -1.110880 | -0.485527 |
| C | 1.908155 | -0.072420 | 0.559502 |
| C | 0.611765 | 0.583056 | 0.154236 |
| C | -0.607850 | -0.256251 | 0.264541 |
| C | -1.802319 | 0.190800 | -0.115894 |
| C | -3.073381 | -0.578728 | -0.031288 |
| O | 0.580240 | 1.723658 | -0.265340 |
| H | 3.262478 | -1.586050 | -0.190190 |
| H | 1.574262 | -1.889214 | -0.596529 |
| H | 2.477073 | -0.639285 | -1.456661 |
| H | 2.667615 | 0.700269 | 0.661450 |
| H | 1.770743 | -0.561200 | 1.526196 |
| H | -0.492372 | -1.253302 | 0.674630 |
| H | -1.856888 | 1.197578 | -0.519953 |
| H | -3.523058 | -0.674282 | -1.021387 |
| H | -2.916856 | -1.572239 | 0.383911 |
| H | -3.796941 | -0.045006 | 0.587840 |

**4-hexene-3-one_4**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -309.848683 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -309.73063 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 45)**

1. 69.8634 cm⁻¹
2. 107.8091 cm⁻¹
3. 164.5924 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
M06-2X/def2tzvpp-IEFPCM(water) Energy
-309.849904

M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)
-309.732747

Number of Imaginary Frequencies
0

Frequencies (Top 3 out of 45)

1. 44.0452 cm⁻¹
2. 96.9466 cm⁻¹
3. 146.8115 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C  1.701100  -1.510056  -0.487142
C  1.453326  -0.503655   0.641575
C  0.763211   0.730416   0.108645
C -0.696005   0.724242  -0.118304
C -1.507198  -0.292128   0.171769
C -2.978133  -0.292461  -0.062982
O  1.409714   1.722679  -0.176794
H  2.239540  -2.376576  -0.107787
H  0.764197  -1.854146  -0.923480
H  2.298394  -1.056714  -1.277893
H  2.401288  -0.180854   1.068150
H  0.863199  -0.963631   1.433293
H -1.089175  1.635262  -0.557138
H -1.094746  -1.195639   0.609401
H -3.509835  -0.456492   0.876004
H -3.314602   0.644281  -0.502232
H -3.253773  -1.115075  -0.725334

4-hexene-3-one_5
### 4-hexene-3-one_HEI_10

| Datum                                           | Value        |
|-------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -748.06377   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910594 |
| Number of Imaginary Frequencies                 | 0            |

**Frequencies** (Top 3 out of 60)

1. 58.5033 cm\(^{-1}\)  
2. 76.7668 cm\(^{-1}\)  
3. 92.9933 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |          |          |          |
|-----|----------|----------|----------|
| C   | 2.481505 | 1.745818 | 0.060023 |
| C   | 1.905487 | 0.573172 | 0.851079 |
| C   | 1.725118 | -0.657355| -0.035869|
| C   | 0.468909 | -1.184746| -0.236611|
| C   | -0.818486| -0.704718| -0.343418|
| C   | -1.859518| -1.814381| 0.412313  |
| O   | 2.800498 | -1.120526| -0.553062|
| H   | 2.659660 | 2.611302 | 0.699337  |
| H   | 3.424847 | 1.461909 | -0.404514|
| H   | 1.791522 | 2.047352 | -0.730653|
| H   | 0.971191 | 0.878693 | 1.320803  |
| H   | 2.603566 | 0.303724 | 1.649188  |
| H   | -0.689152| -0.283809| 1.342069  |
| H   | -1.498914| -2.612748| 1.063752  |
| H   | -2.813594| -1.462481| 0.804073  |
| H   | -2.028601| -2.234450| -0.580513 |
| C   | -2.941460| 1.204836 | 0.228272  |
| H   | -3.243147| 2.183143 | -0.140165 |
| H   | -3.760900| 0.504981 | 0.080568  |
4-hexene-3-one_HEI_11_reopt

| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.062182 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.909141 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 60)**

1. 34.1109 cm\(^{-1}\)
2. 67.8926 cm\(^{-1}\)
3. 95.9302 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|         | X        | Y        | Z       |
|---------|----------|----------|---------|
| C       | 2.476783 | -1.485814| -0.290250|
| C       | 1.989196 | -0.159111| -0.870207|
| C       | 1.497935 | 0.765684 | 0.240112 |
| C       | 0.163079 | 1.094394 | 0.318698 |
| C       | -0.925720| 0.686874 | -0.609049|
| C       | -2.116573| 1.637370 | -0.531236|
| O       | 2.399184 | 1.161743 | 1.058868 |
| H       | 2.900199 | -2.131818| -1.060382|
| H       | 3.239555 | -1.306518| 0.466625 |
| H       | 1.648614 | -2.018849| 0.180847 |
| H       | 1.218267 | -0.351216| -1.615750|
| H       | 2.821125 | 0.341165 | -1.373787|
| H       | -0.586532| 0.639122 | -1.644691|
| H       | -2.533873| 1.645072 | 0.477489 |
| H       | -1.794020| 2.654495 | -0.761405|
| H       | -2.905364| 1.352701 | -1.226159|
| C       | -1.853323| -1.090833| 1.386417 |
| H       | -0.958994| -0.753908| 1.909602 |
| H       | -2.695655| -0.454958| 1.654864 |
| H       | -2.078293| -2.114635| 1.673906 |
| S       | -1.544703| -1.074524| -0.386664|
| H       | -0.141516| 1.701911 | 1.167607 |
4-hexene-3-one_HEI_12_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.062182    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.909142    |
| Number of Imaginary Frequencies | 0              |

**Frequencies** (Top 3 out of 60)

1. 34.0570 cm⁻¹
2. 67.8849 cm⁻¹
3. 95.9239 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

```
C  -2.476803  -1.485836  -0.290213
C  -1.989217  -0.159140  -0.870189
C  -1.497954   0.765671   0.240116
C  -0.163097   1.094379   0.318698
C   0.925697   1.094379  -0.609057
C   2.116534   0.686860  -0.609057
O  -2.399204   1.161747   1.058863
H  -2.900228  -2.131846  -1.060335
H  -1.648631  -2.018868   0.180881
H  -3.239567  -1.306532   0.466668
H  -2.821147   0.341129  -1.373775
H  -1.218290  -0.351256  -1.615731
H   0.586495   0.639089  -1.644693
H   2.905326   1.352706  -1.226195
H   1.793963   2.654492  -0.761466
H   2.533840   1.645113   0.477448
C   1.853450  -1.090021   1.386402
H   0.959171  -0.753778   1.909630
H   2.078386  -2.114572   1.673923
H   2.695832  -0.454927   1.654766
S   1.544708  -1.074524  -0.386658
H   0.141498   1.701914   1.167594
```

4-hexene-3-one_HEI_13
| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.068222    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -747.914827    |
| Number of Imaginary Frequencies                                       | 0              |

**Frequencies** (Top 3 out of 60)

1. 58.8206 cm⁻¹  
2. 80.1931 cm⁻¹  
3. 92.2385 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |   |
|---|---|---|---|---|
| C | -3.310876 | 0.670196 | -0.560158 |
| C | -2.598703 | -0.672160 | 0.410955 |
| C | -1.270187 | -0.520108 | 0.325472 |
| C | -0.120789 | -0.848323 | -0.357231 |
| C | 1.228524 | -0.725919 | 0.237867 |
| C | 2.158821 | -1.884405 | -0.104600 |
| O | -1.337333 | -0.086369 | 1.527373 |
| H | -4.281594 | 0.561617 | -1.045487 |
| H | -3.465453 | 1.124849 | 0.417665 |
| H | -2.709525 | 1.357532 | -1.159270 |
| H | -2.442748 | -1.124048 | -1.392200 |
| H | -3.233405 | -1.350685 | 0.167204 |
| H | 1.132952 | -0.626999 | 1.319168 |
| H | 2.251126 | -1.988968 | -1.187552 |
| H | 3.158091 | -1.744239 | 0.311236 |
| H | 1.747172 | -2.814445 | 0.288319 |
| C | 0.952907 | 2.075316 | 0.147377 |
| H | 1.257312 | 3.007883 | -0.322858 |
| H | 0.913258 | 2.210424 | 1.226179 |
| H | -0.029871 | 1.778741 | -0.217266 |
| S | 2.146864 | 0.807479 | -0.306584 |
| H | -0.186658 | -1.187941 | -1.385399 |

**4-hexene-3-one_HEI_14**

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.068222    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -747.914829    |
Datum | Value  
--- | ---  
Number of Imaginary Frequencies | 0  

### Frequencies (Top 3 out of 60)

1. 58.8685 cm⁻¹  
2. 80.1387 cm⁻¹  
3. 92.2795 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|  |  |  |  |  |
|---|---|---|---|---|
| C | 3.310837 | 0.670106 | -0.559943 |  
| C | 2.598580 | -0.672258 | -0.411222 |  
| C | 1.270119 | -0.520287 | 0.325405 |  
| C | 0.120668 | -0.848596 | -0.357176 |  
| C | -1.228585 | -0.725896 | 0.237984 |  
| C | -2.159205 | -1.884167 | -0.104404 |  
| O | 1.337420 | -0.086429 | 1.527212 |  
| H | 4.281728 | 0.561629 | -1.044945 |  
| H | 2.709705 | 1.357574 | -1.159131 |  
| H | 3.465014 | 1.124500 | 0.418069 |  
| H | 3.233276 | -1.351043 | 0.166649 |  
| H | 2.442504 | -1.123772 | -1.392619 |  
| H | -1.133059 | -0.626885 | 1.319282 |  
| H | -2.251799 | -1.988600 | -1.187338 |  
| H | -1.747803 | -2.814389 | 0.288356 |  
| H | -3.158342 | -1.743743 | 0.311669 |  
| C | -0.952612 | 2.075286 | 0.147543 |  
| H | -1.256784 | 3.007981 | -0.322601 |  
| H | -0.913305 | 2.210198 | 1.226381 |  
| H | 0.030238 | 1.778625 | -0.216823 |  
| S | -2.146624 | 0.807656 | -0.306777 |  
| H | 0.186421 | -1.188261 | -1.385330 |  

Datum | Value  
--- | ---  
M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.06646  
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.913786

Number of Imaginary Frequencies | 0
**Frequencies** (Top 3 out of 60)

1. 44.1539 cm⁻¹  
2. 68.8193 cm⁻¹  
3. 74.1413 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atoms | Coordinates |
|-------|-------------|
| C     | -3.371784   | 1.040947 | -0.261113 |
| C     | -2.697094   | -0.279341| -0.624518 |
| C     | -1.419544   | -0.502700| 0.179470  |
| C     | -0.234568   | -0.612669| -0.511308 |
| C     | 1.061661    | -0.850407| 0.168111  |
| C     | 2.040602    | -1.655876| -0.678178 |
| O     | -1.550698   | -0.567783| 1.449896  |
| H     | -4.306296   | 1.179634 | -0.806116 |
| H     | -3.590192   | 1.072490 | 0.805698  |
| H     | -2.716888   | 1.882934 | -0.495465 |
| H     | -2.482979   | -0.308448| -1.694480 |
| H     | -3.383310   | -1.103144| -0.404652 |
| H     | 0.882806    | -1.358608| 1.117356  |
| H     | 2.247411    | -1.142508| -1.619272 |
| H     | 2.986680    | -1.816350| -0.161647 |
| H     | 1.605453    | -2.626235| -0.924015 |
| C     | 2.064115    | 1.617087 | -0.770972 |
| H     | 2.801925    | 1.166194 | -1.431833 |
| H     | 2.382126    | 2.628141 | -0.526704 |
| H     | 1.097147    | 1.657455 | -1.271255 |
| S     | 1.903447    | 0.705991 | 0.774743  |
| H     | -0.233771   | -0.527408| -1.591621 |

**4-hexene-3-one_HEI_16**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.066459 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.913786 |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 60)
1. 44.0342 cm⁻¹
2. 68.8199 cm⁻¹
3. 74.1534 cm⁻¹

4-hexene-3-one_HEI_17_reopt

| Datum | Value             |
|-------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.06646 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.913787 |

Number of Imaginary Frequencies

| Frequencies | (Top 3 out of 60) |
|-------------|-------------------|
| 1. 44.0971 cm⁻¹ |
| 2. 68.7955 cm⁻¹ |
| 3. 74.1370 cm⁻¹ |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|  |  |  |  |
|---|---|---|---|
| C | 3.371792 | 1.040931 | -0.261000 |
| C | 2.697066 | -0.279299 | -0.624551 |
| C | 1.419525 | -0.502724 | 0.179435 |
| C | 0.234541 | -0.612635 | -0.511338 |
| C | -1.061682 | -0.850412 | 0.168074 |
| C | -2.040620 | -1.655864 | -0.678237 |
| O | 1.550695 | -0.567914 | 1.449853 |
| H | 4.306280 | 1.179675 | -0.806030 |
| H | 2.716897 | 1.882958 | -0.495208 |
| H | 3.590254 | 1.072330 | 0.805805 |
| H | 3.383269 | -1.103143 | -0.404797 |
| H | 2.482930 | -0.308273 | -1.694511 |
| H | -0.882818 | -1.358639 | 1.117303 |
| H | -2.986686 | -1.816379 | -0.161697 |
| H | -2.247456 | -1.142458 | -1.619304 |
| H | -1.605456 | -2.626204 | -0.924124 |
| C | -2.063964 | 1.617198 | -0.770899 |
| H | -1.096925 | 1.657659 | -1.271038 |
| H | -2.382061 | 2.628212 | -0.526578 |
| H | -2.801656 | 1.166334 | -1.431911 |
| S | -1.903489 | 0.705959 | 0.774750 |
| H | 0.233732 | -0.527278 | -1.591645 |

4-hexene-3-one_HEI_18

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.067611 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.914992 |

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 60)

1. 37.1767 cm⁻¹
2. 59.0313 cm⁻¹
3. 73.9908 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
4-hexene-3-one_HEI_19

| Datum | Value              |
|-------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.067612 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.914992 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 60)

1. 37.2731 cm⁻¹
2. 59.0405 cm⁻¹
3. 74.0082 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |     |     |
|-----|-----|-----|
| C   | -3.583711 | -0.857037 | -0.557744 |
| C   | -2.916733 | 0.467799  | -0.197307 |
| C   | -1.525338 | 0.255274  | 0.391817  |
| C   | -0.454563 | 0.803278  | -0.276638 |
4-hexene-3-one_HEI_1

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.064145
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910893

**Number of Imaginary Frequencies**

0

**Frequencies** (Top 3 out of 60)

1. 70.8408 cm⁻¹
2. 75.8046 cm⁻¹
3. 97.6981 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Element | X | Y | Z |
|---|---|---|---|
| C | 0.944999 | 0.663425 | 0.206044 |
| C | 1.811832 | 1.873878 | -0.110499 |
| O | -1.464865 | -0.423984 | 1.473208 |
| H | -3.635657 | -1.502954 | 0.317452 |
| H | -4.596082 | -0.709393 | -0.936010 |
| H | -3.009117 | -1.377864 | -1.327099 |
| H | -2.864994 | 1.113408 | -1.075815 |
| H | -3.525393 | 0.981354 | 0.553358 |
| H | 0.939237 | 0.471349 | 1.280809 |
| H | 1.813062 | 2.065362 | -1.185133 |
| H | 1.408544 | 2.755357 | 0.391743 |
| H | 2.844073 | 1.742303 | 0.214760 |
| C | 3.280563 | -0.974478 | 0.285628 |
| H | 3.154785 | -0.850047 | 1.360827 |
| H | 3.981945 | -0.231005 | -0.086513 |
| H | 3.685066 | -1.966207 | 0.093609 |
| S | 1.674884 | -0.865549 | -0.539890 |
| H | -0.616979 | 1.355992 | -1.194770 |

| Element | X | Y | Z |
|---|---|---|---|
| C | 2.830026 | 1.086876 | -0.475480 |
| C | 1.866308 | -0.010936 | -0.902787 |
| C | 1.344622 | -0.821546 | 0.288936 |
| C | -0.002958 | -1.067472 | 0.443426 |
| C | -1.126612 | -0.627656 | -0.414173 |
| C | -2.200724 | -1.699854 | -0.575852 |
| O | 2.251530 | -1.260303 | 1.079311 |
| H | 3.243564 | 1.608894 | -1.339152 |
| H | 2.330411 | 1.825643 | 0.154349 |
4-hexene-3-one_HEI_2

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.064145    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910889 |
| Number of Imaginary Frequencies            | 0              |

Frequencies (Top 3 out of 60)

1. 70.8500 cm⁻¹
2. 75.9632 cm⁻¹
3. 98.1002 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 3.650777  | 0.659456 | 0.097300 |
| C   | 2.387154  | -0.706535| -1.564197|
| C   | 1.048536  | 0.424921 | -1.482936|
| C   | -0.789434 | -0.316897| -1.401370|
| C   | -2.568935 | -2.015487| 0.402046 |
| C   | -3.048402 | -1.342870| -1.162785|
| C   | -1.775369 | -2.572349| -1.072296|
| C   | -0.705597 | 2.048079 | 0.352949 |
| H   | -0.371639 | 2.358810 | -0.636388|
| H   | 0.125298  | 1.589362 | 0.888285 |
| H   | -1.057459 | 2.918648 | 0.901980 |
| S   | -2.055769 | 0.865882 | 0.247473 |
| H   | -0.288826 | -1.648223| 1.319004 |
### 4-hexene-3-one_HEI_3

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.06377  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910589 |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 60)**

1. 58.5561 cm⁻¹
2. 76.7332 cm⁻¹
3. 93.0653 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          |          |          |          |
|----------|----------|----------|----------|
| C        | 2.481081 | 1.746048 | 0.060115 |
| C        | 1.905989 | 0.573006 | 0.851282 |
| C        | 1.725300 | -0.657248| -0.035956|
| C        | 0.469029 | -1.184480| -0.236758|
| C        | -0.818379| -0.704642| 0.343504 |
| C        | -1.859227| -1.814484| 0.412517 |
| O        | 2.800552 | -1.120391| -0.553454|
| H        | 2.659487 | 2.611497 | 0.699492 |
| H        | 3.424322 | 1.462666 | -0.404969|
| H        | 1.790533 | 2.047380 | -0.730147|
| H        | 0.972016 | 0.878110 | 1.321922 |
| H        | 2.604818 | 0.303492 | 1.648710 |
| H        | -0.688890| -0.283773| 1.342142 |
| H        | -1.498411| -2.612827| 1.063866 |
| H        | -2.813307| -1.462737| 0.804401 |
| H        | -2.028374| -2.234536| -0.580308|
| C        | -2.941896| 1.204522 | 0.228085 |
| H        | -2.720036| 1.285445 | 1.292076 |
| H        | -3.761145| 0.504468 | 0.080269 |
4-hexene-3-one_HEI_4

| Datum | Value       |
|-------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -748.06377  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910593 |
| Number of Imaginary Frequencies          | 0           |

Frequencies (Top 3 out of 60)

1. 58.4939 cm⁻¹
2. 76.7020 cm⁻¹
3. 93.0273 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 1.745927 | 0.060036 |
|-------|----------|----------|
| C     | 0.573078 | 0.851199 |
| C     | -0.657333 | -0.035862 |
| C     | -1.184733 | -0.236612 |
| C     | -0.704776 | 0.343488 |
| C     | -1.814461 | 0.412293 |
| O     | -1.120387 | -0.553244 |
| H     | 2.611444 | 0.699337 |
| H     | 2.047251 | -0.730458 |
| H     | 1.462343 | -0.404758 |
| H     | 0.303674 | 1.649005 |
| H     | 0.878367 | 1.321316 |
| H     | -0.283958 | 1.342162 |
| H     | -2.612908 | 1.063636 |
| H     | -2.234415 | -0.580580 |
| H     | -1.462590 | 0.804096 |
| C     | 1.204797 | 0.228122 |
| H     | 1.285722 | 1.292101 |
| H     | 2.183031 | -0.140478 |
| H     | 0.504855 | 0.080367 |
| S     | 0.708831 | -0.674797 |
| H     | -0.394383 | -0.909022 |
4-hexene-3-one_HEI_5

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.064202            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -747.911126            |

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 60)

1. 36.3523 cm⁻¹
2. 67.6671 cm⁻¹
3. 82.6115 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|        |        |        |
|--------|--------|--------|
| C      | -2.889371 | 0.153940 | 1.314555 |
| C      | -1.826083 | -0.667218 | 0.586739 |
| C      | -1.396164 | 0.015723 | -0.710926 |
| C      | -0.179675 | 0.656751 | -0.792849 |
| C      | 0.859190  | 0.768560 | 0.255603  |
| C      | 1.526050  | 2.141009 | 0.287415  |
| O      | -2.259968 | -0.029638 | -1.655910 |
| H      | -3.278424 | -0.370619 | 2.188087  |
| H      | -2.473657 | 1.105996 | 1.650501  |
| H      | -3.722357 | 0.367789 | 0.645115  |
| H      | -2.243899 | -1.638401 | 0.310307  |
| H      | -0.988054 | -0.859324 | 1.255190  |
| H      | 0.461893  | 0.548349 | 1.245314  |
| H      | 2.328657  | 2.188068 | 1.024965  |
| H      | 1.945237  | 2.379597 | -0.691810 |
| H      | 0.784496  | 2.902476 | 0.530171  |
| C      | 1.397698  | -1.993535 | 0.063354  |
| H      | 1.082228  | -2.262919 | 1.071505  |
| H      | 0.524184  | -1.919702 | -0.584425 |
| H      | 2.061843  | -2.772458 | -0.316540 |
| S      | 2.286267  | -0.435493 | 0.040129  |
| H      | 0.067458  | 1.119660 | -1.746502 |

4-hexene-3-one_HEI_6
### M06-2X/def2tzvpp-IEFPCM(water) Energy

-748.064202

### M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)

-747.911126

### Number of Imaginary Frequencies

0

### Frequencies (Top 3 out of 60)

1. 36.3495 cm⁻¹
2. 67.6657 cm⁻¹
3. 82.6113 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C    | 2.889364 | 0.153958 | 1.314560 |
|------|----------|----------|----------|
| C    | 1.826087 | -0.667217| 0.586746 |
| C    | 1.396167 | 0.015706 | -0.710929|
| C    | 0.179679 | 0.656733 | -0.792860|
| C    | -0.859183| 0.768561 | 0.255592 |
| C    | -1.526028| 2.141017 | 0.287396 |
| O    | 2.259970 | -0.029672| -1.655913|
| H    | 3.278416 | -0.370589| 2.188099 |
| H    | 3.722351 | 0.367808 | 0.645122 |
| H    | 2.473639 | 1.106014 | 1.650493 |
| H    | 0.9888055| -0.859324| 1.255195 |
| H    | 2.243912 | -1.638399| 0.310327 |
| H    | -0.461885| 0.548353 | 1.245305 |
| H    | -1.945216| 2.379601 | -0.691829|
| H    | -2.328632| 2.188090 | 1.024949 |
| H    | -0.784465| 2.902478 | 0.530143 |
| C    | -1.397720 | -1.999349| 0.063371 |
| H    | -1.082246 | -2.262906| 1.071524 |
| H    | -0.524208 | -1.919715| -0.584413|
| H    | -2.061876 | -2.772449| -0.316509|
| S    | -2.286271 | -0.435479| 0.040135 |
| H    | -0.067457 | 1.119627 | -1.746519|

### 4-hexene-3-one_HEI_7

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.063817 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.911014 |
Datum | Value
---|---
Number of Imaginary Frequencies | 0

**Frequencies (Top 3 out of 60)**

1. 40.5235 cm⁻¹  
2. 52.8324 cm⁻¹  
3. 83.9985 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C  | -2.583088 | -1.321078 | 1.104950 |
| C  | -1.863115 | -1.046094 | -0.215009 |
| C  | -1.718065 | 0.456100  | -0.458439 |
| C  | -0.535807 | 1.078527  | -0.127089 |
| C  | 0.665322  | 0.424758  | 0.466247  |
| C  | 1.454404  | 1.370922  | 1.361867  |
| O  | -2.753696 | 1.042016  | -0.929948 |
| H  | -2.773031 | -2.385325 | 1.250005  |
| H  | -1.987618 | -0.966425 | 1.948423  |
| H  | -3.540518 | -0.799522 | 1.127603  |
| H  | -2.452915 | -1.448398 | -1.041055 |
| H  | -0.898130 | -1.554182 | -0.227629 |
| H  | 0.398314  | -0.464288 | 1.040898  |
| H  | 1.744440  | 2.262517  | 0.803525  |
| H  | 0.831457  | 1.682556  | 2.202488  |
| H  | 2.356184  | 0.907336  | 1.761718  |
| C  | 3.062702  | -1.062247 | -0.000401 |
| H  | 2.631314  | -1.703547 | 0.767964  |
| H  | 3.759951  | -0.364798 | 0.458434  |
| H  | 3.603294  | -1.684327 | -0.710775 |
| S  | 1.745203  | -0.210725 | -0.901955 |
| H  | -0.460542 | 2.148553  | -0.303479 |

**4-hexene-3-one_HEI_8**

Datum | Value
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.063817
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.911014
Number of Imaginary Frequencies | 0
**Frequencies** (Top 3 out of 60)

1. 40.5269 cm⁻¹  
2. 52.8405 cm⁻¹  
3. 83.9930 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| C      | 2.583049  | -1.321038 | 1.105014  |
| C      | 1.863054  | -1.046136 | -0.214951 |
| C      | 1.718031  | 0.456045  | -0.458471 |
| C      | 0.535797  | 1.078543  | -0.127135 |
| C      | -0.665375 | 0.424879  | 0.466256  |
| C      | -1.454382 | 1.371152  | 1.361825  |
| O      | 2.753667  | 1.041900  | -0.930043 |
| H      | 2.772995  | -2.385276 | 1.250129  |
| H      | 3.540478  | -0.799479 | 1.127616  |
| H      | 1.987596  | -0.966334 | 1.948478  |
| H      | 0.898064  | -1.554216 | -0.227520 |
| H      | 2.452851  | -1.448493 | -1.040974 |
| H      | -0.398398 | -0.464140 | 1.040956  |
| H      | -0.831472 | 1.682674  | 2.202514  |
| H      | -1.744208 | 2.262804  | 0.803472  |
| H      | -2.356288 | 0.907728  | 1.761582  |
| C      | -3.062453 | -1.062598 | -0.000361 |
| H      | -3.759655 | -0.365351 | 0.458857  |
| H      | -3.603181 | -1.684494 | -0.710793 |
| H      | -2.630824 | -1.704096 | 0.767698  |
| S      | -1.745262 | -0.210636 | -0.901947 |
| H      | 0.460581  | 2.148564  | -0.303580 |

**4-hexene-3-one_HEI_9**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.06377  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.910593 |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 60)
1. 58.4774 cm⁻¹
2. 76.6780 cm⁻¹
3. 93.0373 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -2.480930 | 1.746002 | 0.059972 |
| C | -1.905558 | 0.573133 | 0.851176 |
| C | -1.725196 | -0.657330 | -0.035844 |
| C | -0.469002 | -1.184752 | -0.236613 |
| C | 0.818419 | -0.704794 | 0.343469 |
| C | 1.859438 | -1.814495 | 0.412210 |
| O | -2.800577 | -1.120386 | -0.553142 |
| H | -2.659237 | 2.611549 | 0.699243 |
| H | -1.790592 | 2.047249 | -0.730508 |
| H | -3.424251 | 1.462471 | -0.404838 |
| H | -2.604024 | 0.303804 | 1.648984 |
| H | -0.971363 | 0.878366 | 1.321288 |
| H | 0.689066 | -0.284047 | 1.342182 |
| H | 1.498867 | -2.612939 | 1.063572 |
| H | 2.028461 | -2.234448 | -0.580677 |
| H | 2.813540 | -1.462648 | 0.803951 |
| C | 2.941530 | 1.204758 | 0.228119 |
| H | 3.243122 | 2.183062 | -0.140395 |
| H | 3.760941 | 0.504910 | 0.080227 |
| H | 2.719680 | 1.285550 | 1.292122 |
| S | 1.453915 | 0.708823 | -0.674750 |
| H | -0.394433 | -2.036091 | -0.908951 |

4-hexene-3-one_TS_10_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.05415 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.901434 |

Number of Imaginary Frequencies

| Frequencies (Top 3 out of 60) |
|-------------------------------|
| 1. -205.8737 cm⁻¹ |
| 2. 63.7505 cm⁻¹ |
| 3. 85.5028 cm⁻¹ |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -1.576732 | -1.495907 | -1.079373 |
| C | -2.074502 | -0.055966 | -0.946007 |
| C | -1.653982 | 0.566280 | 0.378691 |
| C | -0.347314 | 1.118296 | 0.524394 |
| C | 0.651160 | 1.095640 | -0.433582 |
| C | 1.756396 | 2.115034 | -0.399129 |
| O | -2.488462 | 0.577344 | 1.301971 |
| H | -1.907809 | -2.095364 | -0.229999 |
| H | -1.963514 | -1.954772 | -1.989282 |
| H | -0.487191 | -1.527487 | -1.111471 |
| H | -3.163703 | -0.034012 | -0.969221 |
| H | -1.711480 | 0.537315 | -1.785581 |
| H | 0.381292 | 0.756318 | -1.425565 |
| H | 1.374633 | 3.070090 | -0.772477 |
| H | 2.109995 | 2.268170 | 0.619928 |
| H | 2.601247 | 1.820887 | -1.018705 |
| C | 1.069321 | -1.710776 | 1.075029 |
| H | 0.721424 | -2.668970 | 0.690120 |
| H | 0.188906 | -1.094886 | 1.300341 |
| H | 1.608466 | -1.883737 | 2.005529 |
| S | 2.083702 | -0.822835 | -0.121474 |
| H | -0.129893 | 1.557457 | 1.494073 |

4-hexene-3-one_TS_11_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.049878 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.899097 |
| Number of Imaginary Frequencies | 1 |

Frequencies (Top 3 out of 60)

1. -172.3877 cm⁻¹
2. 33.7467 cm⁻¹
3. 34.0205 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
4-hexene-3-one_TS_12_reopt

| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.047733            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.895048 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 60)

1. -194.6219 cm⁻¹
2.  57.2530 cm⁻¹
3.  71.2321 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |     |     |     |
|---|-----|-----|-----|
| C | 2.580510 | 0.839417 | -1.124753 |
| C | 1.486436 | -0.218028 | -0.972546 |
| C | 1.357842 | -0.675384 | 0.469226 |
| C | 0.304836 | -0.179180 | 1.304876 |
4-hexene-3-one_TS_13_reopt

Datum Value
M06-2X/def2tzvpp-IEFPCM(water) Energy -748.049819
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) -747.899328

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 60)

1. -223.6411 cm⁻¹
2. 39.0879 cm⁻¹
3. 42.4166 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| C | -4.086403 | -0.092440 | -0.305325 |
| C | -2.930839 | -0.118474 | 0.690983  |
| C | -1.583763 | -0.201670 | -0.012198 |
| C | -0.605021 | 0.789494  | 0.310890  |
| C | 0.632481  | 0.819307  | -0.290030 |
| C | 1.506801  | 2.033378  | -0.185496 |
| C | 1.403162  | -1.117434 | -0.827949 |
| C | -0.046935 | -0.083609 | 0.208542  |
| C | -4.032078 | 0.796082  | -0.936110 |
### 4-hexene-3-one_TS_14_reopt

| Datum                                                                 | Value     |
|-----------------------------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -748.04985 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -747.899076 |
| Number of Imaginary Frequencies                                       | 1         |

**Frequencies** (Top 3 out of 60)

1. -223.4941 cm\(^{-1}\)
2. 44.8797 cm\(^{-1}\)
3. 47.5140 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | -0.999362 | -0.768793 |
|------------|-----------|-----------|
| C          | 0.302994  | -0.032045 |
| C          | 0.258541  | 0.514315  |
| C          | 0.977779  | -0.202473 |
| C          | 0.971208  | 0.184237  |
| C          | 1.974647  | -0.372654 |
| O          | -0.425248 | 1.526165  |
| H          | -0.998915 | -1.142893 |
| H          | -1.851270 | -0.100196 |
| H          | -1.136340 | -1.617829 |
| H          | 1.152835  | -0.703001 |
| H          | 0.425922  | 0.809073  |
| H          | 0.586301  | 1.174177  |
| H          | 1.694279  | -0.195728 |
4-hexene-3-one_TS_15_reopt

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.050298    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.899053 |
| Number of Imaginary Frequencies            | 1              |

**Frequencies** (Top 3 out of 60)

1. -168.7824 cm⁻¹
2. 38.3213 cm⁻¹
3. 60.1603 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atomic Symbol | X Value   | Y Value   | Z Value   |
|---------------|-----------|-----------|-----------|
| C             | 3.127949  | -1.078806 | -0.317210 |
| C             | 2.608872  | 0.051225  | 0.567057  |
| C             | 1.284257  | 0.603062  | 0.052520  |
| C             | 0.197723  | 0.666809  | 0.985246  |
| C             | -1.075613 | 1.117523  | 0.713563  |
| C             | -1.444165 | 2.062032  | -0.393998 |
| O             | 1.224575  | 0.954863  | -1.133538 |
| H             | 4.100652  | -1.429898 | 0.025396  |
| H             | 2.438740  | -1.924817 | -0.305889 |
| H             | 3.226750  | -0.738070 | -1.346387 |
| H             | 3.325622  | 0.877221  | 0.560274  |
| H             | 2.508287  | -0.282941 | 1.599192  |
| H             | -1.746210 | 1.147041  | 1.562579  |
| H             | -2.525642 | 2.132002  | -0.493166 |
| H             | -1.060230 | 3.058362  | -0.149154 |
| H             | -1.009321 | 1.762769  | -1.340622 |
| C             | -1.103770 | -2.081073 | -0.023043 |
| H             | -1.361054 | -2.877787 | 0.674696  |
| H             | -0.191243 | -1.590880 | 0.342992  |
### 4-hexene-3-one_TS_16_reopt

#### Datum

| Datum                                                      | Value       |
|------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -748.049086 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)| -747.898024 |
| Number of Imaginary Frequencies                           | 1           |

#### Frequencies (Top 3 out of 60)

1. -168.4572 cm⁻¹  
2. 15.5218 cm⁻¹   
3. 43.1267 cm⁻¹   

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | -3.016920 | -1.062788 | -0.778567 |
| C   | -2.650692 | -0.151197 | 0.383364  |
| C   | -1.290967 | 0.544686  | 0.364068  |
| C   | -0.446597 | 0.387613  | -0.781520 |
| C   | 0.811291  | 0.930578  | -0.929956 |
| C   | 1.341503  | 2.118788  | -0.180910 |
| O   | -1.001734 | 1.216185  | 1.365419  |
| H   | -4.002943 | -1.498292 | -0.618587 |
| H   | -3.043264 | -0.518612 | -1.722532 |
| H   | -2.303933 | -1.881365 | -0.881946 |
| H   | -2.687926 | -0.705915 | 1.323963  |
| H   | -3.393065 | 0.645138  | 0.483668  |
| H   | 1.271120  | 0.772860  | -1.896686 |
| H   | 2.397303  | 2.266679  | -0.399206 |
| H   | 0.796740  | 3.012862  | -0.503076 |
| H   | 1.200997  | 2.016791  | 0.889005  |
| C   | 1.268292  | -1.946495 | 0.579177  |
| H   | 0.253315  | -1.583704 | 0.331468  |
| H   | 1.309664  | -2.077899 | 1.659995  |
| H   | 1.390383  | -2.921141 | 0.109111  |
| S   | 2.472603  | -0.743292 | -0.005047 |
| H   | -0.783624 | -0.291321 | -1.551713 |
4-hexene-3-one_TS_17_reopt

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.04856     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -747.897033    |
| Number of Imaginary Frequencies                                      | 1              |

**Frequencies** (Top 3 out of 60)

1.  -206.4009 cm⁻¹  
2.   21.8536 cm⁻¹  
3.   43.9455 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |       |       |       |
|-----|-------|-------|-------|
| C   | 2.70552 | -0.833071 | -1.198140 |
| C   | 1.535047 | 0.072635 | -0.852174 |
| C   | 1.378583 | 0.307495 | 0.645135 |
| C   | 0.140711 | 0.812209 | 1.151320 |
| C   | -0.976236 | 1.253689 | 0.453494 |
| C   | -0.983996 | 1.976289 | -0.871036 |
| O   | 2.321304 | 0.010251 | 1.397256 |
| H   | 2.768806 | -0.981873 | -2.275851 |
| H   | 3.646374 | -0.407459 | -0.854049 |
| H   | 2.593459 | -1.808957 | -0.725189 |
| H   | 0.596165 | -0.343628 | -1.228123 |
| H   | 1.653506 | 1.043751 | -1.340069 |
| H   | -1.768242 | 1.604220 | 1.104084 |
| H   | -0.477319 | 2.939601 | -0.756253 |
| H   | -0.493529 | 1.428078 | -1.667475 |
| H   | -2.009443 | 2.169368 | -1.182379 |
| C   | -1.275576 | -1.930682 | 0.377156 |
| H   | -1.807813 | -2.569157 | 1.081293 |
| H   | -0.430203 | -1.470173 | 0.905081 |
| H   | -0.873573 | -2.553660 | -0.421768 |
| S   | -2.322670 | -0.613633 | -0.267602 |
| H   | 0.049582 | 0.734619 | 2.229749 |

4-hexene-3-one_TS_18_reopt
### Datum Value

| Datum                                                                 | Value       |
|-----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -748.048868 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -747.898071 |

**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 60)

1.  -225.5036 cm⁻¹
2.   35.3240 cm⁻¹
3.   62.2193 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|              | X       | Y       | Z       |
|--------------|---------|---------|---------|
| C            | -3.578330 | 0.643323 | 0.779377 |
| C            | -3.032389 | -0.57344 | 0.046423 |
| C            | -1.578631 | -0.540144 | -0.412719 |
| C            | -0.771422 | 0.602139 | -0.117049 |
| C            | 0.536281  | 0.687947 | -0.536183 |
| C            | 1.268281  | 1.995793 | -0.503990 |
| O            | -1.165718 | -1.530276 | -1.035787 |
| H            | -3.506297 | 1.542430 | 0.167185 |
| H            | -4.628184 | 0.493386 | 1.029650 |
| H            | -3.038242 | 0.825937 | 1.708363 |
| H            | -3.627106 | -0.773235 | -0.848279 |
| H            | -3.132437 | -1.465460 | 0.670100 |
| H            | 0.862474  | -0.034714 | -1.274233 |
| H            | 1.052589  | 2.539206 | 0.415410 |
| H            | 2.344044  | 1.868180 | -0.594308 |
| H            | 0.929278  | 2.611398 | -1.343272 |
| C            | 3.492892  | -0.506917 | -0.233386 |
| H            | 4.040394  | -1.448575 | -0.258804 |
| H            | 4.198606  | 0.289375 | 0.004347 |
| H            | 3.109588  | -0.321795 | -1.241488 |
| S            | 2.117801  | -0.570927 | 0.951809 |
| H            | -1.183875 | 1.398117 | 0.487837 |

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**4-hexene-3-one_TS_19**

### Datum Value

| Datum                                                                 | Value       |
|-----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                  | -748.049738 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -747.898521 |
| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| Number of Imaginary Frequencies            | 1                      |

**Frequencies** (Top 3 out of 60)

|   |                          |                        |
|---|--------------------------|------------------------|
| 1 | -247.5574 cm⁻¹           |                        |
| 2 | 46.6275 cm⁻¹             |                        |
| 3 | 62.6886 cm⁻¹             |                        |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C  | -2.359596 | 1.415076 | 1.204432 |
|----|-----------|----------|----------|
| C  | -1.822719 | 1.117120 | -0.197389|
| C  | -1.847069 | -0.376789| -0.479252|
| C  | -0.735941 | -1.175207| -0.087286|
| C  | 0.404369  | -0.692160| 0.530391 |
| C  | 1.341440  | -1.653176| 1.205885 |
| O  | -2.863567 | -0.853738| -1.015215|
| H  | -2.401276 | 2.488250 | 1.388729 |
| H  | -3.366563 | 1.012317 | 1.319143 |
| H  | -1.727299 | 0.963103 | 1.969151 |
| H  | -0.812860 | 1.513321 | -0.310984|
| H  | -2.459764 | 1.593982 | -0.942291|
| H  | 0.370099  | 0.297252 | 0.970093 |
| H  | 2.303476  | -1.200226 | 1.432723 |
| H  | 0.891954  | -1.986193 | 2.146358 |
| H  | 1.504075  | -2.532908 | 0.583989 |
| C  | 3.012130  | 1.088110 | 0.254586 |
| H  | 2.428493  | 1.223488 | 1.178369 |
| H  | 3.887150  | 0.487292 | 0.502657 |
| H  | 3.353699  | 2.071648 | -0.065771|
| S  | 1.985619  | 0.299383 | -1.018087|
| H  | -0.788230 | -2.229406 | -0.341262|

**4-hexene-3-one_TS_1_reopt**

| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.05505             |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903738 |
| Number of Imaginary Frequencies            | 1                      |
**Frequencies** (Top 3 out of 60)

1. -181.1460 cm\(^{-1}\)
2. 36.6120 cm\(^{-1}\)
3. 65.1398 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -3.274951 | 0.762652  | -0.285471 |
| C    | -2.565577 | -0.572269 | -0.490744 |
| C    | -1.260962 | -0.645793 | 0.290002  |
| C    | -0.086035 | -1.072747 | -0.411486 |
| C    | 1.135922  | -1.146352 | 0.209769  |
| C    | 2.296707  | -1.865104 | -0.408955 |
| O    | -1.275536 | -0.342947 | 1.490771  |
| H    | -4.231648 | 0.782718  | -0.806118 |
| H    | -3.454262 | 0.936431  | 0.774077  |
| H    | -2.665108 | 1.584807  | -0.663584 |
| H    | -2.381603 | -0.753763 | -1.549529 |
| H    | -3.203965 | -1.383587 | -0.129006 |
| H    | 1.131954  | -1.077280 | 1.288852  |
| H    | 3.244089  | -1.549321 | 0.022191  |
| H    | 2.187991  | -2.940239 | -0.236020 |
| H    | 2.331366  | -1.700312 | -1.485498 |
| C    | 0.710114  | 2.038004  | -0.420794 |
| H    | 0.262322  | 2.679446  | 0.338646  |
| H    | -0.045349 | 1.301968  | -0.728329 |
| H    | 0.950938  | 2.648823  | -1.290456 |
| S    | 2.157003  | 1.155581  | 0.194972  |
| H    | -0.165793 | -1.265765 | -1.474873 |

**4-hexene-3-one_TS_2_reopt**

| Datum                                         | Value    |
|-----------------------------------------------|----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy         | -748.054767 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903695 |
| Number of Imaginary Frequencies               | 1        |

**Frequencies** (Top 3 out of 60)
1. -183.4377 cm⁻¹
2.  27.4895 cm⁻¹
3.  63.8170 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|       | X          | Y          | Z          |
|-------|------------|------------|------------|
|       | 3.800631   | -0.209970  | 0.033779   |
|       | 2.505057   | -0.005878  | -0.734155  |
|       | 1.295714   | 0.236961   | 0.162837   |
|       | 0.172315   | 0.892505   | -0.436409  |
|       | -0.983654  | 1.142813   | 0.267203   |
|       | -2.006023  | 2.122670   | -0.229039  |
|       | 1.327557   | -0.148116  | 1.339384   |
|       | 4.628452   | -0.404238  | -0.647425  |
|       | 4.046185   | 0.673815   | 0.623454   |
|       | 3.714471   | -1.050332  | 0.719946   |
|       | 2.281889   | -0.892978  | -1.336000  |
|       | 2.593759   | 0.820379   | -1.441520  |
|       | -0.922489  | 1.020155   | 1.340001   |
|       | -2.969045  | 1.984498   | 0.258064   |
|       | -1.662941  | 3.140281   | -0.019203  |
|       | -2.144960  | 2.030219   | -1.305892  |
|       | -1.226549  | -1.993387  | -0.512218  |
|       | -0.891759  | -2.745806  | 0.201945   |
|       | -0.351459  | -1.412874  | -0.831468  |
|       | -1.627667  | -2.502355  | -1.388088  |
|       | -2.430774  | -0.858506  | 0.205519   |
|       | 0.232553   | 1.145974   | -1.489175  |

4-hexene-3-one_TS_3_reopt

|        | Value        |
|--------|--------------|
| Datum  | Value        |
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.05397 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.902637 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 60)

1. -171.2137 cm⁻¹
2.  41.2803 cm⁻¹
3.  58.2918 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |        |        |        |
|---|--------|--------|--------|
| C | 2.997330 | 0.030284 | -1.278872 |
| C | 2.673984 | -0.322935 | 0.165365  |
| C | 1.308498 | 0.079823  | 0.710727  |
| C | 0.414870 | 0.844529  | -0.110307 |
| C | -0.832794 | 1.197721  | 0.335316  |
| C | -1.667520 | 2.220924  | -0.372539 |
| O | 1.036617 | -0.279767 | 1.864659  |
| H | 2.284911 | -0.424627 | -1.967771 |
| H | 2.980055 | 1.107985  | -1.440858 |
| H | 3.991683 | -0.329453 | -1.541575 |
| H | 3.412475 | 0.122671  | 0.837023  |
| H | 2.752032 | -1.402109 | 0.317766  |
| H | -1.030986 | 1.057066  | 1.388724  |
| H | -1.560388 | 2.134269  | -1.453398 |
| H | -2.720968 | 2.128457  | -0.118146 |
| H | -1.335492 | 3.221864  | -0.079911 |
| C | -1.101683 | -1.955784 | -0.553470 |
| H | -0.952564 | -2.733410 | 0.196004  |
| H | -0.152055 | -1.417196 | -0.674448 |
| H | -1.334256 | -2.434329 | -1.504517 |
| S | -2.380472 | -0.777552 | -0.070487 |
| H | 0.704053  | 1.080407  | -1.125699 |

4-hexene-3-one_TS_4

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.055054 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903184 |
| Number of Imaginary Frequencies | 1 |
| Frequencies (Top 3 out of 60) |
| 1. | -202.5888 cm⁻¹ |
| 2. | 51.5162 cm⁻¹ |
| 3. | 62.7588 cm⁻¹ |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### 4-hexene-3-one_TS_5_reopt

| Datum                                           | Value          |
|-------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -748.055637    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy      | -747.90355     |
| (Quasiharmonic)                                |                |
| Number of Imaginary Frequencies                 | 1              |

**Frequencies (Top 3 out of 60)**

1. -212.9409 cm⁻¹
2.  49.6738 cm⁻¹
3.  70.8098 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|        | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| C      | 3.017708  | 0.809079  | -0.783633 |
| C      | 1.677735  | 0.099030  | -0.877300 |
| C      | 1.336166  | -0.716021 |  0.368985 |
| C      | 0.001666  | -1.188957 |  0.511050 |
### 4-hexene-3-one_TS_6_reopt

| Datum | Value         |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -748.05469 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903291 |

**Number of Imaginary Frequencies**

**Frequencies** (Top 3 out of 60)

1. -173.0754 cm\(^{-1}\)
2. 40.2993 cm\(^{-1}\)
3. 64.4200 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | 3.796272 | -0.091806 | -0.054945 |
|---------|----------|-----------|-----------|
| C       | 2.489571 | -0.429577 | -0.649244 |
| C       | 1.295282 | -0.016951 | 0.197600  |
| C       | 0.280671 | 0.784933  | -0.423737 |
| C       | -0.832163| 1.198703  | 0.262157  |
| C       | -1.738192| 2.268710  | -0.266700 |
| O       | 1.260686 | -0.380723 | 1.380526  |
| H       | 3.804492 | 1.182602  | -0.037288 |
| H       | 3.915105 | -0.264612 | 0.967009  |
### 4-hexene-3-one_TS_7

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.055054    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -747.903186    |
| Number of Imaginary Frequencies                                      | 1              |

**Frequencies** (Top 3 out of 60)

1. -202.6039 cm⁻¹
2.  51.4947 cm⁻¹
3.  62.6939 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | 2.590726 | 0.271879 | -1.516124 |
|------------|----------|----------|-----------|
| C          | -1.708381| -0.667972| -0.692069 |
| C          | -1.452559| -0.094234|  0.693405 |
| C          | -0.313603|  0.738124|  0.898629 |
| C          |  0.571050|  1.117525| -0.094047 |
| C          |  1.507870|  2.271244|  0.127613 |
| O          | -2.271913| -0.351863|  1.593042 |
| H          | -3.527206|  0.468600| -0.993445 |
| H          | -2.092390|  1.226955| -1.685204 |
| H          | -2.828819| -0.163251| -2.486288 |
| H          | -0.768972| -0.862153| -1.211653 |
| H          | -2.217961| -1.621793| -0.552771 |
| H          |  0.268074|  0.974884| -1.121307 |
| H          |  0.956486|  3.210621|  0.027994 |
4-hexene-3-one_TS_8_reopt

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -748.05505     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -747.903736    |
| Number of Imaginary Frequencies            | 1              |

**Frequencies** (Top 3 out of 60)

1. -181.1412 cm⁻¹
2. 36.6343 cm⁻¹
3. 65.1604 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 1.935890 | 2.236459 | 1.128897 |
|-------|----------|----------|----------|
| H     | 2.319641 | 2.276714 | -0.597183 |
| C     | 1.392693 | -1.959220 | 0.325882 |
| H     | 0.547879 | -1.556255 | 0.898499 |
| H     | 2.035851 | -2.499246 | 1.019587 |
| H     | 1.002077 | -2.665610 | -0.406531 |
| S     | 2.264968 | -0.583510 | -0.446518 |
| H     | -0.132801 | 1.061073 | 1.919624 |
4-hexene-3-one_TS_9_reopt

| Datum                                                                 | Value        |
|----------------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -748.05397   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -747.902638  |
| Number of Imaginary Frequencies                                      | 1            |

**Frequencies** (Top 3 out of 60)

1. -171.1934 cm⁻¹  
2. 41.2341 cm⁻¹   
3. 58.3964 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | 2.997164 | 0.029733 | -1.279009 |
|---------|----------|----------|-----------|
| C       | 2.674039 | -0.322717| 0.165468  |
| C       | 1.308544 | 0.080114 | 0.710763  |
| C       | 0.414870 | 0.844602 | -0.110426 |
| C       | -0.832809| 1.197844 | 0.335133  |
| C       | -1.667637| 2.220749 | -0.373032 |
| O       | 1.036702 | -0.279185| 1.864795  |
| H       | 3.991477 | -0.330142| -1.541669 |
| H       | 2.284639 | -0.425550| -1.967554 |
| H       | 2.979867 | 1.107345 | -1.441578 |
| H       | 3.412525 | 0.123419 | 0.836781  |
| H       | 2.752312 | -1.401785| 0.318486  |
| H       | -1.031024| 1.057449 | 1.388577  |
| H       | -2.721063| 2.128307 | -0.118536 |
| H       | -1.335651| 3.221817 | -0.080794 |
| H       | -1.560577| 2.133699 | -1.453868 |
| C       | -1.101669| -1.955890| -0.553360 |
| H       | -0.151983| -1.417326| -0.673916 |
| H       | -1.334040| -2.434106| -1.504621 |
| H       | -0.952819| -2.733782| 0.195890  |
| S       | -2.380392| -0.777667| -0.070178 |
| H       | 0.703992 | 1.080198 | -1.125914 |
5_3-methyl-2-cyclopentene-1-one_1

| Datum                                                      | Value      |
|------------------------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -308.660411|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -308.561666|
| Number of Imaginary Frequencies                            | 0          |

Frequencies (Top 3 out of 39)

1. 99.8504 cm⁻¹
2. 140.7928 cm⁻¹
3. 186.3999 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |          |          |          |
|----|----------|----------|----------|
| C  | -0.581171| 1.273116 | 0.000001 |
| C  | 0.946705 | 1.200376 | -0.000001|
| C  | 1.268077 | -0.287146| -0.000001|
| C  | -0.001629| -1.019500| -0.000000|
| C  | -1.032714| -0.164830| 0.000001  |
| H  | -0.980918| 1.788566 | 0.875083 |
| H  | -0.980920| 1.788567 | -0.875081|
| H  | 1.398262 | 1.661104 | 0.877949 |
| H  | 1.398260 | 1.661104 | -0.877951|
| O  | 2.385814 | -0.761401| -0.000002|
| H  | -0.063578| -2.098230| -0.000000|
| C  | -2.479877| -0.502501| 0.000002 |
| H  | -2.647401| -1.576779| 0.000001 |
| H  | -2.963283| -0.065107| 0.875917 |
| H  | -2.963284| -0.065107| -0.875913|

5_3methyl2cyclopentene1one_HEI_1

| Datum                                                      | Value      |
|------------------------------------------------------------|------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -746.870798|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.736194|
| Number of Imaginary Frequencies                            | 0          |
### Frequencies (Top 3 out of 54)

1. 92.5471 cm\(^{-1}\)
2. 116.2500 cm\(^{-1}\)
3. 168.9810 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | C          | H          | O          |
|------|------------|------------|------------|
|      | 1.487548   | -0.151060  | 1.164888   |
|      | 0.165890   | 0.593616   | 1.368476   |
|      | -0.466528  | 0.735466   | -0.038671  |
|      | 0.673414   | 0.500787   | -0.956404  |
|      | 1.782818   | -0.024003  | -0.334600  |
|      | 2.306510   | 0.271972   | 1.749460   |
|      | 1.421986   | -1.210501  | 1.427592   |
|      | 0.363723   | 1.598896   | 1.747269   |
|      | -0.509345  | 0.109730   | 2.074606   |
|      | 2.906045   | -0.387664  | -0.807153  |
|      | 0.587032   | 0.644226   | -2.027605  |
|      | -0.984845  | -2.059217  | 0.067714   |
|      | -0.783289  | -2.174011  | 1.131681   |
|      | -0.046303  | -2.069144  | -0.486750  |
|      | -1.610528  | -2.883771  | -0.266513  |
|      | -1.857491  | -0.524060  | -0.273120  |
|      | -1.187917  | 2.067535   | -0.223108  |
|      | -0.473273  | 2.881385   | -0.091615  |
|      | -1.613719  | 2.147263   | -1.224851  |
|      | -1.993568  | 2.191476   | 0.504090   |

### 5_3methyl2cyclopentene1one_HEI_2

| Datum                                      | Value           |
|--------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.869627     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy | -746.735811     |

Number of Imaginary Frequencies

### Frequencies (Top 3 out of 54)

1. 65.3372 cm\(^{-1}\)
2. 104.1520 cm\(^{-1}\)
3. 141.3933 cm\(^{-1}\)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 1.787965 | -0.520758 | -0.934288 |
| C | 0.630526 | -1.444478 | -0.561363 |
| C | -0.295811 | -0.583850 | 0.320339 |
| C | 0.627500 | 0.432041 | 0.886938 |
| C | 1.816473 | 0.517035 | 0.196193 |
| H | 2.745909 | -1.035678 | -1.019572 |
| H | 1.608335 | -0.005448 | -1.882883 |
| H | 0.998993 | -2.267982 | 0.05143 |
| H | 0.110036 | -1.881562 | -1.416387 |
| O | 2.816551 | 1.284040 | 0.353578 |
| C | 0.349676 | 1.083195 | 1.706795 |
| C | -2.233427 | 1.492734 | 0.110775 |
| H | -2.770196 | 1.116605 | 0.980255 |
| H | -1.430532 | 2.153353 | 0.433932 |
| H | -2.926876 | 2.052440 | -0.513277 |
| S | -1.562190 | 0.151031 | -0.884492 |
| C | -1.072793 | -1.404190 | 1.341796 |
| H | -0.373234 | -1.877187 | 2.034706 |
| H | -1.747487 | -0.775458 | 1.925258 |
| H | -1.664587 | -2.182296 | 0.856939 |

5_3methyl2cyclopentene1one_HEI_3

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -746.867217 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.733283 |

Number of Imaginary Frequencies | 0

Frequencies (Top 3 out of 54)

1. 59.7448 cm⁻¹
2. 75.4790 cm⁻¹
3. 134.2102 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
5_3methyl2cyclopentene1one_TS_1

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -746.862263 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.729397 |
| Number of Imaginary Frequencies            | 1         |

**Frequencies** (Top 3 out of 54)

1. -219.4180 cm⁻¹
2.  61.9380 cm⁻¹
3.  96.3570 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

C  1.433113  0.003805  1.219717
C  0.362060  1.090795  1.203330
C -0.219776  0.992720 -0.197472
C  0.739393  0.403938 -1.020050
C  1.771217 -0.200596 -0.256705
H  2.322401  0.244971  1.800308
5_3methyl2cyclopentene1one_TS_2

| Datum                                                        | Value                  |
|--------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                        | -746.862263            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  | -746.729394            |
| Number of Imaginary Frequencies                              | 1                      |
| **Frequencies** (Top 3 out of 54)                            |                        |
| 1. -219.3785 cm⁻¹                                           |                        |
| 2.  62.1772 cm⁻¹                                            |                        |
| 3.  96.3748 cm⁻¹                                            |                        |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|         |          |          |          |
|---------|----------|----------|----------|
| C       | 1.432899 | -0.002864| -1.219741|
| C       | 0.362256 | -1.090238| -1.203652|
| C       | -0.219424| -0.992907|  0.197240|
| C       |  0.739655| -0.404197|  1.019959|
| C       |  1.771360|  0.200694|  0.256708|
| H       |  2.322060| -0.243235| -1.800847|
| H       |  1.023145|  0.937834| -1.600402|
| H       |  0.825300| -2.078186| -1.300948|
| H       | -0.391968| -0.993576| -1.979800|
| O       |  2.782469| -0.807190| -0.642964|
| H       |  0.680764|  0.349447| -2.099029|
| C       | -1.051060| -2.117792| -0.163612|
| H       | -0.791227| -2.659177|  0.746085|
| H       | -0.122427| -1.846775| -0.679309|
| H       | -1.613724| -2.785423| -0.815085|
| S       | -1.970236| -0.604597|  0.181102|
5_3methyl2cyclopentene1one_TS_3

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -746.85844 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -746.726421 |
| Number of Imaginary Frequencies | 1 |
| Frequencies (Top 3 out of 54) | |
| 1. | -256.6556 cm⁻¹ |
| 2. | 75.8278 cm⁻¹ |
| 3. | 81.5561 cm⁻¹ |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Datum | Value          |
|-------|----------------|
| H     | -0.122688      | 1.846629 | 0.679469 |
| H     | -0.791433      | 2.658599 | -0.746205 |
| S     | -1.134547      | -2.087537 | 0.660857 |
| C     | -1.543860      | -1.874031 | 1.646401 |
| H     | -1.958775      | -2.239108 | -0.035909 |
### 6_3pentene2one_HEI_1

| Datum                                           | Value              |
|------------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -708.760776        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.635078        |
| Number of Imaginary Frequencies                 | 0                  |

#### Frequencies (Top 3 out of 51)

1. 65.5606 cm⁻¹
2. 86.5236 cm⁻¹
3. 97.8224 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 2.993217 | 0.019702 | -0.731518 |
|-------|----------|----------|-----------|
| C     | 1.729053 | 0.050976 | 0.117794  |
| C     | 0.613341 | 0.653837 | -0.415766 |
| C     | -0.671622| 0.757231 | 0.311136  |
| O     | 1.820706 | -0.488611| 1.274441  |
| C     | -1.347512| 2.117383 | 0.173047  |
| H     | 3.807191 | 0.508958 | -0.192054 |
| H     | 3.296134 | -1.017399| -0.893241 |
| H     | 2.868934 | 0.504788 | -1.699342 |
| H     | 0.654447 | 1.063161 | -1.419433 |
| H     | -0.50833 | 0.526610 | 1.363408  |
| H     | -2.312809| 2.148782 | 0.681358  |
| H     | -0.706795| 2.890271 | 0.598289  |
| H     | -1.507983| 2.355929 | -0.880260 |
| S     | -1.953357| -0.476734| -0.259539 |
| C     | -1.038958| -2.012308| -0.047305 |
| H     | -0.042987| -1.886025| -0.470312 |
| H     | -0.957051| -2.281212| 1.004061  |
| H     | -1.570292| -2.798166| -0.579703 |

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### 6_3pentene2one_HEI_2_reopt2

| Datum | Value |
|-------|-------|
|       |       |
### M06-2X/def2tzvpp-IEFPCM(water) Properties

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.759249 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.633682 |

Number of Imaginary Frequencies: 0

Frequencies (Top 3 out of 51)

1. 45.5116 cm⁻¹
2. 77.8442 cm⁻¹
3. 106.5720 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X | Y | Z |
|------|---|---|---|
| C    | -3.033129 | -0.331326 | 0.834564 |
| C    | -1.854014 | -0.047554 | -0.085620 |
| C    | -0.694482 | 0.433602  | 0.476358  |
| C    |  0.497005 | 0.776590  | -0.337065 |
| O    | -2.042655 | -0.275954 | -1.329714 |
| C    |  1.304896 | 1.930747  | 0.244763  |
| H    | -3.894005 | 0.261327  | 0.516975  |
| H    | -3.320023 | -1.381842 | 0.748673  |
| H    | -2.818830 | -0.109573 | 1.879733  |
| H    | -0.637157 | 0.577949  | 1.548718  |
| H    |  0.180154 | 1.016723  | -1.353569 |
| H    |  2.177088 | 2.163841  | -0.365628 |
| H    |  0.678347 | 2.821529  | 0.316966  |
| H    |  1.647433 | 1.689667  | 1.252976  |
| S    |  1.637678 | -0.667835 | -0.674496 |
| C    |  2.060728 | -1.152521 | 1.008287  |
| H    |  2.716470 | -0.427045 | 1.485782  |
| H    |  1.149180 | -1.266534 | 1.593893  |
| H    |  2.573703 | -2.110271 | 0.957400  |

### 6_3pentene2one_HEI_3 Properties

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.757306 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.631745 |

Number of Imaginary Frequencies: 0
**Frequencies** (Top 3 out of 51)

| Rank | Frequency (cm⁻¹) |
|------|------------------|
| 1.   | 62.9190          |
| 2.   | 90.5919          |
| 3.   | 95.5811          |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| C    | 1.990940     | -0.612095    | 1.123559     |
| C    | 1.796405     | 0.195803     | -0.154623    |
| C    | 0.587877     | 0.791920     | -0.437478    |
| C    | -0.663481    | 0.744959     | 0.351633     |
| O    | 2.834123     | 0.266828     | -0.902281    |
| C    | -1.436782    | 2.060031     | 0.316621     |
| H    | 1.124478     | -0.654628    | 1.779172     |
| H    | 2.262510     | -1.634603    | 0.851855     |
| H    | 2.832412     | -0.194049    | 1.679498     |
| H    | 0.522225     | 1.323990     | -1.385120    |
| H    | -0.479876    | 0.471227     | 1.389174     |
| H    | -0.835327    | 2.850903     | 0.765324     |
| H    | -2.382460    | 1.991777     | 0.856356     |
| H    | -1.650590    | 2.344149     | -0.715400    |
| S    | -1.895905    | -0.537925    | -0.252274    |
| C    | -0.886929    | -2.022274    | -0.134063    |
| H    | 0.062527     | -1.851808    | -0.640812    |
| H    | -0.701202    | -2.291614    | 0.904576     |
| H    | -1.421378    | -2.833227    | -0.623894    |

**6_3pentene2one_HEI_4**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.760358   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.635046 |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 51)

| Rank | Frequency (cm⁻¹) |
|------|------------------|
| 1.   | 56.9514          |
| 2.   | 77.4122          |
| 3.   | 88.5218          |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| C | 3.320579| -0.016012| -0.515824|
| C | 1.960482| -0.172719| 0.149887 |
| C | 0.927654| 0.616324 | -0.300121|
| C | -0.436183| 0.560473 | 0.290184 |
| O | 1.893528| -1.032009| 1.094126 |
| C | -1.135698| 1.912266 | 0.310984 |
| H | 3.322593| 0.731570 | -1.308567|
| H | 4.063060| 0.262683 | 0.235200 |
| H | 3.634247| -0.975086| -0.934117|
| H | 1.092590| 1.305896 | -1.119788|
| H | -0.376889| 0.148815| 1.299627 |
| H | -0.570399| 2.607718 | 0.934354 |
| S | -2.149194| 1.850253| 0.708003 |
| H | -1.187446| 2.324882| -0.698245|
| S | -1.438857| -0.670426| -0.661816|
| C | -2.908755| -0.731336| 0.281889 |
| H | -3.542609| -1.599374| -0.056951|
| H | -2.762601| -0.848087| 1.343082 |
| H | -3.586338| 0.159630 | 0.131456 |

6_3pentene2one_HEI_5_reopt

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -708.75541   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.629217|
| Number of Imaginary Frequencies            | 0            |

Frequencies (Top 3 out of 51)

1. 77.9228 cm⁻¹
2. 106.8922 cm⁻¹
3. 107.7473 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| C | -2.970519| -0.562500| -0.535610|
| C | -1.661830| -0.012390| 0.026880 |
| C | -0.682170| 0.316681 | -0.882910|
### 6_3pentene2one_HEI_6

| Datum                                                                 | Value         |
|-----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -708.754933   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.629884   |
| Number of Imaginary Frequencies                                       | 0             |
| **Frequencies (Top 3 out of 51)**                                      |               |
| 1. 43.3364 cm⁻¹                                                      |               |
| 2. 55.2989 cm⁻¹                                                      |               |
| 3. 94.6534 cm⁻¹                                                      |               |

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -2.154089 | -0.641382 | -1.115518 |
| C     | -1.888782 | 0.040607  | 0.221217  |
| C     | -0.676099 | 0.647847  | 0.454063  |
| C     | 0.478715  | 0.736584  | -0.478046 |
| O     | -2.858538 | -0.010066 | 1.055341  |
| C     | 1.373747  | 1.930640  | -0.161986 |
| H     | -2.485194 | -1.687275 | -0.928017 |
| H     | -3.027481 | -0.182113 | -1.583193 |
| H     | -1.321081 | -0.611261 | -1.814348 |
| H     | -0.529631 | 1.088064  | 1.437141  |
| H     | 0.160122  | 0.807555  | -1.518425 |
| Datum                                      | Value          |
|-------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy     | -708.751492    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.626048 |
| Number of Imaginary Frequencies           | 0              |

Frequencies (Top 3 out of 51)

1. 53.6420 cm⁻¹
2. 83.6133 cm⁻¹
3. 106.6484 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -1.773787 | 0.295894 | 1.294528 |
| C     | -1.760805 | -0.340239 | -0.091297 |
| C     | -0.678278 | -0.171609 | -0.926406 |
| C     | 0.551728  | 0.649999  | -0.720142 |
| O     | -2.806585 | -1.017602 | -0.380616 |
| C     | 0.355246  | 2.128606  | -0.380827 |
| H     | -2.392762 | 1.196743  | 1.286054  |
| H     | -2.234671 | -0.408621 | 1.987739  |
| H     | -0.783538 | 0.555607  | 1.661973  |
| H     | -0.727470 | -0.705119 | -1.871081 |
| H     | 1.123415  | 0.609483  | -1.648880 |
| H     | -0.251360 | 2.596201  | -1.156966 |
| H     | 1.312044  | 2.651794  | -0.327601 |
| H     | -0.158093 | 2.263545  | 0.569453  |
| S     | 1.770689  | 0.001581  | 0.544387  |
| C     | 1.991661  | -1.666769 | -0.090735 |
| H     | 2.644424  | -2.204700 | 0.593073  |
| H     | 1.026774  | -2.167739 | -0.146828 |
| H     | 2.448317  | -1.646967 | -1.079734 |
### 6_3pentene2one_TS_1_reopt

| Datum |
|-------|
| Datum |
| Value |
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.747583 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.623927 |
| Number of Imaginary Frequencies | 1 |

#### Frequencies (Top 3 out of 51)

1. -175.8704 cm\(^{-1}\)
2. 49.9216 cm\(^{-1}\)
3. 64.3090 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 2.940720 | -0.277989 | -0.647222 |
|-------|----------|-----------|-----------|
| C     | 1.739465 | 0.093813  | 0.200620  |
| C     | 0.685062 | 0.838087  | -0.425292 |
| C     | -0.448051| 1.195633  | 0.259273  |
| O     | 1.726784 | -0.262471 | 1.386248  |
| C     | -1.407687| 2.217079  | -0.271312 |
| H     | 3.845735 | 0.100220  | -0.178766 |
| H     | 3.023288 | -1.365210 | -0.685250 |
| H     | 2.878086 | 0.109863  | -1.661448 |
| H     | 0.772833 | 1.060176  | -1.482238 |
| H     | -0.423058| 1.068867  | 1.332778  |
| H     | -2.384485| 2.136113  | 0.200132  |
| H     | -1.015820| 3.218481  | -0.068159 |
| H     | -1.530846| 2.117060  | -1.349233 |
| S     | -2.046209| -0.771776 | 0.201685  |
| C     | -0.897393| -1.963524 | -0.516393 |
| H     | 0.012066 | -1.432605 | -0.827800 |
| H     | -0.607400| -2.737036 | 0.195089  |
| H     | -1.318019| -2.446342 | -1.398089 |

### 6_3pentene2one_TS_2_reopt

| Datum |
|-------|
| Datum |
| Value |
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.747583 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.623927 |
| Number of Imaginary Frequencies | 1 |

#### Frequencies (Top 3 out of 51)

1. -175.8704 cm\(^{-1}\)
2. 49.9216 cm\(^{-1}\)
3. 64.3090 cm\(^{-1}\)
### SI_ketones.md

#### Datum

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -708.747583 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.623933 |
| Number of Imaginary Frequencies                                      | 1           |

#### Frequencies (Top 3 out of 51)

|   |                        |
|---|------------------------|
| 1 | -175.8163 cm⁻¹         |
| 2 |  49.1787 cm⁻¹          |
| 3 |  64.3348 cm⁻¹          |

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |          |
|---|----------|
| C |  2.940469 |
| C |  1.739439 |
| C |  0.684971 |
| C | -0.448295 |
| O |  1.726711 |
| C | -1.408144 |
| H |  3.846380 |
| H |  3.018496 |
| H |  2.880694 |
| H |  0.772841 |
| H | -0.423382 |
| H | -2.384969 |
| H | -1.016565 |
| H | -1.531162 |
| S | -2.045962 |
| C | -0.896705 |
| H | -1.317249 |
| H |  0.012453 |
| H | -0.606247 |

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#### 6_3pentene2one_TS_3

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -708.748244 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.623547 |
| Number of Imaginary Frequencies                                      | 1           |
**Frequencies (Top 3 out of 51)**

1.  -207.7977 cm⁻¹
2.   72.8449 cm⁻¹
3.   95.2196 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|    |   x    |   y    |   z    |
|----|--------|--------|--------|
| C  | 1.794647 | -0.523181 | 1.287317 |
| C  | 1.822495 | 0.109832  | -0.093716 |
| C  | 0.692278 | 0.869538  | -0.507162 |
| C  | -0.419105 | 1.101241  | 0.287991  |
| O  | 2.828854 | -0.057837 | -0.805724 |
| C  | -1.380763 | 2.201758  | -0.064818 |
| H  | 0.858599 | -1.059769 | 1.453277 |
| H  | 2.635177 | -1.205645 | 1.385457 |
| H  | 1.871534 | 0.244256  | 2.059830 |
| H  | 0.701957 | 1.236573  | -1.528923 |
| H  | -0.316565 | 0.917909 | 1.348505 |
| H  | -0.942103 | 3.166850  | 0.204295 |
| H  | -2.325570 | 2.099341  | 0.465648 |
| H  | -1.582872 | 2.210359  | -1.135533 |
| S  | -1.966300 | -0.719430 | 0.160121 |
| C  | -0.873829 | -1.939710 | -0.591116 |
| H  | 0.039206 | -1.427015 | -0.919508 |
| H  | -0.592307 | -2.728227 | 0.106683 |
| H  | -1.331418 | -2.397924 | -1.466852 |

**6_3pentene2one_TS_4**

| Datum                                           | Value     |
|-------------------------------------------------|-----------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -708.742738 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.619556 |
| Number of Imaginary Frequencies                 | 1         |

**Frequencies (Top 3 out of 51)**

1.  -225.0791 cm⁻¹
2.   57.7762 cm⁻¹
3.   74.1111 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |    |    |
|----|----|----|
| C  | 3.427344 | -0.182356 | -0.457626 |
| C  | 2.049146 | -0.233771 | 0.173533 |
| C  | 1.104815 | 0.768282 | -0.210219 |
| C  | -0.163605 | 0.818043 | 0.321146 |
| O  | 1.811209 | -1.141502 | 0.983510 |
| C  | -1.016196 | 2.040158 | 0.154358 |
| H  | 3.575504 | 0.699143 | -1.077343 |
| H  | 4.182974 | -0.205479 | 0.327801 |
| H  | 3.568018 | -1.074076 | -1.070932 |
| H  | 1.392527 | 1.477881 | -0.976491 |
| H  | -0.349107 | 0.211723 | 1.199784 |
| H  | -0.663900 | 2.814217 | 0.843389 |
| H  | -2.062950 | 1.846206 | 0.374186 |
| H  | -0.935079 | 2.434196 | -0.858219 |
| S  | -1.737220 | -0.797116 | -0.760873 |
| C  | -3.001739 | -0.632365 | 0.532636 |
| H  | -3.457288 | -1.593674 | 0.768034 |
| H  | -2.548719 | -0.248761 | 1.451883 |
| H  | -3.794720 | 0.056548 | 0.240831 |

6_3pentene2one_TS_5_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -708.742808 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.619483 |
| Number of Imaginary Frequencies | 1 |
| Frequencies (Top 3 out of 51) | |
| 1. | -175.7306 cm⁻¹ |
| 2. | 42.6136 cm⁻¹ |
| 3. | 52.5006 cm⁻¹ |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    |    |    |
|----|----|----|
| C  | 2.815094 | -1.032800 | 0.257843 |
| C  | 1.714380 | -0.043977 | -0.085632 |
| C  | 0.741131 | 0.229355 | 0.931018 |
### 6_3pentene2one_TS_6

| Datum                                                                 | Value              |
|----------------------------------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -708.748244        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -708.623547        |
| Number of Imaginary Frequencies                                       | 1                  |

#### Frequencies (Top 3 out of 51)

1.  -207.7085 cm⁻¹  
2.  72.8461 cm⁻¹  
3.  95.2144 cm⁻¹  

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -1.794615 | -0.523349 | -1.287267 |
| C | -1.822507 | 0.109812 | 0.093680  |
| C | -0.692330 | 0.869641 | 0.507074  |
| C | 0.419013  | 1.101373 | -0.288027 |
| O | -2.828846 | -0.057840 | 0.805704  |
| C | 1.380711  | 2.201846 | 0.064708  |
| H | -2.635109 | -1.205867 | -1.385317 |
| H | -1.871528 | 0.243986 | -2.059880 |
| H | -0.858535 | -1.059907 | -1.453135 |
| H | -0.702084 | 1.236775 | 1.528800  |
| H | 0.316632  | 0.917898 | -1.348530 |
### 6_3pentene2one_TS_7

| Datum                                                | Value             |
|------------------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                | -708.74125        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -708.616396       |

**Number of Imaginary Frequencies**

1

**Frequencies (Top 3 out of 51)**

1. -198.4299 cm⁻¹  
2. 54.1396 cm⁻¹  
3. 62.6093 cm⁻¹ 

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -1.609273 | 0.017212 | 1.374915 |
| C | -1.771389 | -0.223234 | -0.112933 |
| C | -0.781805 | 0.259886 | -1.025131 |
| C | 0.308655 | 1.075839 | -0.770680 |
| O | -2.753433 | -0.879712 | -0.496280 |
| C | 0.397970 | 2.165014 | 0.267666 |
| H | -1.879039 | 1.043024 | 1.629653 |
| H | -2.268487 | -0.660083 | 1.912898 |
| H | -0.573992 | -0.142876 | 1.681361 |
| H | -0.871224 | -0.152643 | -2.024398 |
| H | 0.880633 | 1.314491 | -1.658947 |
| H | -0.315044 | 2.956753 | 0.017234 |
| H | 1.396859 | 2.597967 | 0.266871 |
| H | 0.184601 | 1.824200 | 1.274476 |
| S | 2.170981 | -0.244587 | 0.100783 |
| C | 1.340049 | -1.844176 | 0.097398 |
| H | 1.251265 | -2.254253 | 1.103220 |
| H | 0.326779 | -1.706358 | -0.301874 |
| H | 1.854164 | -2.572389 | -0.529109 |
6_cis_3pentene2one_1

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -270.537274 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -270.447003 |
| Number of Imaginary Frequencies                                      | 0           |

**Frequencies (Top 3 out of 36)**

1.  47.6694 cm⁻¹  
2.  68.6799 cm⁻¹  
3.  137.3835 cm⁻¹  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C  | -2.297330  | -0.270427  | 0.190285  |
| C  | -0.877956  | 0.163455   | -0.064601 |
| C  | 0.115789   | -0.931828  | -0.154908 |
| C  | 1.439537   | -0.791365  | -0.051023 |
| O  | -0.587188  | 1.336696   | -0.196230 |
| C  | 2.218169   | 0.460970   | 0.177659  |
| H  | -2.950021  | 0.593647   | 0.270490  |
| H  | -2.630285  | -0.913982  | -0.626019 |
| H  | -2.345033  | -0.865500  | 1.103410  |
| H  | -0.294953  | -1.926410  | -0.281055 |
| H  | 2.030225   | -1.698747  | -0.131480 |
| H  | 3.083167   | 0.251393   | 0.805612  |
| H  | 2.600410   | 0.834666   | -0.776161 |
| H  | 1.614732   | 1.246532   | 0.620576  |

6_cis_3pentene2one_2

| Datum                                                                 | Value       |
|----------------------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -270.535588 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -270.444392 |
| Number of Imaginary Frequencies                                      | 0           |
### Frequencies (Top 3 out of 36)

1. 46.4002 cm⁻¹
2. 75.9100 cm⁻¹
3. 257.0370 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |          |          |          |
|---|----------|----------|----------|
| C | -0.828335| 1.409395 | 0.068758 |
| C | -1.042312| -0.078658| -0.002052|
| C | 0.094371 | -1.025869| 0.050808 |
| C | 1.408043 | -0.785000| 0.034622 |
| O | -2.170030| -0.530659| -0.084383|
| C | 2.161182 | 0.503480 | -0.072233|
| H | -1.783606| 1.892983 | 0.252528 |
| H | -0.115452| 1.672463 | 0.848043 |
| H | -0.429163| 1.766307 | -0.881986|
| H | -0.235514| -2.056093| 0.118462 |
| H | 2.039661 | -1.664170| 0.115096 |
| H | 2.354033 | 0.908086 | 0.924809 |
| H | 3.129838 | 0.322547 | -0.534010|
| H | 1.642743 | 1.263062 | -0.647298|
1_methylacrolein_1_am1_HEI

| Datum                                      | Value  |
|--------------------------------------------|--------|
| AM1 Energy                                 | -0.111465 |
| AM1 Free Energy (Quasiharmonic)            | -0.012505 |
| Number of Imaginary Frequencies            | 0      |

**Frequencies (Top 3 out of 42)**

1. 33.8223 cm\(^{-1}\)
2. 67.6256 cm\(^{-1}\)
3. 94.2264 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -1.793440 | -0.611816 | -0.145821 |
| C   | -0.983371 | 0.504765  | 0.093542  |
| C   | 0.121048  | 0.454914  | 1.013883  |
| O   | -1.694333 | -1.761703 | 0.364529  |
| H   | 0.287096  | 1.413363  | 1.563507  |
| H   | 0.033409  | -0.400702 | 1.723716  |
| C   | 1.595488  | -0.986981 | -0.952579 |
| H   | 2.128265  | -1.915301 | -0.651493 |
| H   | 0.506357  | -1.208773 | -1.070584 |
| H   | 2.008764  | -0.631460 | -1.921429 |
| S   | 1.812877  | 0.255989  | 0.267323  |
| H   | -2.632465 | -0.444109 | -0.874513 |
| C   | -1.245816 | 1.772468  | -0.605024 |
| H   | -1.496364 | 2.592931  | 0.118909  |
### 1_methylacrolein_2_am1_HEI

| Datum                                        | Value         |
|----------------------------------------------|---------------|
| AM1 Energy                                   | -0.112426     |
| AM1 Free Energy (Quasiharmonic)              | -0.013337     |
| Number of Imaginary Frequencies              | 0             |

#### Frequencies (Top 3 out of 42)

1. 38.7715 cm⁻¹  
2. 75.5113 cm⁻¹  
3. 95.8763 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| C     | 1.633504 | -0.544295 | 0.623332 |
| C     | 0.811971 | 0.491707  | 0.151696 |
| C     | -0.386869| 0.858647  | 0.849006 |
| O     | 2.709521 | -0.959607 | 0.115737 |
| H     | -0.378983| 0.574227  | 1.927608 |
| H     | -0.648711| 1.937788  | 0.737000 |
| C     | -1.509996| -1.183099 | -0.860055|
| H     | -0.394638| -1.208210 | -0.950576|
| H     | -1.874607| -2.168460 | -0.496458|
| H     | -1.954026| -0.979597 | -1.858814|
| S     | -1.984894| 0.074587  | 0.265083 |
| H     | 1.279892 | -1.043979 | 1.565088 |
| C     | 1.164222 | 1.225276  | -1.074073|
| H     | 2.147352 | 0.871695  | -1.473594|
| H     | 0.389698 | 1.082346  | -1.873004|
| H     | 1.239158 | 2.328248  | -0.883913|

### 1_methylacrolein_3_am1_HEI

| Datum       | Value       |
|--------------|-------------|
| AM1 Energy   | -0.111465   |
### AM1 Free Energy (Quasiharmonic)

-0.012504

### Number of Imaginary Frequencies

0

### Frequencies (Top 3 out of 42)

1. 33.8382 cm\(^{-1}\)
2. 67.7514 cm\(^{-1}\)
3. 94.2407 cm\(^{-1}\)

### AM1 Molecular Geometry in Cartesian Coordinates

| C  | 1.793396 | -0.611883 | -0.145788 |
| C  | 0.983385 | 0.504748  | 0.093531  |
| C  | -0.121053| 0.454974  | 1.013856  |
| O  | 1.694173 | -1.761769 | 0.364548  |
| H  | -0.033462| -0.400621 | 1.723720  |
| H  | -0.287055| 1.413446  | 1.563456  |
| C  | -1.595476| -0.987031 | -0.952499 |
| H  | -2.008619| -0.631575 | -1.921432 |
| H  | -0.566358| -1.208944 | -1.070378 |
| H  | -2.128395| -1.915253 | -0.651361 |
| S  | -1.812858| 0.256083  | 0.267264  |
| H  | 2.632481 | -0.444237 | -0.874425 |
| C  | 1.245927 | 1.772431  | -0.605026 |
| H  | 2.102207 | 1.680845  | -1.320097 |
| H  | 1.496186 | 2.592965  | 0.118930  |
| H  | 0.348280 | 2.110757  | -1.185469 |

### 1_methylacrolein_4_reopt_am1_HEI

### AM1 Energy

-0.112426

### AM1 Free Energy (Quasiharmonic)

-0.013337

### Number of Imaginary Frequencies

0

### Frequencies (Top 3 out of 42)

1. 38.7637 cm\(^{-1}\)
2. 75.5166 cm\(^{-1}\)
### AM1 Molecular Geometry in Cartesian Coordinates

|   | X   | Y   | Z   |
|---|-----|-----|-----|
| C | -1.633539 | -0.544290 | 0.623309 |
| C | -0.811977 | 0.491699 | 0.151698 |
| C | 0.386857 | 0.858617 | 0.849037 |
| O | -2.709552 | -0.959581 | 0.115691 |
| H | 0.648679 | 1.937771 | 0.737102 |
| H | 0.378975 | 0.574131 | 1.927620 |
| C | 1.510014 | -1.183211 | -0.859929 |
| H | 0.394662 | -1.208263 | -0.950550 |
| H | 1.954151 | -0.979923 | -1.858685 |
| H | 1.874526 | -2.168529 | -0.496116 |
| S | 1.984896 | 0.074650 | 0.265014 |
| H | -1.279955 | -1.043987 | 1.565069 |
| C | -1.164177 | 1.225296 | -1.074067 |
| H | -2.147296 | 0.871737 | -1.473634 |
| H | -1.239106 | 2.328265 | -0.883885 |
| H | -0.389621 | 1.082375 | -1.872968 |

### 1_methylacrolein_5_am1_HEI

| Datum                                    | Value       |
|------------------------------------------|-------------|
| AM1 Energy                               | -0.106715   |
| AM1 Free Energy (Quasiharmonic)          | -0.008644   |
| Number of Imaginary Frequencies          | 0           |

**Frequencies (Top 3 out of 42)**

1. 36.1511 cm\(^{-1}\)
2. 57.3415 cm\(^{-1}\)
3. 60.3798 cm\(^{-1}\)

### AM1 Molecular Geometry in Cartesian Coordinates

|   | X   | Y   | Z   |
|---|-----|-----|-----|
| C | -2.108547 | -0.522424 | -0.182084 |
| C | -1.122298 | 0.401441 | 0.191233 |
| C | 0.138257 | -0.026896 | 0.732704 |
| O | -2.077187 | -1.776816 | -0.063038 |
| H | 0.509190 | 0.611176 | 1.570723 |
H  0.130668  -1.098963  1.039685
C  2.886076  -0.429610  0.255454
H  3.131561   0.209078  1.133732
H  2.768424  -1.477160  0.613358
H  3.730179  -0.387833 -0.467888
S  1.444234   0.130311 -0.563550
H  -3.042281 -0.070098 -0.614742
C  -1.364978  1.844390  0.041443
H  -1.446822  2.350979  1.040633
H  -2.314410  2.046937 -0.515879
H  -0.527813  2.344029 -0.511022

1_methylacrolein_6_reopt_am1_HEI

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.112426 |
| AM1 Free Energy (Quasiharmonic)            | -0.013337 |
| Number of Imaginary Frequencies            | 0         |

Frequencies (Top 3 out of 42)

1.      38.7617 cm⁻¹
2.      75.5160 cm⁻¹
3.      95.8874 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

C  -1.633525  -0.544301  0.623307
C  -0.811980   0.491703  0.151701
C   0.386860   0.858623  0.849032
O  -2.789538  -0.959598  0.115692
H   0.648678   1.937778  0.737095
H   0.378984   0.574139  1.927616
C   1.510014  -1.183215 -0.859927
H   0.394662  -1.208274 -0.950545
H   1.954146  -0.979933 -1.858686
H   1.874533  -2.168529 -0.496107
S   1.984894   0.074655  0.265007
H  -1.279926  -1.044007  1.565057
C  -1.164199   1.225309 -1.074054
H  -2.147334   0.871766 -1.473596
H  -1.239104   2.328279 -0.883869
H  -0.389665   1.082374 -1.872974
### 1_methylacrolein_7_am1_HEI

| Datum                        | Value      |
|------------------------------|------------|
| AM1 Energy                   | -0.10788   |
| AM1 Free Energy (Quasiharmonic) | -0.009611 |
| Number of Imaginary Frequencies | 0        |

**Frequencies** (Top 3 out of 42)

1. 45.0407 cm\(^{-1}\)
2. 59.6497 cm\(^{-1}\)
3. 74.3969 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 1.829284 | -0.856094 | 0.163841 |
| C | 0.998038  | 0.270104  | 0.280274 |
| C | -0.331044 | 0.151427  | 0.805721 |
| O | 3.019094  | -0.889394 | -0.248999 |
| H | -0.472311 | -0.714985 | 1.494552 |
| H | -0.700206 | 1.082648  | 1.297176 |
| C | -3.078409 | -0.198856 | 0.193459 |
| H | -3.138525 | -1.019845 | 0.942966 |
| H | -3.303503 | 0.759214  | 0.713856 |
| H | -3.847382 | -0.371611 | -0.591669 |
| S | -1.511245 | -0.153322 | -0.583569 |
| H | 1.370178  | -1.825563 | 0.496312 |
| C | 1.469441  | 1.596042  | -0.148739 |
| H | 2.515453  | 1.530696  | -0.539746 |
| H | 0.818890  | 2.024439  | -0.954499 |
| H | 1.460713  | 2.327571  | 0.702812 |

### 1_methylacrolein_8_am1_HEI_reopt

| Datum                        | Value      |
|------------------------------|------------|
| AM1 Energy                   | -0.10788   |
| AM1 Free Energy (Quasiharmonic) | -0.009612 |
| Number of Imaginary Frequencies | 0        |
**Frequencies (Top 3 out of 42)**

1. 45.0342 cm⁻¹  
2. 59.6120 cm⁻¹  
3. 74.3758 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -1.829292 | -0.856074 | 0.163875 |
|------------|-----------|-----------|----------|
| C          | -0.998062 | 0.270138  | 0.280284 |
| C          | 0.330986  | 0.151494  | 0.805778 |
| O          | -3.019073 | -0.889432 | -0.249056|
| H          | 0.700140  | 1.082745  | 1.297178 |
| H          | 0.472238  | -0.714884 | 1.494651 |
| C          | 3.078450  | -0.198862 | 0.193436 |
| H          | 3.138329  | -1.019301 | 0.943561 |
| H          | 3.847273  | -0.372493 | -0.591645|
| H          | 3.303979  | 0.759517  | 0.713075 |
| S          | 1.511228  | -0.153361 | -0.583492|
| H          | -1.370214 | -1.825507 | 0.496495 |
| C          | -1.469402 | 1.596049  | -0.148878|
| H          | -0.819130 | 2.024136  | -0.955023|
| H          | -2.515587 | 1.530763  | -0.539428|
| H          | -1.460175 | 2.327792  | 0.702479 |

**1_methylacrolein_conf2_min_am1**

| Datum                                | Value    |
|--------------------------------------|----------|
| AM1 Energy                           | -0.038056|
| AM1 Free Energy (Quasiharmonic)      | 0.026225 |
| Number of Imaginary Frequencies      | 0        |

**Frequencies (Top 3 out of 27)**

1. 19.0539 cm⁻¹  
2. 82.7581 cm⁻¹  
3. 269.6063 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**
1_methylacrolein_min_am1

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.038885   |
| AM1 Free Energy (Quasiharmonic)      | 0.025987    |
| Number of Imaginary Frequencies      | 0           |

Frequencies (Top 3 out of 27)

1. 68.2365 cm⁻¹
2. 81.5885 cm⁻¹
3. 287.2702 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 0.441184 | 1.450224 | -0.000006 |
| H | -0.483749 | 2.045955 | -0.000007 |
| H | 1.378878  | 2.021578 | -0.000009 |
| C | 0.412792  | 0.111807 | -0.000001 |
| C | -0.862632 | -0.630288 | 0.000004 |
| H | -0.760873 | -1.739832 | 0.000009 |
| O | -1.971137 | -0.090016 | 0.000001 |
| C | 1.635846  | -0.724023 | 0.000002 |
| H | 1.656485  | -1.379658 | 0.906251 |
| H | 1.656484  | -1.379667 | -0.906241 |
| H | 2.558732  | -0.094567 | -0.000002 |
**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | -2.110854 | -0.034781 | 0.362736 |
| C | -0.899730 | 0.570354 | 0.693749 |
| C | 0.155098 | 0.807865 | -0.246418 |
| O | -2.499732 | -0.447170 | -0.765553 |
| H | -0.729175 | 0.863941 | 1.734502 |
| H | -0.189063 | 0.683859 | -1.303101 |
| C | 0.797283 | -1.963731 | 0.222020 |
| H | -0.279171 | -1.777531 | 0.463048 |
| H | 0.863331 | -2.650180 | -0.650215 |
| H | 1.295081 | -2.439986 | 1.094660 |
| S | 1.587399 | -0.442515 | -0.143122 |
| H | -2.825241 | -0.148501 | 1.223807 |
| C | 0.915421 | 2.092620 | -0.054037 |
| H | 1.226703 | 2.214569 | 1.011291 |
| H | 1.829633 | 2.119124 | -0.697075 |
| H | 0.264054 | 2.958343 | -0.330841 |

**2_crotonaldehyde-2-0_am1_HEI**

| Datum                                      | Value    |
|--------------------------------------------|----------|
| AM1 Energy                                 | -0.104518 |
| AM1 Free Energy (Quasiharmonic)            | -0.005567 |
| Number of Imaginary Frequencies            | 0        |

**Frequencies** (Top 3 out of 42)

1. 41.5973 cm⁻¹
2. 77.3142 cm⁻¹
3. 118.8495 cm⁻¹
| Datum                          | Value       |
|-------------------------------|-------------|
| AM1 Energy                    | -0.106264   |
| AM1 Free Energy (Quasiharmonic)| -0.007377   |
| Number of Imaginary Frequencies | 0           |

**Frequencies (Top 3 out of 42)**

1. 43.4230 cm⁻¹
2. 91.2258 cm⁻¹
3. 140.2700 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C    | 1.926143 | -0.072589 | -0.234608 |
|------|----------|-----------|-----------|
| C    | 0.928001 | 0.110254  | 0.726353  |
| C    | -0.260781| 0.878050  | 0.546318  |
| O    | 2.981658 | -0.749702 | -0.096753 |
| H    | 1.048676 | -0.397996 | 1.690541  |
| H    | -0.657453| 1.277017  | 1.515253  |
| C    | -1.201325| -1.751831 | -0.323272 |
| H    | -0.089405| -1.773438 | -0.191217 |
| H    | -1.665384| -2.504845 | 0.350374  |
| H    | -1.452858| -2.006828 | -1.375894 |
| S    | -1.812280| -0.156467 | 0.063582  |
| H    | 1.772270 | 0.444521  | -1.219129 |
| C    | -0.242674| 1.958335  | -0.498991 |
| H    | -1.217154| 2.505357  | -0.517093 |
| H    | -0.063606| 1.532539  | -1.515268 |
| H    | 0.571944 | 2.691438  | -0.275656 |

| Datum                          | Value       |
|-------------------------------|-------------|
| AM1 Molecular Geometry in Cartesian Coordinates |            |
### 2_crotonaldehyde-4-0_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.104518   |
| AM1 Free Energy (Quasiharmonic)           | -0.005566   |
| Number of Imaginary Frequencies            | 0           |

#### Frequencies (Top 3 out of 42)

1. 41.2155 cm⁻¹
2. 82.6342 cm⁻¹
3. 136.6572 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

| C   | -1.926156 | -0.072531 | 0.234593 |
| C   | -0.927984 | 0.110270  | -0.726338|
| C   | 0.260811  | 0.878036  | -0.546310|
| O   | -2.981702 | -0.749595 | 0.096707 |
| H   | -1.048676 | -0.397963 | -1.690534|
| H   | 0.657452  | 1.277046  | -1.515243|
| C   | 1.201199  | -1.751810 | 0.323374 |
| H   | 1.452509  | -2.006629 | 1.376091 |
| H   | 0.089311  | -1.773366 | 0.191127 |
| H   | 1.665356  | -2.504959 | -0.350049|
| S   | 1.812292  | -0.156527 | -0.063671|
| H   | -1.772302 | 0.444576  | 1.219118 |
| C   | 0.242803  | 1.958269  | 0.499064 |
| H   | 1.217409  | 2.505060  | 0.517355 |
2_crotonaldehyde-5-0_am1_HEI

| Datum                          | Value          |
|-------------------------------|----------------|
| AM1 Energy                    | -0.104412      |
| AM1 Free Energy (Quasiharmonic)| -0.005408      |
| Number of Imaginary Frequencies| 0              |

Frequencies (Top 3 out of 42)

1. 41.5496 cm⁻¹
2. 77.2744 cm⁻¹
3. 118.7466 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|       |             |             |             |
|-------|-------------|-------------|-------------|
| C     | -2.110888   | -0.035291   | 0.362813    |
| C     | -0.899771   | 0.569806    | 0.693862    |
| C     | 0.154952    | 0.807716    | -0.246356   |
| O     | -2.499890   | -0.447378   | -0.765547   |
| H     | -0.729146   | 0.863181    | 1.734660    |
| H     | -0.189276   | 0.683609    | -1.303005   |
| C     | 0.797973    | -1.963604   | 0.221736    |
| H     | 1.295994    | -2.439970   | 1.094184    |
| H     | -0.278509   | -1.777823   | 0.462965    |
| H     | 0.864166    | -2.649752   | -0.650719   |
| S     | 1.587615    | -0.442059   | -0.143042   |
| H     | -2.825158   | -0.149309   | 1.223941    |
| C     | 0.914662    | 2.092864    | -0.054080   |
| H     | 1.226004    | 2.214999    | 1.011203    |
| H     | 1.828789    | 2.119831    | -0.697213   |
| H     | 0.262842    | 2.958259    | -0.330827   |

2_crotonaldehyde-6-1_am1_HEI

| Datum       | Value    |
|-------------|----------|
| AM1 Energy  | -0.099891|

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Free Energy (Quasiharmonic)            | -0.001275   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 42)**

1. 46.2292 cm⁻¹
2. 69.6864 cm⁻¹
3. 78.8464 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | C             | O              | H             | C             | H             | H             | S             | H             | C             | H             | H             | H             |
|---|---------------|----------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| C | 2.384314      | -0.256252      | -0.263008     | 1.228589      | 0.434765      | -0.626075     | 0.070064      | 0.532338      | 0.216999      | 2.648944      | -0.819781     | 0.834700      |
| C | 1.228589      | 0.434765       | -0.626075     | 0.070064      | 0.532338      | 0.216999      | 2.648944      | -0.819781     | 0.834700      | 1.180093      | 0.900757      | -1.614771     |
| C | 0.070064      | 0.532338       | 0.216999      | 2.648944      | -0.819781     | 0.834700      | 1.180093      | 0.900757      | -1.614771     | 0.260242      | 0.147084      | 1.249963      |
| O | 2.648944      | -0.819781      | 0.834700      | 1.180093      | 0.900757      | -1.614771     | 0.260242      | 0.147084      | 1.249963      | -2.552347     | -0.680974     | 0.494459      |
| H | 0.260242      | 0.147084       | 1.249963      | -2.552347     | -0.680974     | 0.494459      | -2.552347     | -0.680974     | 0.494459      | -2.259029     | -0.754648     | 1.565483      |
| H | -2.259029     | -0.754648      | 1.565483      | -3.181465     | 0.229342      | 0.370262      | -3.181465     | 0.229342      | 0.370262      | -3.159738     | -1.572871     | 0.223077      |
| H | -3.159738     | -1.572871      | 0.223077      | -3.145518     | -0.649701     | -0.546676     | -1.145518     | -0.649701     | -0.546676     | -3.183000     | -0.274959     | -1.054593     |
| S | -3.183000     | -0.274959      | -1.054593     | -0.576123     | 1.892194      | 0.261447      | -0.791989     | 2.263328      | -0.769042     | -1.533975     | 1.864000      | 0.837038      |
| H | -1.533975     | 1.864000       | 0.837038      | 0.112615      | 2.619002      | 0.758869      | 0.112615      | 2.619002      | 0.758869      |                         |               |               |

**2_crotonaldehyde-7-0_am1_HEI**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.10172    |
| AM1 Free Energy (Quasiharmonic)            | -0.00331    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 42)**

1. 54.3570 cm⁻¹
2. 69.9752 cm⁻¹
### AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | 2.213577 | -0.340538 | 0.363146 |
| C    | 1.217529  | 0.417991  | -0.259696 |
| C    | -0.080504 | 0.610090  | 0.311347 |
| O    | 3.382713  | -0.543257 | -0.063661 |
| H    | 1.421165  | 0.853910  | -1.242387 |
| H    | -0.118724 | 0.443283  | 1.417537 |
| C    | -2.706475 | -0.674248 | 0.323236 |
| H    | -2.649078 | -0.521112 | 1.424163 |
| H    | -3.298146 | 0.163226  | -0.110673 |
| H    | -3.239019 | -1.629479 | 0.118418 |
| S    | -1.110794 | -0.781080 | -0.387691 |
| H    | 1.938771  | -0.791794 | 1.354348 |
| C    | -0.745086 | 1.913348  | -0.045056 |
| H    | -1.795234 | 1.945280  | 0.336494 |
| H    | -0.764575 | 2.056455  | -1.152038 |
| H    | -0.178404 | 2.763701  | 0.408627 |

### 2-crotonaldehyde-8-1_am1_HEI

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.102333 |
| AM1 Free Energy (Quasiharmonic)            | -0.003211 |
| Number of Imaginary Frequencies            | 0       |

#### Frequencies (Top 3 out of 42)

1. 38.5170 cm⁻¹
2. 56.0144 cm⁻¹
3. 121.8176 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X  | Y  | Z  |
|------|----|----|----|
| C    | -1.902353 | -0.691288 | -0.377288 |
| C    | -0.837719  | -0.105813 | -1.059677 |
| C    | 0.077690   | 0.876446  | -0.561981 |
| O    | -2.316040  | -0.488085 | 0.797599 |
| H    | -0.647160  | -0.459437 | -2.081221 |
### 2_crotonaldehyde_min_am1

| Datum                              | Value            |
|------------------------------------|------------------|
| AM1 Energy                         | -0.043079        |
| AM1 Free Energy (Quasiharmonic)    | 0.021628         |
| Number of Imaginary Frequencies    | 0                |

**Frequencies (Top 3 out of 27)**

1. 77.5650 cm\(^{-1}\)
2. 119.5921 cm\(^{-1}\)
3. 208.0285 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C       | 0.841994 | -0.320672 | 0.000012 |
|---------|----------|-----------|----------|
| H       | 0.506684 | -1.374814 | 0.000113 |
| C       | -0.059071| 0.671425  | -0.000061|
| H       | 0.245643 | 1.729967  | -0.000162|
| C       | -1.504586| 0.430888  | -0.000007|
| H       | -2.133685| 1.350639  | -0.000057|
| O       | -2.021177| -0.690765 | 0.000087 |
| C       | 2.300687 | -0.111120 | -0.000025|
| H       | 2.753115 | -0.587832 | 0.906316 |
| H       | 2.753065 | -0.587797 | -0.906410|

### 2_crotonaldehyde_min_conf2_am1
| Datum                                      | Value   |
|-------------------------------------------|---------|
| AM1 Energy                                | -0.04312|
| AM1 Free Energy (Quasiharmonic)           | 0.021706|
| Number of Imaginary Frequencies           | 0       |

**Frequencies** (Top 3 out of 27)

1.  71.1397 cm⁻¹
2.  109.8476 cm⁻¹
3.  227.3218 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 1.055342 | 0.415507 | 0.000001 |
| H   | 1.039740 | 1.520263 | -0.000004|
| C   | -0.082293| -0.289596| 0.000005 |
| H   | -0.087453| -1.392392| 0.000011 |
| C   | -1.401413| 0.353030 | 0.000002 |
| H   | -1.400537| 1.467741 | 0.000006 |
| O   | -2.457200| -0.284499| -0.000004|
| C   | 2.398485 | -0.192880| -0.000002|
| H   | 2.966292 | 0.136681 | -0.906666|
| H   | 2.966366 | 0.136827 | 0.906563 |
| H   | 2.352462 | -1.309496| 0.000089 |

**3_4methyl2pentenal_10_reopt_am1_HEI**

| Datum                                      | Value   |
|-------------------------------------------|---------|
| AM1 Energy                                | -0.114671|
| AM1 Free Energy (Quasiharmonic)           | 0.038561|
| Number of Imaginary Frequencies           | 0       |

**Frequencies** (Top 3 out of 60)

1.  39.4706 cm⁻¹
2.  60.0635 cm⁻¹
3.  92.5093 cm⁻¹
**AM1 Molecular Geometry in Cartesian Coordinates**

| Datum         | Value               |
|---------------|---------------------|
| AM1 Energy    | -0.115303           |
| AM1 Free Energy (Quasiharmonic) | 0.037662 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 60)

1. 25.8360 cm⁻¹
2. 49.5258 cm⁻¹
3. 94.9828 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Datum         | Value               |
|---------------|---------------------|
| C             | -0.342243           |
| C             | 1.908955            |
| C             | 0.255753            |
3_4methyl2pentenal_12_reopt_am1_HEI

**Datum** | **Value**
--- | ---
AM1 Energy | -0.118533
AM1 Free Energy (Quasiharmonic) | 0.034329
Number of Imaginary Frequencies | 0

**Frequencies** (Top 3 out of 60)

1. 34.1181 cm⁻¹
2. 55.0023 cm⁻¹
3. 66.4440 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |     |     |     |
|---|-----|-----|-----|
| C | -2.208969 | -1.219727 | -0.310557 |
| C | -0.908109 | -0.882192 | -0.680486 |
| C | 0.066885 | -0.365310 | 0.235645 |
| O | -2.740749 | -1.157063 | 0.833091 |
| H | -0.275737 | -0.467345 | 1.297135 |
| C | -1.298155 | 2.125583 | -0.216629 |
| H | -1.272628 | 2.804109 | -1.097051 |
| H | -1.988824 | 1.270915 | -0.425485 |
**3_4methyl2pentenal_13_am1_HEI**

| Datum                                | Value        |
|--------------------------------------|--------------|
| AM1 Energy                           | -0.117561    |
| AM1 Free Energy (Quasiharmonic)      | 0.035664     |
| Number of Imaginary Frequencies      | 0            |

**Frequencies** (Top 3 out of 60)

1. 36.2756 cm⁻¹
2. 69.9440 cm⁻¹
3. 79.1900 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | 0.322323 | 2.199386 | 0.155432 |
|-------------|-----------|----------|----------|
| C           | -0.033008 | 1.147951 | 0.998521 |
| C           | -0.055549 | -0.257954 | 0.737341 |
| O           | -0.827008 | 2.168930 | -1.001000 |
| H           | -0.144020 | -0.860310 | 1.679492 |
| C           | 2.508646 | 0.344145 | -0.539939 |
| H           | 2.674513 | 0.154509 | -1.623021 |
| H           | 1.932797 | 1.295316 | -0.417475 |
| H           | 3.494769 | 0.442928 | -0.035563 |
| S           | 1.622881 | -0.98037 | 0.171503 |
| H           | -0.127894 | 3.217462 | 0.595530 |
| H           | 0.486410 | 1.419118 | 1.961458 |
| C           | -1.108766 | -0.788184 | -0.261728 |
| H           | -0.906486 | -0.178270 | -1.236937 |
### 3_4methyl2pentenal_14_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.115214   |
| AM1 Free Energy (Quasiharmonic)            | 0.037266    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 60)

1. 46.7949 cm⁻¹  
2. 50.0865 cm⁻¹  
3. 65.0255 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -1.074639 | -2.06698 | -0.483497 |
|-----|-----------|----------|-----------|
| H   | -1.338951 | -2.750765| 0.455616  |
| H   | -1.808204 | -2.496387| -1.274371 |
| H   | -0.051424 | -2.525646| -0.803987 |
| C   | -2.488791 | -0.297824| 0.218799  |
| H   | -2.704195 | -0.730989| 1.224958  |
| H   | -2.539114 | 0.816919 | 0.283710  |
| H   | -3.269531 | -0.655664| -0.495026 |
3_4methyl2pentenal_1_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.118533   |
| AM1 Free Energy (Quasiharmonic)            | 0.034329    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 60)**

1. 34.1720 cm⁻¹
2. 54.8981 cm⁻¹
3. 66.4173 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |         |         |         |
|-----|---------|---------|---------|
| C   | -2.209214 | -1.219307 | -0.310678 |
| C   | -0.908376 | -0.881686 | -0.680608 |
| C   | 0.066770  | -0.365320 | 0.235647  |
| O   | -2.740863 | -1.157143 | 0.833056  |
| H   | -0.275860 | -0.467600 | 1.297106  |
| C   | -1.297615 | 2.125835  | -0.216578 |
| H   | -1.672521 | 2.690423  | 0.664962  |
| H   | -1.271631 | 2.805152  | -1.096366 |
| H   | -1.988135 | 1.271323  | -0.426528 |
| S   | 0.317500  | 1.521382  | 0.098416  |
| H   | -2.846664 | -1.606850 | -1.151963 |
| H   | -0.619153 | -0.997096 | -1.729652 |
| C   | 1.472126  | -0.931934 | 0.084004  |
| H   | 1.368961  | -2.053371 | 0.169062  |
| C   | 2.097632  | -0.620855 | -1.258798 |
| H   | 2.118490  | 0.484727  | -1.425250 |
| H   | 3.142022  | -1.015701 | -1.303624 |
| H   | 1.504222  | -1.090308 | -2.079393 |
| C   | 2.374508  | -0.457235 | 1.206512  |
| H   | 2.464232  | 0.657160  | 1.185397  |
| H   | 1.953775  | -0.758214 | 2.195897  |
| H   | 3.394173  | -0.901606 | 1.104239  |
3_4methyl2pentenal_1_am1

| Datum                              | Value         |
|------------------------------------|---------------|
| AM1 Energy                         | -0.0595       |
| AM1 Free Energy (Quasiharmonic)    | 0.058979      |
| Number of Imaginary Frequencies    | 0             |

**Frequencies (Top 3 out of 45)**

1. 40.5471 cm⁻¹  
2. 94.5033 cm⁻¹  
3. 150.0735 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|          | C           | C           | C           | C           | O           | C           | H           | H           | H           | H           | H           | H           | H           | H           |
|----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| Datum    | 2.308364    | -0.406565   | -0.018314   | -0.054599   | 0.251712    | 1.407533    | 0.183649    | 0.152765    | -0.320681   | -0.398157   | -0.224771   | -0.518398   | 0.045966    | 0.152765    |
| Number of Imaginary Frequencies    | 0

3_4methyl2pentenal_2_am1

| Datum                              | Value         |
|------------------------------------|---------------|
| AM1 Energy                         | -0.060516     |
| AM1 Free Energy (Quasiharmonic)    | 0.057565      |
| Number of Imaginary Frequencies    | 0             |
**Frequencies (Top 3 out of 45)**

1. 36.4524 cm⁻¹  
2. 96.3614 cm⁻¹  
3. 139.2734 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | C        | C        | C        | C        | O        | C        | H        | H        | H        | H        | H        | H        | H        | H        | H        |
|---|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| C | -1.378596| -1.949080| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000| -0.000000|
| C | -0.182447| -1.098397| 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  |
| C | -0.257362| 0.237222 | 1.132730  | 1.997666  | 1.246657  | 1.246657  | 1.246657  | 1.246657  | 1.246657  | 1.246657  | 1.246657  | 1.246657  | 1.246657  | 1.246657  | 1.246657  |
| C | 0.934177 | 1.997666 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 |
| C | 0.934177 | 1.997666 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 | -1.246657 |
| O | -1.324645| -3.181269| 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  |
| H | -2.356831| -1.414670| 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  |
| H | 0.783122 | -1.631343| 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  |
| H | -1.230808| 0.759299 | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  |
| H | 1.874682 | 0.509738 | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  | 0.000000  |
| H | 1.833848 | 2.658914 | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  | 1.250210  |
| H | 0.021741 | 2.640273 | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  | 1.280201  |
| H | 0.955287 | 1.360962 | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  | 2.163196  |
| H | 1.833848 | 2.658914 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 | -1.250210 |
| H | 0.955287 | 1.360962 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 | -2.163196 |
| H | 0.021741 | 2.640273 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 | -1.280201 |

**3_4methyl2pentenal_2_reopt_am1_HEI**

| Datum                              | Value          |
|------------------------------------|----------------|
| AM1 Energy                         | -0.120311      |
| AM1 Free Energy (Quasiharmonic)    | 0.032632       |
| Number of Imaginary Frequencies    | 0              |

**Frequencies (Top 3 out of 60)**

1. 42.0022 cm⁻¹  
2. 49.7860 cm⁻¹  
3. 65.7084 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
3_4methyl2pentenal_3_am1_HEI

| Datum                                  | Value       |
|----------------------------------------|-------------|
| AM1 Energy                             | -0.119508   |
| AM1 Free Energy (Quasiharmonic)        | 0.033398    |
| Number of Imaginary Frequencies        | 0           |

Frequencies (Top 3 out of 60)

1. 39.3768 cm⁻¹
2. 42.0036 cm⁻¹
3. 66.0175 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Datum | X          | Y          | Z          |
|-------|------------|------------|------------|
| C     | -1.368152  | 1.829605   | 0.563201   |
| C     | -0.365324  | 0.879601   | 0.756224   |
| C     | 0.187783   | 0.089491   | -0.301761  |
| O     | -1.925818  | 2.173437   | -0.515955  |
| H     | -0.121864  | 0.474150   | -1.306746  |
3_4methyl2pentenal_3_reopt2_am1

| Datum                              | Value    |
|------------------------------------|----------|
| AM1 Energy                         | -0.059426|
| AM1 Free Energy (Quasiharmonic)    | 0.059013 |
| Number of Imaginary Frequencies    | 0        |

**Frequencies** (Top 3 out of 45)

1. 38.1875 cm⁻¹
2. 95.7473 cm⁻¹
3. 151.4256 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```markdown
|   |    |    |    |
|---|----|----|----|
| C | 2.380350 | 0.383617 | 0.165876 |
| C | 0.942203 | 0.649172 | 0.063601 |
| C | 0.056622 | -0.300495 | -0.264764 |
| C | -1.411666 | -0.111448 | -0.409947 |
| C | -2.151356 | -1.206851 | 0.337802 |
| O | 2.901267 | -0.715643 | -0.046871 |
| C | -1.899367 | 1.250307 | 0.037356 |
| H | 2.999671 | 1.263090 | 0.457296 |
| H | 0.638394 | 1.686060 | 0.277329 |
| H | 0.409192 | -1.330989 | -0.465144 |
| H | -1.642339 | -0.221632 | -1.512546 |
```
### 3_4methyl2pentenal_4_am1_HEI

| Datum                        | Value       |
|------------------------------|-------------|
| AM1 Energy                   | -0.116439   |
| AM1 Free Energy (Quasiharmonic) | 0.036341   |
| Number of Imaginary Frequencies | 0          |

#### Frequencies (Top 3 out of 60)

1. 32.8887 cm⁻¹
2. 57.6985 cm⁻¹
3. 90.8456 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

| C          | -2.051115 | 0.861722 | 0.079141 |
| C          | -1.207611 | 0.201163 | -0.815431 |
| C          | 0.220889  | 0.164155 | -0.780890 |
| O          | -3.313018 | 0.867562 | 0.046910  |
| H          | 0.653400  | 0.144383 | -1.818124 |
| C          | -0.40975  | -2.341501| 0.574446  |
| H          | -0.149948 | -2.475072| 1.647497  |
| H          | -1.337222 | -1.719884| 0.492361  |
| H          | -0.593149 | -3.339248| 0.119981  |
| S          | 0.980107  | -1.554531| -0.271501 |
| H          | -1.559686 | 1.459159 | 0.892628  |
| H          | -1.682308 | -0.364827| -1.627783 |
| C          | 0.937461  | 1.229338 | 0.038297  |
| H          | 0.348060  | 2.185091 | -0.079807 |
| C          | 1.024385  | 0.910016 | 1.516073  |
| H          | 1.678366  | 0.018231 | 1.679621  |
| H          | 1.450161  | 1.779926 | 2.073393  |
| H          | 0.012776  | 0.680025 | 1.927949  |
| C          | 2.332787  | 1.470409 | -0.509817 |
| H          | 2.281660  | 1.835770 | -1.563520 |
| H          | 2.866464  | 2.235286 | 0.184265  |
| H          | 2.921918  | 0.521344 | -0.490639 |
### 3_4methyl2pentenal_4_am1

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.060367   |
| AM1 Free Energy (Quasiharmonic)      | 0.057704    |
| Number of Imaginary Frequencies      | 0           |

**Frequencies** (Top 3 out of 45)

1. 39.1490 cm⁻¹  
2. 81.0092 cm⁻¹  
3. 139.5450 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C  | 2.465483 | 0.000005 | 0.331562 |
|----|----------|----------|----------|
| C  | 1.065671 | 0.00007  | 0.766433 |
| C  | 0.039146 | -0.00002 | -0.093908|
| C  | -1.392150| 0.00002  | 0.319764 |
| C  | -2.082458| -1.246674| -0.201738|
| O  | 2.826053 | -0.00010 | -0.849404|
| C  | -2.082457| 1.246672 | -0.201754|
| H  | 3.213138 | 0.00018  | 1.158001 |
| H  | 0.908406 | 0.00017  | 1.856763 |
| H  | 0.219733 | -0.00012 | -1.184494|
| H  | -1.461828| 0.00009  | 1.445654 |
| H  | -3.152845| -1.249294| 0.115786 |
| H  | -2.042702| -1.280689| -1.317078|
| H  | -1.588093| -2.163256| 0.199900 |
| H  | -3.152844| 1.249297 | 0.115770 |
| H  | -1.588091| 2.163258 | 0.199872 |
| H  | -2.042700| 1.280672 | -1.317095|

### 3_4methyl2pentenal_5_am1

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.0595     |
| AM1 Free Energy (Quasiharmonic)      | 0.058979    |
### Number of Imaginary Frequencies

**Datum** | **Value**
--- | ---
Number of Imaginary Frequencies | 0

### Frequencies (Top 3 out of 45)

1. 40.5472 cm⁻¹  
2. 94.5033 cm⁻¹  
3. 150.0735 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| C          |          |          |          |
|------------|----------|----------|----------|
| -2.308364  | -0.406565| -0.018314|
| -0.964685  | 0.183649 | -0.054599|
| 0.123368   | -0.547587| -0.320681|
| 1.517808   | -0.032935| -0.398157|
| 1.660465   | 1.407533 | 0.045966 |
| -3.322862  | 0.251712 | 0.224256 |
| 2.445554   | -0.925634| 0.407001 |
| -2.366977  | -1.500476| -0.224770|
| -0.915765  | 1.265646 | 0.152764 |
| 0.035048   | -1.632273| -0.518398|
| 1.825424   | -0.096282| -1.485386|
| 2.731108   | 1.720050 | -0.014524|
| 1.058337   | 2.082406 | -0.608919|
| 1.314876   | 1.531919 | 1.100413 |
| 3.501459   | -0.582482| 0.289032 |
| 2.180627   | -0.889476| 1.490807 |
| 2.373883   | -1.983500| 0.057633 |

---

### AM1 Energy and Free Energy

| Datum | Value |
|-------|-------|
| AM1 Energy | -0.120342 |
| AM1 Free Energy (Quasiharmonic) | 0.032401 |

### Number of Imaginary Frequencies

**Datum** | **Value**
--- | ---
Number of Imaginary Frequencies | 0

### Frequencies (Top 3 out of 60)

1. 37.6703 cm⁻¹  
2. 63.4984 cm⁻¹  
3. 85.7800 cm⁻¹
**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 2.308400 | -0.773182 | -0.443171 |
| C | 1.065563 | -0.762059 | 0.198250  |
| C | -0.137412 | -0.357023 | -0.455729 |
| O | 3.412027 | -1.114526 | 0.062538  |
| H | -0.054696 | -0.375400 | -1.572577 |
| C | 0.865896 | 2.236493  | 0.450057  |
| H | 1.262723 | 3.013587  | -0.239178 |
| H | 0.615751 | 2.712052  | 1.423454  |
| H | 1.647682 | 1.451375  | 0.613317  |
| S | -0.571912 | 1.514445  | -0.242170 |
| H | 2.308805 | -0.453278 | -1.519929 |
| H | 1.018751 | -1.063257 | 1.249238  |
| C | -1.397485 | -1.094650 | -0.025642 |
| H | -1.189950 | -2.193660 | -0.183580 |
| C | -1.738528 | -0.888949 | 1.434424  |
| H | -1.847337 | 0.203159  | 1.648597  |
| H | -2.695122 | -1.407767 | 1.687720  |
| H | -0.928365 | -1.299280 | 2.083388  |
| C | -2.575435 | -0.707665 | -0.899133 |
| H | -2.773335 | 0.389940  | -0.814455 |
| H | -2.363299 | -0.947802 | -1.968666 |
| H | -3.493218 | -1.262365 | -0.587246 |

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**3_4methyl2pentenal_6_reopt2_am1**

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.059426 |
| AM1 Free Energy (Quasiharmonic)            | 0.059013  |
| Number of Imaginary Frequencies            | 0         |

**Frequencies (Top 3 out of 45)**

1. 38.1875 cm⁻¹
2. 95.7473 cm⁻¹
3. 151.4256 cm⁻¹

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**AM1 Molecular Geometry in Cartesian Coordinates**
### 3_4methyl2pentenal_6_reopt_am1_HEI

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| AM1 Energy                                 | -0.120129      |
| AM1 Free Energy (Quasiharmonic)            | 0.032937       |
| Number of Imaginary Frequencies            | 0              |

**Frequencies** (Top 3 out of 60)

1. 41.3156 cm\(^{-1}\)
2. 73.9241 cm\(^{-1}\)
3. 92.9126 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | -1.747792 | -1.117022 | -0.298630 |
| C | -1.029035 | -0.489182 | 0.723288  |
| C | 0.311820  | -0.010831 | 0.625480  |
| O | -2.933720 | -1.540583 | -0.225562 |
| H | 0.788002  | 0.119787  | 1.630071  |
| C | -1.223099 | 2.332769  | -0.256426 |
| H | -1.307316 | 2.735522  | -1.289425 |
| H | -1.917001 | 1.461835  | -0.140185 |
| H | -1.510837 | 3.128323  | 0.465151  |
| S | 0.428279  | 1.829322  | 0.038211  |
### 3_4methyl2pentenal_7_reopt_am1.HEI

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.122345 |
| AM1 Free Energy (Quasiharmonic)      | 0.030568  |
| Number of Imaginary Frequencies      | 0         |

**Frequencies (Top 3 out of 60)**

1. 42.1697 cm⁻¹  
2. 57.1149 cm⁻¹  
3. 83.0870 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|      |          |          |          |
|------|----------|----------|----------|
| C    | -2.077533| 1.016237 | -0.453758|
| C    | -0.926422| 0.736847 | 0.288762 |
| C    | 0.245317  | 0.154534 | -0.285332|
| O    | -3.147617 | 1.523561 | -0.019923|
| H    | 0.289990  | 0.241751 | -1.398779|
| C    | -1.286959 | -2.245020| 0.380262 |
| H    | -1.729199 | -2.910893| -0.392712|
| H    | -1.235445 | -2.796671| 1.344228 |
| H    | -1.936480 | -1.341634| 0.506847 |
| S    | 0.324366  | -1.762191| -0.107539|
| H    | -2.028043 | 0.768337 | -1.548186|
| H    | -0.926108 | 0.955700 | 1.361407 |
| C    | 1.560235  | 0.594454 | 0.342981 |
| H    | 1.558000  | 0.270586 | 1.421680 |
| C    | 2.758551  | -0.038137| -0.350269|
| H    | 2.786079  | 0.265136 | -1.424457|
### 3_4methyl2pentenal_8_reopt_am1_HEI

| Datum                                    | Value     |
|------------------------------------------|-----------|
| AM1 Energy                               | -0.12123  |
| AM1 Free Energy (Quasiharmonic)          | 0.031473  |
| Number of Imaginary Frequencies          | 0         |

#### Frequencies (Top 3 out of 60)

1. 34.7543 cm⁻¹
2. 50.5304 cm⁻¹
3. 80.3257 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

| C    | -1.785349 | 1.418348 | -0.286990 |
| C    | -0.632958 | 0.852384 | 0.268959  |
| C    | 0.276125  | 0.056942 | -0.488953 |
| O    | -2.641079 | 2.123672 | 0.313179  |
| H    | 0.153228  | 0.187133 | -1.594384 |
| C    | -1.651573 | -2.002683| 0.275269  |
| H    | -2.310799 | -2.494907| -0.472746 |
| H    | -1.628113 | -2.622770| 1.197801  |
| H    | -2.061469 | -0.989875| 0.521552  |
| S    | -0.031104 | -1.844687| -0.369710 |
| H    | -1.948079 | 1.227044 | -1.381979 |
| H    | -0.440211 | 1.006258 | 1.335158  |
| C    | 1.752261  | 0.134680 | -0.128848 |
| H    | 2.271140  | -0.749038| -0.604379 |
| C    | 2.351380  | 1.402237 | -0.709347 |
| H    | 1.798012  | 2.294330 | -0.328137 |
| H    | 3.426255  | 1.493179 | -0.420712 |
| H    | 2.281969  | 1.392431 | -1.823461 |
| C    | 2.003762  | 0.073754 | 1.362315  |
| H    | 1.665195  | 1.014404 | 1.859232  |
| H    | 1.442888  | -0.786372| 1.802446  |
| H    | 3.094398  | -0.060172| 1.565108  |
### 3_4methyl2pentenal_9_am1_HEI

| Datum                             | Value       |
|-----------------------------------|-------------|
| AM1 Energy                        | -0.117561   |
| AM1 Free Energy (Quasiharmonic)   | 0.035662    |
| Number of Imaginary Frequencies   | 0           |

#### Frequencies (Top 3 out of 60)

1. 36.2424 cm\(^{-1}\)
2. 69.9317 cm\(^{-1}\)
3. 79.2250 cm\(^{-1}\)

#### AM1 Molecular Geometry in Cartesian Coordinates

|   |       |       |       |
|---|-------|-------|-------|
| C | -0.323851 | -2.199222 | -0.155472 |
| C | 0.032654  | -1.148027 | -0.998519 |
| C | -0.055443 | 0.257902  | -0.737399 |
| O | -0.828796 | -2.168373 | 1.000833  |
| H | -0.143426 | 0.860323  | -1.679530 |
| C | 2.508473  | -0.345584 | 0.540190  |
| H | 2.674269  | -0.156032 | 1.623293  |
| H | 3.494620  | -0.445011 | 0.035998  |
| H | 1.932005  | -1.296364 | 0.417623  |
| S | 1.623652  | 0.988062  | -0.171543 |
| H | -0.129975 | -3.217435 | -0.595480 |
| H | 0.485868  | -1.419521 | -1.961308 |
| C | -1.108276 | 0.708844  | 0.261729  |
| H | -0.906228 | 0.178892  | 1.236953  |
| C | -1.073160 | 2.207361  | 0.483319  |
| H | -1.337588 | 2.751469  | -0.455734 |
| H | -1.806189 | 2.497558  | 1.274496  |
| H | -0.049583 | 2.525685  | 0.803273  |
| C | -2.488614 | 0.299319  | -0.218620 |
| H | -2.703864 | 0.732545  | -1.224782 |
| H | -2.539642 | -0.815394 | -0.283422 |
| H | -3.269033 | 0.657724  | 0.495268  |

### 4_3-methyl-2-butenal_1_am1
### AM1 Energy

| Datum                                   | Value     |
|-----------------------------------------|-----------|
| AM1 Energy                              | -0.054069 |
| AM1 Free Energy (Quasiharmonic)         | 0.036886  |

### Number of Imaginary Frequencies

| Datum                                   | Value     |
|-----------------------------------------|-----------|
| Number of Imaginary Frequencies         | 0         |

### Frequencies (Top 3 out of 36)

1. 60.0704 cm⁻¹
2. 77.3123 cm⁻¹
3. 112.7599 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| Datum                                   | Value     |
|-----------------------------------------|-----------|
| C                                       | 1.588740  |
| C                                       | 0.367788  |
| O                                       | 2.718980  |
| C                                       | -0.875395 |
| C                                       | -2.068956 |
| C                                       | -2.692692 |
| C                                       | -1.156956 |
| C                                       | -2.257023 |
| C                                       | -0.714633 |
| C                                       | -0.715064 |

| Datum                                   | Value     |
|-----------------------------------------|-----------|
| H                                       | 0.528534  |
| H                                       | -2.692611 |
| H                                       | -1.787206 |
| H                                       | -0.240165 |
| H                                       | 1.345933  |
| H                                       | -0.733189 |
| H                                       | -2.018660 |
| H                                       | 1.400896  |
| H                                       | 1.885933  |
| H                                       | 1.885566  |

### 4_3methyl2butenal_1_reopt_am1_HEI

| Datum                                   | Value     |
|-----------------------------------------|-----------|
| AM1 Energy                              | -0.107762 |
| AM1 Free Energy (Quasiharmonic)         | 0.017065  |

### Number of Imaginary Frequencies

| Datum                                   | Value     |
|-----------------------------------------|-----------|
| Number of Imaginary Frequencies         | 0         |

### Frequencies (Top 3 out of 51)

1. 39.9937 cm⁻¹
2. 86.1156 cm⁻¹
3. 139.0825 cm⁻¹
AM1 Molecular Geometry in Cartesian Coordinates

| Datum   | Value         |
|---------|---------------|
| 4_3-methyl-2-butenal_2_am1  |               |
| AM1 Energy | -0.054229   |
| AM1 Free Energy (Quasiharmonic) | 0.036991   |
| Number of Imaginary Frequencies | 0           |

Frequencies (Top 3 out of 36)

1. 70.6709 cm⁻¹
2. 99.9176 cm⁻¹
3. 123.2436 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Datum   | Value         |
|---------|---------------|
| C       | -2.060942     |
|         | -0.016149     |
|         | -0.234404     |
| C       | -0.963021     |
|         | 0.338423      |
|         | 0.558441      |
| C       | 0.299940      |
|         | 0.782940      |
|         | 0.068253      |
| O       | -3.180766     |
|         | -0.416344     |
|         | 0.184236      |
| C       | 0.682602      |
|         | -2.167454     |
|         | 0.067595      |
| H       | 1.077921      |
|         | -2.759016     |
|         | 0.922120      |
| H       | -0.389258     |
|         | -1.908231     |
|         | 0.263968      |
| H       | 0.748597      |
|         | -2.782687     |
|         | -0.856404     |
| S       | 1.619125      |
|         | -0.701662     |
|         | -0.123062     |
| H       | -1.930400     |
|         | 0.077427      |
|         | -1.344895     |
| H       | -1.069740     |
|         | 0.235661      |
|         | 1.645420      |
| C       | 0.337537      |
|         | 1.355403      |
|         | -1.325432     |
| H       | -0.008448     |
|         | 0.603608      |
|         | -2.074112     |
| H       | -0.329331     |
|         | 2.251304      |
|         | -1.386701     |
| H       | 1.376163      |
|         | 1.666442      |
|         | -1.596636     |
| C       | 1.077818      |
|         | 1.377738      |
|         | 1.040470      |
| H       | 2.136315      |
|         | 1.763264      |
|         | 0.704820      |
| H       | 0.606112      |
|         | 2.649573      |
|         | 1.112217      |
| H       | 1.078600      |
|         | 1.174592      |
|         | 2.055771      |
### 4_3methyl2butenal_2_reopt_am1_HEI

| Datum                          | Value       |
|-------------------------------|-------------|
| AM1 Energy                    | -0.107762   |
| AM1 Free Energy (Quasiharmonic) | 0.017064   |
| Number of Imaginary Frequencies | 0           |

#### Frequencies (Top 3 out of 51)

1. 39.9537 cm⁻¹
2. 86.1197 cm⁻¹
3. 139.0786 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|          |          |          |          |
|----------|----------|----------|----------|
| C        | 2.061000 | -0.016250| 0.234489 |
| C        | 0.963082 | 0.338096 | -0.558487|
| C        | -0.299767| 0.783043 | -0.068420|
| O        | 3.180734 | -0.416816| -0.184017|
| C        | -0.683045| -2.167374| -0.067926|
| H        | 0.388876 | -1.908201| -0.264038|
| H        | -0.749247| -2.783171| 0.855684 |
| H        | -1.078355| -2.758356| -0.922861|
| S        | -1.619265| -0.701542| 0.123648 |
| H        | 1.930525 | 0.077932 | 1.344935 |
| H        | 1.069717 | 0.234764 | -1.645419|
| C        | -0.337282| 1.355882 | 1.325097 |
| H        | 0.008535 | 0.604209 | 2.073983 |
| H        | 0.329763 | 2.251667 | 1.386122 |
| H        | -1.375856| 1.667199 | 1.596190 |
| C        | -1.077553| 1.637631 | -1.040863|
| H        | -2.136142| 1.763042 | -0.705445|
4_3methyl2butenal_3_am1_HEI

| Datum                          | Value       |
|-------------------------------|-------------|
| AM1 Energy                    | -0.107762   |
| AM1 Free Energy (Quasiharmonic) | 0.017065    |
| Number of Imaginary Frequencies | 0           |

**Frequencies (Top 3 out of 51)**

1. 40.0050 cm⁻¹
2. 86.1110 cm⁻¹
3. 139.0805 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C    | -2.060954 | -0.016182 | -0.234406 |
|------|-----------|-----------|-----------|
| C    | -0.963031 | 0.338376  | 0.558444  |
| C    | 0.299906  | 0.782949  | 0.068264  |
| O    | -3.180765 | -0.416420 | 0.184228  |
| C    | 0.682692  | -2.167451 | 0.067607  |
| H    | 1.078037  | -2.758989 | 0.922136  |
| H    | -0.389174 | -1.908258 | 0.263986  |
| H    | 0.748699  | -2.782696 | -0.856383 |
| S    | 1.619159  | -0.701626 | -0.123086 |
| H    | -1.930428 | 0.077450  | -1.344893 |
| H    | -1.069739 | 0.235560  | 1.645419  |
| C    | 0.337482  | 1.355427  | -1.325415 |
| H    | -0.008499 | 0.603635  | -2.074099 |
| H    | -0.329398 | 2.251320  | -1.386663 |
| H    | 1.376101  | 1.666482  | -1.596623 |
| C    | 1.077761  | 1.637768  | 1.040480  |
| H    | 2.136271  | 1.763273  | 0.704859  |
| H    | 0.606064  | 2.649610  | 1.112180  |
| H    | 1.078512  | 1.174655  | 2.055796  |

4_3methyl2butenal_4_am1_HEI
| Datum                        | Value       |
|------------------------------|-------------|
| AM1 Energy                   | -0.103311   |
| AM1 Free Energy (Quasiharmonic) | 0.021565   |
| Number of Imaginary Frequencies | 0          |

**Frequencies (Top 3 out of 51)**

1. 51.7373 cm⁻¹
2. 70.0890 cm⁻¹
3. 88.9743 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
|   |   |   |   |
| C | -2.251965 | -0.322875 | 0.272186 |
| C | -1.225323 | 0.200006  | -0.520385 |
| C | 0.065116  | 0.605660  | -0.039347 |
| O | -3.395833 | -0.673226 | -0.127445 |
| C | 2.724038  | -0.736458 | 0.206529  |
| H | 3.243331  | -0.014363 | -0.463066 |
| H | 2.799115  | -0.354075 | 1.249294  |
| H | 3.243628  | -1.718500 | 0.144801  |
| S | 1.058100  | -0.983280 | -0.270698 |
| H | -2.040303 | -0.418951 | 1.370123  |
| H | -1.395199 | 0.264190  | -1.601387 |
| C | 0.157992  | 0.980385  | 1.420769  |
| H | -0.111137 | 0.113020  | 2.069676  |
| H | 1.195447  | 1.306113  | 1.681243  |
| H | -0.542519 | 1.822437  | 1.642423  |
| C | 0.725593  | 1.659439  | -0.901946 |
| H | 0.700745  | 1.355812  | -1.975559 |
| H | 0.181466  | 2.629993  | -0.794954 |
| H | 1.789776  | 1.815680  | -0.598700 |

**4_3methyl2butenal_5_am1_HEI**

| Datum                        | Value       |
|------------------------------|-------------|
| AM1 Energy                   | -0.105601   |
| AM1 Free Energy (Quasiharmonic) | 0.019419   |
| Number of Imaginary Frequencies | 0          |

**Frequencies (Top 3 out of 51)**
1. 38.6334 cm⁻¹
2. 54.5255 cm⁻¹
3. 118.5943 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|       | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| C     | 2.066963  | 0.273444  | -0.613084 |
| C     | 0.845656  | -0.310492 | -0.948040 |
| C     | -0.171142 | -0.771070 | -0.048794 |
| O     | 2.568011  | 0.500729  | 0.522171  |
| C     | -0.868244 | 2.084495  | -0.067241 |
| H     | -0.902228 | 2.645646  | 0.892221  |
| H     | 0.198792  | 1.944992  | -0.373812 |
| H     | -1.402206 | 2.670839  | -0.846677 |
| S     | -1.635479 | 0.521202  | 0.116789  |
| H     | 2.685639  | 0.567389  | -1.506892 |
| H     | 0.612661  | -0.393439 | -2.017665 |
| C     | 0.258321  | -0.998744 | 1.376750  |
| H     | 0.729367  | -0.072104 | 1.787831  |
| H     | -0.611230 | -1.287910 | 2.014963  |
| H     | 1.021184  | -1.815734 | 1.413267  |
| C     | -0.987059 | -1.929270 | -0.577972 |
| H     | -1.307308 | -1.738672 | -1.629912 |
| H     | -0.370360 | -2.861784 | -0.557977 |
| H     | -1.897709 | -2.094461 | 0.048929  |

4_3methyl2butenal_6_am1_HEI_reopt

| Datum                                      | Value    |
|--------------------------------------------|----------|
| AM1 Energy                                 | -0.105601|
| AM1 Free Energy (Quasiharmonic)            | 0.019417 |
| Number of Imaginary Frequencies            | 0        |

Frequencies (Top 3 out of 51)

1. 38.6253 cm⁻¹
2. 54.5084 cm⁻¹
3. 118.4650 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
4_3methyl2butenal_7_reopt_am1_HEI

| Datum                              | Value       |
|------------------------------------|-------------|
| AM1 Energy                         | -0.103311   |
| AM1 Free Energy (Quasiharmonic)    | 0.021565    |
| Number of Imaginary Frequencies    | 0           |

**Frequencies** (Top 3 out of 51)

1. 51.7376 cm⁻¹
2. 70.0892 cm⁻¹
3. 88.9747 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C       | 2.066923 | 0.273430 | -0.613266 |
| C       | 2.845539 | -0.310434| -0.948040 |
| C       | -0.171138| -0.770995| -0.048645 |
| O       | 2.568137 | 0.500688 | 0.521928  |
| C       | -0.868315| 2.084389 | -0.066825 |
| H       | 0.198855 | 1.944854 | -0.372891 |
| H       | -1.401822| 2.671025 | -0.846353 |
| H       | -0.902774| 2.645232 | 0.892794  |
| S       | -1.635687| 0.521031 | 0.116214  |
| H       | 2.685492 | 0.567341 | -1.507156 |
| C       | 0.612378 | -0.393396| -2.017626 |
| H       | 0.258438 | -0.998065| 1.376964  |
| H       | 0.728827 | -0.071020| 1.787856  |
| H       | -0.610919| -1.287716| 2.015211  |
| H       | 1.021902 | -1.814478| 1.413663  |
| C       | -0.986753| -1.929596| -0.577418 |
| H       | -1.306872| -1.739545| -1.629494 |
| H       | -0.369867| -2.861972| -0.556890 |
| H       | -1.897470| -2.094709| 0.049414  |
4_3methyl2butenal_8_reopt_am1_HEI

| Datum                              | Value     |
|------------------------------------|-----------|
| AM1 Energy                         | -0.101531 |
| AM1 Free Energy (Quasiharmonic)    | 0.023557  |
| Number of Imaginary Frequencies    | 0         |

**Frequencies (Top 3 out of 51)**

1. 45.2673 cm⁻¹
2. 58.7695 cm⁻¹
3. 85.7882 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C       | 2.342417 | -0.373082 | -0.513739 |
|---------|----------|-----------|-----------|
| C       | 1.141117 | 0.228752  | -0.887244 |
| C       | 0.034357 | 0.551416  | -0.024626 |
| O       | 2.765902 | -0.682146 | 0.633568  |
| C       | -2.675269| -0.612634 | 0.383746  |
| H       | -2.505075| -0.493745 | 1.477293  |
| H       | -3.234435| 0.279959  | 0.022760  |
| H       | -3.298676| -1.518227 | 0.211944  |
| S       | -1.169450| -0.830897 | -0.481800 |
| H       | 3.032388 | -0.577271 | -1.379867 |
| H       | 0.994243 | 0.441315  | -1.953461 |
| C       | -0.660832| 1.847357  | -0.382982 |
| H       | -0.901358| 1.876427  | -1.472272 |
| H       | -1.608954| 1.966325  | 0.196544  |
| H       | 0.088707 | 2.710193  | -0.144743 |
| C       | 0.306659 | 0.474403  | 1.455450  |
| H       | 0.707946 | -0.535242 | 1.718660  |
5_trans-2-methyl-2-butenal_1_am1

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| AM1 Energy                                 | -0.053372    |
| AM1 Free Energy (Quasiharmonic)            | 0.037279     |
| Number of Imaginary Frequencies            | 0            |

Frequencies (Top 3 out of 36)

1. 23.0622 cm⁻¹
2. 68.1120 cm⁻¹
3. 101.4815 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|        |          |          |          |
|--------|----------|----------|----------|
| C      | 1.362737 | -0.712663| 0.000036 |
| C      | 0.066348 | -0.005233| 0.000006 |
| O      | 2.456845 | -0.144760| -0.00047 |
| C      | -1.071915| -0.722142| -0.00006 |
| C      | -2.433065| -0.158334| -0.00018 |
| H      | 1.295333 | -1.825981| 0.00130  |
| H      | -1.030131| -1.826794| -0.00004 |
| C      | 0.102242 | 1.475521 | 0.00020  |
| H      | -2.989381| -0.509152| 0.906327 |
| H      | -2.428993| 0.959363 | -0.00106 |
| H      | -2.989424| -0.509299| -0.906278|
| H      | -0.414130| 1.879807 | -0.906370|
| H      | -0.413960| 1.879767 | 0.906526 |
| H      | 1.157835 | 1.847473 | -0.00080 |

5_trans2methyl2butenal_1_reopt_am1_HEI

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| AM1 Energy                                 | -0.116606    |
| AM1 Free Energy (Quasiharmonic)            | 0.008834     |
| Datum                               | Value                                      |
|-------------------------------------|--------------------------------------------|
| Number of Imaginary Frequencies     | 0                                          |

**Frequencies (Top 3 out of 51)**

1. 36.3045 cm\(^{-1}\)
2. 73.2536 cm\(^{-1}\)
3. 104.6237 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| C | -1.951259 | -0.573187 | -0.058607 |
| C | -0.971456 | 0.388925  | 0.222040  |
| C | 0.175435  | 0.554687  | -0.636580 |
| O | -1.990623 | -1.374517 | -1.032346 |
| C | 1.229403  | -1.803552 | 0.626503  |
| H | 0.112150  | -1.838719 | 0.635885  |
| H | 1.616313  | -2.629721 | -0.009321 |
| H | 1.612202  | -1.935392 | 1.661997  |
| S | 1.765737  | -0.257313 | -0.003245 |
| H | -2.800691 | -0.614621 | 0.675771  |
| C | 0.656660  | 1.967083  | -0.834597 |
| H | 0.898394  | 2.447240  | 0.144529  |
| H | 1.570843  | 1.989680  | -1.477442 |
| H | -0.143369 | 2.568988  | -1.332170 |
| H | 0.018501  | 0.036196  | -1.616570 |
| C | -1.190451 | 1.240477  | 1.414191  |
| H | -0.160645 | 1.241645  | 2.018923  |
| H | -1.318313 | 2.306870  | 1.134521  |
| H | -1.937823 | 0.894373  | 2.076867  |

**5_trans2methyl2butenal_2_am1_HEI**

| Datum                               | Value          |
|-------------------------------------|----------------|
| AM1 Energy                           | -0.117426      |
| AM1 Free Energy (Quasiharmonic)      | 0.008212       |
| Number of Imaginary Frequencies      | 0              |

**Frequencies (Top 3 out of 51)**
1. 37.4126 cm⁻¹
2. 63.7547 cm⁻¹
3. 116.6724 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|  |  |  |  |
|---|---|---|---|
| C | -1.778300 | -0.393026 | -0.731005 |
| C | -0.850535 | 0.390527 | -0.022498 |
| C | 0.423062 | 0.709899 | -0.606966 |
| O | -2.923756 | -0.751777 | -0.348652 |
| C | 1.082158 | -1.875572 | 0.581990 |
| H | -0.021951 | -1.705495 | 0.654572 |
| H | 1.276057 | -2.790397 | -0.019556 |
| H | 1.498168 | -2.020273 | 1.602887 |
| S | 1.847132 | -0.494028 | -0.176373 |
| H | -1.448449 | -0.721692 | -1.752999 |
| C | 1.028368 | 2.027006 | -0.205032 |
| H | 1.140267 | 2.090492 | 0.904207 |
| H | 2.035270 | 2.159924 | -0.671712 |
| H | 0.366845 | 2.864484 | -0.539754 |
| H | 0.421385 | 0.600257 | -1.721334 |
| C | -1.177039 | 0.876082 | 1.327487 |
| H | -2.170145 | 0.479003 | 1.655723 |
| H | -1.223100 | 1.996924 | 1.360362 |
| H | -0.404682 | 0.555941 | 2.074941 |

5_trans-2-methyl-2-butenal_2_am1

| Datum | Value |
|-------|-------|
| AM1 Energy | -0.054036 |
| AM1 Free Energy (Quasiharmonic) | 0.036459 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 36)

1. 28.2389 cm⁻¹
2. 74.0283 cm⁻¹
3. 79.5065 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
5_trans2methyl2butenal_3_am1_HEI

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.111744     |
| AM1 Free Energy (Quasiharmonic)            | 0.01323       |
| Number of Imaginary Frequencies            | 0             |

Frequencies (Top 3 out of 51)

1. 36.8456 cm⁻¹
2. 58.3821 cm⁻¹
3. 81.7791 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| C   | 2.156158 | -0.708557 | -0.086203 |
| C   | 1.190888 | 0.309202  | -0.095520 |
| C   | -0.083811| 0.121993  | 0.556095  |
| O   | 2.099616 | -1.821751 | 0.502538  |
| C   | -2.783068| -0.712463 | 0.835846  |
| H   | -2.561112| -1.423105 | 0.863298  |
| H   | -3.323791| 0.161136  | 0.465214  |
| H   | -3.446011| -1.213106 | -0.704414 |
| S   | -1.319086| -0.230693 | -0.794475 |
| H   | 3.096177 | -0.474698 | -0.656013 |
| C   | -0.594621| 1.304648  | 1.336885  |
| H   | -0.682852| 2.205418  | 0.682867  |
| H   | -1.597107| 1.087453  | 1.781259  |
5_trans2methyl2butenal_4_am1_HEI_reopt

| Datum                          | Value          |
|-------------------------------|----------------|
| AM1 Energy                    | -0.116627      |
| AM1 Free Energy (Quasiharmonic) | 0.008795      |
| Number of Imaginary Frequencies | 0             |

**Frequencies** (Top 3 out of 51)

1. 38.8314 cm⁻¹
2. 58.1472 cm⁻¹
3. 98.4130 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C     | 1.673431 | 0.240940 | -0.711696 |
|-------|----------|----------|-----------|
| C     | 0.855181 | 0.129313 | 0.423889  |
| C     | -0.404457| 0.809608 | 0.553092  |
| O     | 2.788209 | -0.315794| -0.901685 |
| C     | -1.299604| -1.675240| -0.697266 |
| H     | -1.680264| -1.799770| -1.734462 |
| H     | -0.180861| -1.642543| -0.711558 |
| H     | -1.630909| -2.541548| -0.083930 |
| S     | -1.930637| -0.188424| -0.017783 |
| H     | 1.286005 | 0.903481 | -1.530104 |
| C     | -0.569766| 2.107141 | -0.189691 |
| H     | -0.529782| 1.951102 | -1.294298 |
| H     | -1.553019| 2.577647 | 0.058620  |
| H     | 0.245696 | 2.816647 | 0.096693  |
| H     | -0.691181| 0.941176 | 1.629070  |
| C     | 1.272630 | -0.736330| 1.542021  |
| H     | 2.271849 | -1.194180| 1.331258  |
| H     | 0.535488 | -1.564320| 1.713799  |
| H     | 1.347818 | -0.159150| 2.500829  |
**5_trans2methyl2butenal_5_am1_HEI**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.116627 |
| AM1 Free Energy (Quasiharmonic)            | 0.008793 |
| Number of Imaginary Frequencies            | 0       |

**Frequencies** (Top 3 out of 51)

1. 38.8066 cm⁻¹
2. 58.1445 cm⁻¹
3. 98.4129 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|    | X          | Y          | Z          |
|----|------------|------------|------------|
| C  | 1.673534   | 0.240911   | -0.711624  |
| C  | 0.855278   | 0.129393   | 0.423978   |
| C  | -0.404311  | 0.809755   | 0.553117   |
| O  | 2.788211   | -0.316001  | -0.901656  |
| C  | -1.299765  | -1.675030  | -0.697636  |
| H  | -0.181018  | -1.642521  | -0.711836  |
| H  | -1.631194  | -2.541604  | -0.84739   |
| H  | -1.680377  | -1.799027  | -1.734912  |
| S  | -1.930680  | -0.188474  | -0.017495  |
| H  | 1.286219   | 0.903583   | -1.529981  |
| C  | -0.569691  | 2.107076   | -0.189979  |
| H  | -0.529542  | 1.950801   | -1.294548  |
| H  | -1.553022  | 2.577537   | 0.058104   |
| H  | 0.245665   | 2.816731   | 0.096345   |
| H  | -0.691074  | 0.941471   | 1.629055   |
| C  | 1.272554   | -0.736362  | 1.542086   |
| H  | 2.271010   | -1.194184  | 1.331451   |
| H  | 0.535366   | -1.564369  | 1.713601   |
| H  | 1.347560   | -0.159296  | 2.500972   |

**5_trans2methyl2butenal_6_reopt_am1_HEI**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.117426 |
| AM1 Free Energy (Quasiharmonic)            | 0.008211 |
| Number of Imaginary Frequencies            | 0       |
**Frequencies (Top 3 out of 51)**

1. 37.4269 cm⁻¹
2. 63.7176 cm⁻¹
3. 116.5954 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -1.778368 | -0.392262 | -0.731306 |
| C          | -0.850355 | 0.390680  | -0.022464 |
| C          | 0.423249  | 0.710104  | -0.606860 |
| O          | -2.923820 | -0.751047 | -0.348976 |
| C          | 1.081578  | -1.875319 | 0.582346  |
| H          | 1.497161  | -2.019159 | 1.603541  |
| H          | -0.022527 | -1.705133 | 0.654394  |
| H          | 1.275731  | -2.79629  | -0.018375 |
| S          | 1.846836  | -0.494501 | -0.177053 |
| H          | -1.448764 | -0.720287 | -1.753585 |
| C          | 1.028818  | 2.026938  | -0.204389 |
| H          | 1.140482  | 2.090077  | 0.904887  |
| H          | 2.035869  | 2.159710  | -0.670793 |
| H          | 0.367615  | 2.864699  | -0.539026 |
| H          | 0.421433  | 0.601087  | -1.721298 |
| C          | -1.176533 | 0.875171  | 1.327998  |
| H          | -2.169693 | 0.478067  | 1.656031  |
| H          | -1.222299 | 1.995986  | 1.361904  |
| H          | -0.404150 | 0.554102  | 2.075021  |

**5_trans2methyl2butenal_7_reopt_am1_HEI**

| Datum                      | Value       |
|---------------------------|-------------|
| AM1 Energy                | -0.11277    |
| AM1 Free Energy (Quasiharmonic) | 0.01257     |
| Number of Imaginary Frequencies | 0          |

**Frequencies (Top 3 out of 51)**

1. 49.3630 cm⁻¹
2. 62.4772 cm⁻¹
3. 75.2676 cm⁻¹
### AM1 Molecular Geometry in Cartesian Coordinates

|  | X          | Y          | Z          |
|---|------------|------------|------------|
| C | -1.903124  | -0.830654  | -0.502674  |
| C | -1.079513  |  0.225677  | -0.073682  |
| C |  0.264302  |  0.342926  | -0.576634  |
| O | -3.098391  | -1.048413  | -0.170439  |
| C |  2.949565  | -0.643483  | -0.096749  |
| H |  2.941249  | -0.820319  | -1.195688  |
| H |  3.451180  |  0.332539  |  0.091554  |
| H |  3.539944  | -1.448221  |  0.395113  |
| S |  1.329998  | -0.681272  |  0.565789  |
| H | -1.432365  | -1.539955  | -1.234651  |
| C |  0.826764  |  1.738401  | -0.621702  |
| H |  0.832195  |  2.196380  |  0.396776  |
| H |  1.873184  |  1.732572  | -1.015213  |
| H |  0.199112  |  2.378445  | -1.289922  |
| H |  0.402846  | -0.156521  | -1.570357  |
| C | -1.581327  |  1.200714  |  0.906854  |
| H | -2.603988  |  0.910099  |  1.255418  |
| H | -1.645857  |  2.230659  |  0.463587  |
| H | -0.910341  |  1.270490  |  1.801799  |

### 6_2ethylacrolein_10_reopt_am1_HEI

| Datum                        | Value     |
|------------------------------|-----------|
| AM1 Energy                   | -0.121377 |
| AM1 Free Energy (Quasiharmonic) | 0.005255  |
| Number of Imaginary Frequencies | 0         |

#### Frequencies (Top 3 out of 51)

1. 32.5404 cm⁻¹
2. 55.7350 cm⁻¹
3. 76.5164 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

|  | X          | Y          | Z          |
|---|------------|------------|------------|
| C |  1.414404  | -1.261217  | -0.050301  |
| O |  2.524349  | -1.220538  | -0.644763  |
| C |  0.738565  | -0.198618  |  0.572268  |
| C | -0.509369  | -0.419532  |  1.244794  |
| C |  1.334363  |  1.154066  |  0.581519  |
### 6_2ethylacrolein_11_reopt_am1_HEI

#### Datum

|                       | Value     |
|-----------------------|-----------|
| AM1 Energy            | -0.120847 |
| AM1 Free Energy (Quasiharmonic) | 0.005594 |
| Number of Imaginary Frequencies | 0        |

#### Frequencies (Top 3 out of 51)

1. 34.3893 cm⁻¹
2. 51.0513 cm⁻¹
3. 85.6959 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|       |       |       |
|-------|-------|-------|
| C     | -1.505974 | -1.145253 | -0.240060 |
| O     | -1.154786 | -2.341667 | -0.425362 |
| C     | -0.844006 | -0.160319 | 0.506980  |
| C     | 0.390716  | -0.436154 | 1.189070  |
| C     | -1.440225 | 1.188688  | 0.606646  |
| C     | -1.274093 | 2.005227  | -0.657278 |
| H     | -2.468252 | -0.809944 | -0.713750 |
| H     | 0.563638  | -1.532044 | 1.305056  |
| H     | 0.492314  | 0.086753  | 2.171144  |
| H     | -2.541032 | 1.110011  | 0.831821  |
| H     | -0.976179 | 1.753271  | 1.460637  |
| H     | -1.704905 | 3.028622  | -0.533125 |
| H     | -1.790644 | 1.504388  | -1.511270 |
| H     | -0.190455 | 2.099142  | -0.912350 |
### 6_2ethylacrolein_1_am1

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.047014     |
| AM1 Free Energy (Quasiharmonic)            | 0.044819      |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 36)

1. 36.5757 cm\(^{-1}\)
2. 67.7121 cm\(^{-1}\)
3. 160.3459 cm\(^{-1}\)

### AM1 Molecular Geometry in Cartesian Coordinates

|        |        |        |
|--------|--------|--------|
| C      | 1.348875 | -0.330276 | -0.156736 |
| O      | 1.309480 | -1.530756 | 0.118017  |
| C      | 0.239838 | 0.611902  | 0.100649  |
| C      | 0.404546 | 1.921446  | -0.119824 |
| C      | -1.033120| 0.036342  | 0.618212  |
| C      | -1.820540| -0.656036 | -0.468639 |
| H      | 2.253443 | 0.123369  | -0.625584 |
| H      | -0.393794| 2.652404  | 0.066988  |
| H      | 1.346314 | 2.343528  | -0.497123 |
| H      | -0.787799| -0.706828 | 1.425938  |
| H      | -1.659817| 0.845205  | 1.079935  |
| H      | -2.757555| -1.088877 | -0.042658 |
| H      | -2.097077| 0.060785  | -1.278403 |
| H      | -1.217150| -1.483806 | -0.915200 |

### 6_2ethylacrolein_1_reopt_am1_HEI

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.120847     |
| Datum                                | Value     |
|-------------------------------------|-----------|
| AM1 Free Energy (Quasiharmonic)     | 0.005594  |
| Number of Imaginary Frequencies     | 0         |

**Frequencies (Top 3 out of 51)**

1. 34.2873 cm⁻¹  
2. 51.0915 cm⁻¹  
3. 85.7007 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|          |          |          |
|----------|----------|----------|
| C        | -1.506147| 1.145129 | 0.240155 |
| O        | -1.155057| 2.341603 | 0.425243 |
| C        | -0.844199| 0.160174 | -0.506881|
| C        | 0.390415 | 0.436064 | -1.189133|
| C        | -1.440320| -1.18894 | -0.606321|
| C        | -1.273064| -2.00566 | 0.657311 |
| H        | -2.468306| 0.809776 | 0.714056 |
| H        | 0.563205 | 1.531954 | -1.305301|
| H        | 0.491986 | -0.08698 | -2.171136|
| H        | -2.541317| -1.11033 | -0.830616|
| H        | -0.976857| -1.75324 | -1.460777|
| H        | -1.703480| -3.02922 | 0.533171 |
| H        | -0.189231| -2.09915 | 0.911690 |
| H        | -1.789326| -1.50528 | 1.511743 |
| C        | 1.652804 | 0.000104 | 1.341122 |
| H        | 2.286884 | 0.811497 | 1.759944 |
| H        | 0.575210 | 0.249594 | 1.507727 |
| H        | 1.895411 | -0.95397 | 1.858132 |
| S        | 1.951209 | -0.17993 | -0.378006|

**6_2ethylacrolein_2_am1_HEI_reopt**

| Datum                                | Value     |
|-------------------------------------|-----------|
| AM1 Energy                          | -0.12141  |
| AM1 Free Energy (Quasiharmonic)     | 0.004745  |
| Number of Imaginary Frequencies     | 0         |

**Frequencies (Top 3 out of 51)**

1. 34.2873 cm⁻¹  
2. 51.0915 cm⁻¹  
3. 85.7007 cm⁻¹
1. 33.1763 cm\(^{-1}\)
2. 46.2138 cm\(^{-1}\)
3. 92.4143 cm\(^{-1}\)

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -0.817237 | 1.621743 | 0.155635 |
| O | -0.144772 | 2.525887 | -0.412173 |
| C | -0.729547 | 0.237910 | -0.041018 |
| C | 0.201118  | -0.335167 | -0.976376 |
| C | -1.595589 | -0.671720 | 0.737349  |
| C | -2.814370 | -1.132320 | -0.034286 |
| H | -1.588339 | 1.947915  | 0.905045  |
| H | 0.553611  | 0.413649  | -1.723842 |
| H | -0.183627 | -1.253599 | -1.483390 |
| H | -1.008606 | -1.579303 | 1.050112  |
| H | -1.944511 | -0.168207 | 1.680786  |
| H | -2.504388 | -1.653585 | -0.971639 |
| H | -3.430488 | -1.837544 | 0.575637  |
| H | -3.450430 | -0.259492 | -0.315806 |
| C | 2.296032  | 0.187020  | 0.881342  |
| H | 2.500799  | -0.287227 | 1.865712  |
| H | 1.497349  | 0.960045  | 0.998490  |
| H | 3.226058  | 0.673473  | 0.514335  |
| S | 1.765519  | -1.038001 | -0.258371 |

6_2ethylacrolein_2_am1

| Datum                                | Value      |
|--------------------------------------|------------|
| AM1 Energy                           | -0.047014  |
| AM1 Free Energy (Quasiharmonic)      | 0.044819   |
| Number of Imaginary Frequencies      | 0          |

Frequencies (Top 3 out of 36)

1. 36.5535 cm\(^{-1}\)
2. 67.7163 cm\(^{-1}\)
3. 160.3848 cm\(^{-1}\)

AM1 Molecular Geometry in Cartesian Coordinates
### AM1 Molecular Geometry in Cartesian Coordinates

| C   | 1.586100 | 0.213522 | 0.000001 |
| O   | 2.106915 | -0.903217 | -0.000001 |
| C   | 0.123348 | 0.436836 | 0.000000  |
| C   | -0.358699 | 1.684647 | -0.000001 |
| C   | -0.789031 | -0.796025 | -0.000000 |
| C   | -2.195215 | -0.552809 | 0.000001   |
| H   | 2.206905  | 1.139631  | 0.000004   |
| H   | -1.434463 | 1.905767  | -0.000001  |
| H   | 0.297176  | 2.566744  | -0.000000  |
| H   | -0.426545 | -1.408053 | -0.901401  |
| H   | -0.426543 | -1.408055 | 0.901399   |
| H   | -2.506631 | 0.021160  | 0.906171   |

---

**6_2ethylacrolein_3_am1**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.04719    |
| AM1 Free Energy (Quasiharmonic)            | 0.044666    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 36)

1. 28.6850 cm⁻¹
2. 72.7218 cm⁻¹
3. 207.0465 cm⁻¹
### 6_2ethylacrolein_3_reopt_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.120847   |
| AM1 Free Energy (Quasiharmonic)            | 0.005594    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 51)

1. 34.2914 cm-1  
2. 51.0985 cm-1  
3. 85.6876 cm-1

**AM1 Molecular Geometry in Cartesian Coordinates**

| C      | -1.505999 | -1.145243 | 0.240149 |
|--------|-----------|-----------|----------|
| O      | -1.154783 | -2.341661 | 0.425355 |
| C      | -0.844127 | -0.160271 | -0.506926|
| C      | 0.390533  | -0.436073 | 1.189138 |
| C      | -1.440343 | 1.188749  | -0.606478|
| C      | -1.273468 | 2.005491  | 0.657219 |
| H      | -2.468216 | -0.809960 | 0.713978 |
| H      | 0.492086  | 0.86965   | 2.171141 |
| H      | 0.563399  | -1.531953 | 1.305281 |
| H      | -0.976734 | 1.753162  | -1.460821|
| H      | -2.541270 | 1.110095  | -0.831038|
| H      | -1.789842 | 1.504993  | 1.511511 |
| H      | -1.703999 | 3.028996  | 0.533035 |
| H      | -0.189696 | 2.099093  | 0.911852 |
| C      | 1.652627  | 0.000328  | 1.341181 |
| H      | 0.575019  | -0.249146 | 1.507660 |
| H      | 2.286666  | -0.810957 | 1.760265 |
| H      | 1.895120  | 0.954512  | 1.858057 |
| S      | 1.951275  | 0.179976  | -0.377935|

### 6_2ethylacrolein_4_am1
### AM1 Molecular Geometry in Cartesian Coordinates

| C    | 1.007171 | -0.765542 | 0.175666 |
|------|----------|-----------|----------|
| O    | 2.198485 | -0.735738 | -0.142938|
| C    | 0.122178 | 0.415169  | 0.153357 |
| C    | 0.581853 | 1.621352  | -0.201901|
| C    | -1.290965| 0.177674  | 0.560125 |
| C    | -2.055089| -0.616840 | -0.471758|
| H    | 0.522094 | -1.712059 | 0.508097 |
| H    | -0.056296| 2.514759  | -0.222336|
| H    | 1.632141 | 1.774164  | -0.492134|
| H    | -1.301942| -0.373945 | 1.539733 |
| H    | -1.809102| 1.159704  | 0.729932 |
| H    | -3.100787| -0.792506 | -0.121192|
| H    | -2.094948| -0.067773 | -1.443184|
| H    | -1.569930| -1.607317 | -0.648351|

### 6_2ethylacrolein_4_reopt_am1_HEI

| Datum                  | Value  |
|------------------------|--------|
| AM1 Energy             | -0.12141 |
| AM1 Free Energy (Quasiharmonic) | 0.004744 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 51)

1. 33.1236 cm⁻¹
2. 46.2683 cm⁻¹
3. 92.4119 cm⁻¹
AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -0.816912 | -1.621969 | -0.155637 |
| O | -0.144279 | -2.525904 | 0.412314  |
| C | -0.729613 | -0.238108 | 0.040930  |
| C | 0.200932  | 0.335295  | 0.976211  |
| C | -1.595874 | 0.671253  | -0.737502 |
| H | -1.587833 | -1.948405 | -0.905120 |
| H | 0.553577  | -0.413362 | 1.723766  |
| H | -0.184019 | 1.253708  | 1.483107  |
| H | -1.945221 | 0.167363  | -1.680574 |
| H | -1.008934 | 1.578653  | -1.050893 |
| H | -3.430571 | 1.837348  | -0.575552 |
| H | -3.450363 | 0.259682  | 0.316563  |
| H | -2.503895 | 1.653922  | 0.971441  |
| C | 2.296221  | -0.186900 | -0.881037 |
| H | 1.498043  | -0.960531 | -0.97549  |
| H | 2.500367  | 0.286906  | -1.865748 |
| H | 3.226703  | -0.672450 | -0.514000 |
| S | 1.765229  | 1.038321  | 0.258232  |

6_2ethylacrolein_5_am1

|            | Value    |
|------------|----------|
| AM1 Energy | -0.048143|
| AM1 Free Energy (Quasiharmonic) | 0.043885 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 36)

1.  51.4614 cm⁻¹
2.  89.0563 cm⁻¹
3.  150.0484 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -1.007171 | -0.765542 | 0.175666 |
| O | -2.198484 | -0.735739 | -0.142938 |
| C | -0.122178 | 0.415169  | 0.153357  |
| Datum                          | Value       |
|--------------------------------|-------------|
| AM1 Energy                     | -0.12141    |
| AM1 Free Energy (Quasiharmonic)| 0.004745    |
| Number of Imaginary Frequencies| 0           |

**Frequencies (Top 3 out of 51)**

1. 33.1417 cm⁻¹
2. 46.1704 cm⁻¹
3. 92.4727 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -0.816594 | -1.621832 | -0.155511 |
| O   | -0.143651 | -2.525616 | 0.412309  |
| C   | -0.729550 | -0.237940 | 0.041035  |
| C   | 0.200978  | 0.335643  | 0.976223  |
| C   | -1.596051 | 0.671227  | -0.737351 |
| C   | -2.814963 | 1.131403  | 0.034325  |
| H   | -1.587592 | -1.948426 | -0.904847 |
| H   | 0.553609  | -0.412857 | 1.723940  |
| H   | -0.183953 | 1.254167  | 1.482922  |
| H   | -1.944834 | 0.167459  | -1.680702 |
| H   | -1.009497 | 1.579029  | -1.050280 |
| H   | -2.505133 | 1.652905  | 0.971595  |
| H   | -3.450635 | 0.258340  | 0.315990  |
| H   | -3.431417 | 1.836301  | -0.575633 |
| C   | 2.296185  | -0.187109 | -0.880846 |
| H   | 3.226210  | -0.673191 | -0.513345 |
| H   | 1.497626  | -0.960314 | -0.997625 |
| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| AM1 Energy                                 | -0.122157              |
| AM1 Free Energy (Quasiharmonic)            | 0.004061               |
| Number of Imaginary Frequencies            | 0                      |

**Frequencies** (Top 3 out of 51)

1. 31.0704 cm⁻¹
2. 52.2710 cm⁻¹
3. 74.3407 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 1.016382 | 1.406437  | 0.532189 |
|-----|----------|-----------|----------|
| O   | 1.933849 | 2.048892  | -0.044824|
| C   | 0.620162 | 0.080850  | 0.290910 |
| C   | -0.459219| -0.509271 | 1.029375 |
| C   | 1.295205 | -0.719039 | -0.752313|
| C   | 2.194486 | -1.798344 | -0.189804|
| H   | 0.440502 | 1.937823  | 1.336847 |
| H   | -0.635141| -0.027499 | 2.020005 |
| H   | -0.360066| -1.614255 | 1.150818 |
| H   | 0.529284 | -1.206467 | -1.418133|
| H   | 1.913588 | -0.036078 | -1.397048|
| H   | 2.677664 | -2.379843 | -1.012952|
| H   | 2.996004 | -1.344852 | 0.440570 |
| H   | 1.610385 | -2.507740 | 0.444530 |
| C   | -2.012084| 0.671296  | -1.104188|
| H   | -2.681121| 1.547666  | -0.961152|
| H   | -0.952567| 1.021857  | -1.191261|
| H   | -2.302382| 0.144077  | -2.038979|
| S   | -2.164783| -0.419837 | 0.259271 |
| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.0478 |
| AM1 Free Energy (Quasiharmonic)            | 0.044415|
| Number of Imaginary Frequencies            | 0       |

**Frequencies (Top 3 out of 36)**

1. 40.8091 cm⁻¹
2. 80.1476 cm⁻¹
3. 209.0824 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -1.402758 | -0.627386 | -0.000000 |
| O          | -2.505664 | -0.075343 | 0.000001  |
| C          | -0.117929 | 0.102718  | -0.000000 |
| C          | -0.091714 | 1.440871  | -0.000000 |
| C          | 1.086533  | -0.771344 | 0.000000  |
| C          | 2.397994  | -0.029291 | 0.000000  |
| H          | -1.314319 | -1.738210 | -0.000002 |
| H          | 0.840117  | 2.021436  | 0.000000  |
| H          | -1.021542 | 2.029980  | -0.000001 |
| H          | 1.041220  | -1.440262 | 0.903904  |
| H          | 1.041220  | -1.440262 | -0.903904 |
| H          | 3.245373  | -0.757435 | 0.000001  |
| H          | 2.490240  | 0.617045  | -0.906220 |
| H          | 2.490240  | 0.617046  | 0.906220  |

**6_2ethylacrolein_7_am1_HEI**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.116826|
| AM1 Free Energy (Quasiharmonic)            | 0.008927|
| Number of Imaginary Frequencies            | 0       |

**Frequencies (Top 3 out of 51)**

1. 35.6026 cm⁻¹
2. 56.6112 cm⁻¹
3. 63.4974 cm⁻¹
AM1 Molecular Geometry in Cartesian Coordinates

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -1.803685  | 1.164397   | -0.200998  |
| O       | -1.498572  | 2.367340   | -0.419470  |
| C       | -1.011970  | 0.172608   | 0.397504   |
| C       | 0.342475   | 0.441247   | 0.794551   |
| C       | -1.574871  | -1.174415  | 0.624380   |
| C       | -1.277526  | -2.140376  | -0.502694  |
| H       | -2.839229  | 0.834833   | -0.486980  |
| H       | 0.626279   | -0.014735  | 1.773585   |
| H       | 0.576841   | 1.531865   | 0.795645   |
| H       | -2.690689  | -1.111784  | 0.756121   |
| H       | -1.161786  | -1.605183  | 1.578794   |
| H       | -1.788695  | -1.812873  | -1.439328  |
| H       | -0.175348  | -2.167349  | -0.697817  |
| H       | -1.627524  | -3.171386  | -0.250885  |
| C       | 3.073125   | 0.304016   | 0.091344   |
| H       | 3.352514   | -0.044981  | 1.110876   |
| H       | 3.069277   | 1.417197   | 0.096030   |
| H       | 3.838241   | -0.052389  | -0.633199  |
| S       | 1.520213   | -0.334175  | -0.404476  |

6_2ethylacrolein_8_am1_HEI_reopt

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.122157 |
| AM1 Free Energy (Quasiharmonic)      | 0.004061  |
| Number of Imaginary Frequencies      | 0         |

Frequencies (Top 3 out of 51)

1. 31.0667 cm⁻¹
2. 52.2730 cm⁻¹
3. 74.3440 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 1.016403   | 1.406437   | -0.532190  |
| O       | 1.933871   | 2.048889   | 0.044824   |
| C       | 0.620172   | 0.080854   | -0.290909  |
### 6_2ethylacrolein_9_am1_HEI

| Datum                          | Value    |
|-------------------------------|----------|
| AM1 Energy                    | -0.116771|
| AM1 Free Energy (Quasiharmonic) | 0.0085   |
| Number of Imaginary Frequencies | 0        |

**Frequencies (Top 3 out of 51)**

1. 33.7046 cm⁻¹
2. 44.4282 cm⁻¹
3. 59.3733 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C     | O       | S       |
|-------|---------|---------|
| 1.548439 | 1.385731 | -0.214039 |
| 1.196497 | 2.516058 | 0.217737  |
| 0.896294 | 0.156835 | -0.036292 |
| -0.361634 | 0.069820 | 0.653425  |
| 1.499212 | -1.080408 | -0.573426 |
| 2.303080 | -1.841612 | 0.460394  |
| 2.510393 | 1.331606 | -0.792761 |
| -0.607630 | 1.001924 | 1.213962  |
| -0.448168 | -0.818021 | 1.325391  |
| 2.175162 | -0.841117 | -1.440106 |
| 0.692169 | -1.758536 | -0.966133 |
| 3.148548 | -1.216356 | 0.834431  |
7_transtrans24hexadienal_10_am1_HEI

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| AM1 Energy                                 | -0.081815        |
| AM1 Free Energy (Quasiharmonic)            | 0.047273         |
| Number of Imaginary Frequencies            | 0                |

**Frequencies (Top 3 out of 54)**

1. 56.9784 cm⁻¹
2. 59.3386 cm⁻¹
3. 79.6730 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |    |     |     |
|---|----|-----|-----|
| C | 2.704025 | -0.589498 | 0.400566 |
| C | 1.504698 | -0.634595 | -0.321890 |
| C | 0.268508 | -0.162043 | 0.215212 |
| C | -0.945163 | -0.820199 | -0.312901 |
| C | -2.029530 | -1.096795 | 0.423465 |
| C | -3.241320 | -1.746982 | -0.110183 |
| O | 3.830595 | -0.992369 | 0.007058 |
| H | 2.635845 | -0.168301 | 1.439109 |
| H | 1.522034 | -1.007398 | -1.350420 |
| H | 0.253648 | -0.077432 | 1.329837 |
| H | -0.904544 | -1.079158 | -1.384957 |
| H | -2.065584 | -0.847945 | 1.495707 |
| H | -4.132321 | -1.083614 | 0.027527 |
| H | -3.142889 | -1.976520 | -1.199785 |
| H | -3.439397 | -2.705920 | 0.432055 |
| C | -1.320919 | 2.306219 | 0.340049 |
| H | -1.091192 | 2.791825 | 1.314850 |
| H | -1.737516 | 3.074986 | -0.347756 |
| H | -2.088832 | 1.516469 | 0.512563 |
| S | 0.119012 | 1.622832 | -0.383194 |
### 7_transtrans24hexadienal_11_am1_HEI_reopt

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.075392 |
| AM1 Free Energy (Quasiharmonic)            | 0.053366  |
| Number of Imaginary Frequencies            | 0         |

#### Frequencies (Top 3 out of 54)

1. 38.333 cm$^{-1}$
2. 61.021 cm$^{-1}$
3. 66.577 cm$^{-1}$

#### AM1 Molecular Geometry in Cartesian Coordinates

```
C    -2.354901  0.343284  -0.213504
C    -1.589019 -0.543017  0.550504
C    -0.181472 -0.397985  0.785587
C     0.343186  0.986786  0.705680
C     1.200649  1.463339 -0.200717
C     1.685905  2.856787 -0.221064
O    -3.592834  0.261158 -0.438032
H    -1.805335  1.221564 -0.645967
H    -2.072226 -1.436383  0.959241
H     0.137341  0.835173  1.771255
H    -0.059796  1.645376  1.496709
H     1.574740  0.812884 -1.010909
H     2.803358  2.880374 -0.163205
H     1.279188  3.454147  0.631852
H     1.379101  3.356898 -1.174193
C     2.262829 -1.804062  0.003936
H     2.871334 -0.884620 -0.150692
H     2.671940 -2.617160 -0.635998
H     2.356898 -2.103918  1.071749
S     0.587691 -1.563378 -0.444257
```

### 7_transtrans24hexadienal_1_am1_HEI

| Datum          | Value     |
|----------------|-----------|
| AM1 Energy     | -0.085897 |
### AM1 Free Energy (Quasiharmonic)

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Free Energy (Quasiharmonic)    | 0.043568|
| Number of Imaginary Frequencies    | 0       |

#### Frequencies (Top 3 out of 54)

1. 42.4177 cm⁻¹
2. 51.4748 cm⁻¹
3. 82.0654 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

| C     | -2.146958 | -1.342730 | -0.351770 |
|-------|-----------|-----------|-----------|
| C     | -1.010369 | -0.891744 | 0.331276  |
| O     | -3.135623 | -1.938195 | 0.152858  |
| H     | -3.161693 | -1.154691 | -1.458486 |
| C     | 0.062611  | -0.217559 | -0.322363 |
| C     | 1.388378  | -0.366303 | 0.312019  |
| C     | 2.519573  | -0.597696 | -0.366608 |
| C     | 3.842939  | -0.743460 | 0.268274  |
| C     | -1.315623 | -1.938195 | 0.152858  |
| H     | -2.161693 | -1.154691 | -1.458486 |
| H     | -0.949021 | -1.053068 | 1.412205  |
| H     | 0.089088  | -0.368390 | -1.429308 |
| H     | 1.391521  | -0.281853 | 1.411983  |
| H     | 2.514076  | -0.685162 | -1.464293 |
| H     | 3.781530  | -0.653812 | 1.380840  |
| H     | 4.285501  | -1.741687 | 0.022202  |
| H     | 4.542863  | 0.045456  | -0.106843 |
| C     | -1.617235 | 2.065495  | 0.419292  |
| C     | -1.496314 | 2.627968  | 1.370690  |
| C     | -2.213061 | 2.680608  | -0.289978 |
| C     | -2.159210 | 1.106709  | 0.624010  |
| S     | -0.048370 | 1.721716  | -0.277287 |

### 7_transtans24hexadienal_1_am1

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.022103|
| AM1 Free Energy (Quasiharmonic)    | 0.073558|
| Number of Imaginary Frequencies    | 0       |

#### Frequencies (Top 3 out of 39)
1. 50.6400 cm⁻¹
2. 96.1091 cm⁻¹
3. 116.1256 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -2.610090 | 0.339895 | -0.000001 |
| C          | -1.304913 | -0.328406| -0.000000 |
| C          | -0.150916 | 0.358426 | -0.000001 |
| C          | 1.148288  | -0.278994| -0.000001 |
| C          | 2.298098  | 0.412251 | 0.000001  |
| C          | 3.631492  | -0.217373| 0.000000  |
| O          | -3.678919 | -0.276279| 0.000001  |
| H          | -2.587603 | 1.454418 | -0.000003 |
| H          | -1.328159 | -1.430737| -0.000000 |
| H          | -0.153602 | 1.464254 | -0.000001 |
| H          | 1.151295  | -1.383055| -0.000003 |
| H          | 2.297934  | 1.515999 | 0.000002  |
| H          | 4.205480  | 0.103924 | 0.905999  |
| H          | 3.568761  | -1.333302| -0.000007 |
| H          | 4.205486  | 0.103936 | -0.905989 |

**7_transtrans24hexadienal_2_am1_HEI**

| Datum                               | Value   |
|-------------------------------------|---------|
| AM1 Energy                          | -0.085897 |
| AM1 Free Energy (Quasiharmonic)     | 0.043559 |
| Number of Imaginary Frequencies     | 0       |

**Frequencies (Top 3 out of 54)**

1. 42.2303 cm⁻¹
2. 51.6123 cm⁻¹
3. 82.1985 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -2.148135 | -1.342076 | -0.351696 |
| C          | -1.011083 | -0.891874 | 0.331245  |
| C          | 0.062334  | -0.218835 | -0.322574 |
### AM1 Energy

AM1 Energy: $-0.022074$

### AM1 Free Energy (Quasiharmonic)

AM1 Free Energy (Quasiharmonic): $0.07348$

### Number of Imaginary Frequencies

Number of Imaginary Frequencies: $0$

### Frequencies (Top 3 out of 39)

1. $66.1883 \text{ cm}^{-1}$
2. $87.6745 \text{ cm}^{-1}$
3. $107.6312 \text{ cm}^{-1}$

### AM1 Molecular Geometry in Cartesian Coordinates

| C     | 2.720489 | 0.299356 | -0.000000 |
|-------|----------|----------|------------|
| C     | 1.333915 | 0.769801 | -0.000000 |
| C     | 0.283354 | -0.069352| 0.000000   |
| C     | -1.091966| 0.378647 | 0.000000   |
| C     | -2.131219| -0.470205| -0.000001  |
| C     | -3.541099| -0.038599| -0.000000  |
| O     | 3.050650 | -0.890959| 0.000000   |
| H     | 3.489570 | 1.105899 | -0.000001  |
| H     | 1.200326 | 1.862903 | -0.000001  |
| H     | 0.454358 | -1.163198| 0.000001   |
| H     | -1.253214| 1.470685 | 0.000001   |
### AM1 Energy

| Datum                  | Value         |
|------------------------|---------------|
| AM1 Energy             | -0.084016     |
| AM1 Free Energy (Quasiharmonic) | 0.045272     |
| Number of Imaginary Frequencies | 0            |

### Frequencies (Top 3 out of 54)

1. 31.4341 cm\(^{-1}\)
2. 56.9131 cm\(^{-1}\)
3. 77.1270 cm\(^{-1}\)

### AM1 Molecular Geometry in Cartesian Coordinates

| C   | -1.839051 | -1.550589 | -0.371570 |
|-----|----------|----------|-----------|
| C   | -0.667043 | -0.943108 | 0.098379  |
| C   | 0.051864  | 0.023003  | -0.658569 |
| C   | 1.512909  | 0.132327  | -0.473138 |
| C   | 2.269513  | -0.740344 | 0.201809  |
| C   | 3.728394  | -0.599658 | 0.373550  |
| O   | -2.537331 | -2.402686 | 0.239001  |
| H   | -2.171395 | -1.246688 | -1.400283 |
| H   | -0.310803 | -1.201765 | 1.100793  |
| H   | -0.210346 | 0.031620  | -1.746734 |
| H   | 1.970749  | 1.019568  | -0.947907 |
| H   | 1.817527  | -1.627609 | 0.675316  |
| H   | 4.124745  | 0.308978  | -0.143226 |
| H   | 3.983058  | -0.520822 | 1.460675  |
| H   | 4.256707  | -1.495682 | -0.039684 |
| C   | -1.793659 | 1.774343  | 0.814186  |
| H   | -1.558314 | 2.235614  | 1.798045  |
| H   | -2.653530 | 2.313142  | 0.359394  |
| H   | -2.068589 | 0.699275  | 0.967290  |
| S   | -0.403670 | 1.883126  | -0.243974 |
### 7_transtrans24hexadienal_3_am1

| Datum                              | Value     |
|------------------------------------|-----------|
| AM1 Energy                         | -0.022103 |
| AM1 Free Energy (Quasiharmonic)    | 0.073542  |
| Number of Imaginary Frequencies    | 0         |

#### Frequencies (Top 3 out of 39)

1. 49.8125 cm⁻¹  
2. 94.9446 cm⁻¹  
3. 115.7269 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -2.610022 | 0.339903 | -0.000019 |
| C | -1.304864 | -0.328403 | 0.000029  |
| C | -0.150869 | 0.358447 | 0.000070  |
| C | 1.148322  | -0.278994 | 0.000109  |
| C | 2.298183  | 0.412192 | 0.000040  |
| C | 3.631168  | -0.217319 | -0.000084 |
| O | -3.678827 | -0.276279 | -0.000077 |
| H | -2.587561 | 1.454402 | 0.000001  |
| H | -1.328120 | -1.430696 | 0.000026  |
| H | -0.153623 | 1.464239 | 0.000071  |
| H | 1.151426  | -1.383015 | 0.000246  |
| H | 2.297869  | 1.515913 | -0.000047 |
| H | 4.204904  | 0.103426 | -0.906438 |
| H | 4.205684  | 0.104262 | 0.905469  |
| H | 3.568531  | -1.333249 | 0.000423  |

### 7_transtrans24hexadienal_4_am1_HEI

| Datum                              | Value     |
|------------------------------------|-----------|
| AM1 Energy                         | -0.079759 |
| AM1 Free Energy (Quasiharmonic)    | 0.049279  |
| Number of Imaginary Frequencies    | 0         |

#### Frequencies (Top 3 out of 54)

1. 49.8125 cm⁻¹  
2. 94.9446 cm⁻¹  
3. 115.7269 cm⁻¹
1. 15.7915 cm⁻¹
2. 41.7560 cm⁻¹
3. 66.4766 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | X (Å)  | Y (Å)  | Z (Å)  |
|------|--------|--------|--------|
| C    | -2.135080 | -1.467010 | 0.450345 |
| C    | -0.83986 | -0.993331 | 0.647998 |
| C    | -0.080858 | -0.319685 | -0.371238 |
| C    | 1.344824 | -0.719633 | -0.438925 |
| C    | 2.363323 | -0.118838 | 0.183738 |
| C    | 3.763555 | -0.577197 | 0.098418 |
| O    | -2.835413 | -1.414422 | -0.599857 |
| H    | -2.591895 | -1.965251 | 1.348194 |
| H    | -0.375612 | -1.117192 | 1.630528 |
| H    | -0.566913 | -0.430896 | -1.376456 |
| H    | 1.516298 | -1.621381 | -1.054272 |
| H    | 2.190662 | 0.780046 | 0.801628 |
| H    | 4.410363 | 0.229074 | -0.330809 |
| H    | 4.152396 | -0.824072 | 1.118490 |
| H    | 3.867920 | -1.486681 | -0.543335 |
| C    | -1.674675 | 1.968223 | 0.237022 |
| H    | -2.246237 | 1.037332 | 0.477015 |
| H    | -1.682353 | 2.644965 | 1.119068 |
| H    | -2.161653 | 2.484738 | -0.618849 |
| S    | -0.017268 | 1.559345 | -0.163531 |

**7_transtrans24hexadienal_4_am1**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.020978     |
| AM1 Free Energy (Quasiharmonic)            | 0.073896      |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 39)

1. 18.3256 cm⁻¹
2. 87.9607 cm⁻¹
3. 103.5453 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
### 7_transttrans24hexadienal_5_am1_HEI

| Datum                              | Value       |
|------------------------------------|-------------|
| AM1 Energy                         | -0.085897   |
| AM1 Free Energy (Quasiharmonic)    | 0.043559    |
| Number of Imaginary Frequencies    | 0           |

#### Frequencies (Top 3 out of 54)

1. 42.2768 cm⁻¹  
2. 51.4706 cm⁻¹  
3. 81.9709 cm⁻¹  

#### AM1 Molecular Geometry in Cartesian Coordinates

|  |  |  |
|---|---|---|
| C | 2.147504 | -1.342576 | 0.351740 |
| C | 1.010846 | -0.891652 | -0.331301 |
| C | -0.062433 | -0.218259 | 0.322407 |
| C | -1.388086 | -0.366968 | -0.312009 |
| C | -2.519324 | -0.598328 | 0.366597 |
| C | -3.842671 | -0.743833 | -0.268330 |
| O | 3.136432 | -1.937456 | -0.153006 |
| H | 2.161957 | -1.155099 | 1.458559 |
| H | 0.949875 | -1.052238 | -1.412367 |
| H | -0.088816 | -0.368940 | 1.429343 |
| H | -1.391222 | -0.282363 | -1.411966 |
| H | -2.513825 | -0.685883 | 1.464280 |
### 7_transtranstrans24hexadienal_5_am1

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.020978 |
| AM1 Free Energy (Quasiharmonic)    | 0.073896 |
| Number of Imaginary Frequencies    | 0       |

**Frequencies** (Top 3 out of 39)

1. 18.3259 cm⁻¹
2. 87.9607 cm⁻¹
3. 103.5453 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

|         |         |         |         |
|---------|---------|---------|---------|
| C       | -2.523946 | 0.158452 | 0.012217 |
| C       | -1.078045 | -0.084206 | -0.018522 |
| C       | -0.187839 | 0.920653 | 0.009006 |
| C       | 1.250248  | 0.773324 | -0.018008 |
| C       | 1.909696  | -0.394739 | 0.024879 |
| C       | 3.379992  | -0.502410 | -0.002831 |
| O       | -3.356441 | -0.751932 | -0.008061 |
| H       | -2.839307 | 1.226733 | 0.055660 |
| H       | -0.773413 | -1.142325 | -0.067155 |
| H       | -0.541942 | 1.968314 | 0.053241 |
| H       | 1.812917  | 1.722693 | -0.075434 |
| H       | 1.370184  | -1.355611 | 0.086863 |
| H       | 3.700862  | -1.111220 | -0.886050 |
| H       | 3.874490  | 0.497890 | -0.066026 |
| H       | 3.742298  | -1.017469 | 0.922951 |

### 7_transtranstrans24hexadienal_6_am1_HEI
### AM1 Molecular Geometry in Cartesian Coordinates

|   | C          | C          | C          | C          | C          | O          | H          | H          | H          | H          | H          | S          |
|---|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|   | -1.992730  | -1.660480  | 0.344489   | -0.909771  | -0.902060  | 0.793626   | 0.005732   | -0.235292  | -0.082857  | 1.409554   | -0.199397  | 0.381324   |
|   | 2.463722   | -0.426932  | -0.412080  | 3.863717   | -0.396626  | 0.051921   | 3.863717   | -0.396626  | 0.051921   | 2.339286   | -1.902748  | -0.843113  |
|   | 3.65008    | 1.164988   | 1.872388   | 0.753662   | -0.802102  | 1.872388   | -0.102301  | -0.565169  | -1.145443  | 1.541966   | 0.020737   | 1.454245   |
|   | -0.753662  | -0.802102  | 1.872388   | 0.753662   | -0.802102  | 1.872388   | -0.102301  | -0.565169  | -1.145443  | 1.541966   | 0.020737   | 1.454245   |
|   | 2.328096   | -0.650592  | -1.481999  | 4.356556   | -1.384599  | -0.132172  | 4.440579   | 0.384782   | -0.504462  | 3.934535   | -0.169772  | 1.144242   |
|   | 4.356556   | -1.384599  | -0.132172  | 4.440579   | 0.384782   | -0.504462  | 3.934535   | -0.169772  | 1.144242   | 4.356556   | -1.384599  | -0.132172  |
|   | 4.440579   | 0.384782   | -0.504462  | 3.934535   | -0.169772  | 1.144242   | 4.356556   | -1.384599  | -0.132172  | 4.440579   | 0.384782   | -0.504462  |
|   | 3.934535   | -0.169772  | 1.144242   | 4.356556   | -1.384599  | -0.132172  | 4.440579   | 0.384782   | -0.504462  | 3.934535   | -0.169772  | 1.144242   |
|   | -1.983708  | 1.863272   | 0.136061   | -2.423949  | 0.883629   | 0.450886   | -2.106325  | 2.603491   | 0.956658   | -2.519353  | 2.231616   | -0.766094  |
|   | -2.423949  | 0.883629   | 0.450886   | -2.106325  | 2.603491   | 0.956658   | -2.519353  | 2.231616   | -0.766094  | -2.106325  | 2.603491   | 0.956658   |
|   | -2.106325  | 2.603491   | 0.956658   | -2.519353  | 2.231616   | -0.766094  | -2.106325  | 2.603491   | 0.956658   | -2.519353  | 2.231616   | -0.766094  |
|   | -2.519353  | 2.231616   | -0.766094  | -2.106325  | 2.603491   | 0.956658   | -2.519353  | 2.231616   | -0.766094  | -2.106325  | 2.603491   | 0.956658   |
|   | -0.281620  | 1.657907   | -0.221452  | -0.281620  | 1.657907   | -0.221452  | -0.281620  | 1.657907   | -0.221452  | -0.281620  | 1.657907   | -0.221452  |
**Frequencies (Top 3 out of 39)**

1. 26.1641 cm⁻¹  
2. 85.6211 cm⁻¹  
3. 106.4550 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C   2.505440  -0.574456  -0.016743
C   1.041640  -0.547403  -0.059399
C   0.338380   0.597725  -0.009183
C  -1.101875   0.706690  -0.047614
C  -1.958328  -0.321472   0.052911
C  -3.424465  -0.169241   0.014783
O   3.217441   0.431664   0.062224
H   2.956989  -1.592322  -0.061429
H   0.552319  -1.530380  -0.139059
H   0.884071   1.559783   0.062336
H  -1.485831   1.736645  -0.162943
H  -1.597451  -1.356891   0.177348
H  -3.873257  -0.553392   0.965859
H  -3.733379   0.897041  -0.114899
H  -3.847741  -0.764859  -0.833535
```

**7_transtrans24hexadienal_7_am1_HEI**

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.075597 |
| AM1 Free Energy (Quasiharmonic)    | 0.053444 |
| Number of Imaginary Frequencies    | 0       |

**Frequencies (Top 3 out of 54)**

1. 40.7924 cm⁻¹  
2. 57.8590 cm⁻¹  
3. 71.7327 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
7_transtrans24hexadienal_7_am1

| Datum                        | Value   |
|------------------------------|---------|
| AM1 Energy                   | -0.020743 |
| AM1 Free Energy (Quasiharmonic) | 0.074417 |
| Number of Imaginary Frequencies | 0       |

Frequencies (Top 3 out of 39)

1. 26.1642 cm⁻¹
2. 85.6212 cm⁻¹
3. 106.4552 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   |       |       |       |
|---|-------|-------|-------|
| C | -2.505440 | -0.574456 | -0.016743 |
| C | -1.041640 | -0.547403 | -0.059399 |
| C | -0.338380 | 0.597725  | -0.009183 |
| C | 1.101875  | 0.796690  | -0.047614 |
| C | 1.958328  | -0.321472 | 0.052911  |
| C | 3.424465  | -0.169241 | 0.014783  |
| O | -3.217441 | 0.431664  | 0.062224  |
7_transttrans24hexadienal_8_am1_HEI

| Datum                          | Value    |
|-------------------------------|----------|
| AM1 Energy                    | -0.082232|
| AM1 Free Energy (Quasiharmonic) | 0.047285 |
| Number of Imaginary Frequencies | 0       |

**Frequencies** (Top 3 out of 54)

1. 32.5298 cm⁻¹
2. 51.8990 cm⁻¹
3. 71.5754 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|       |         |         |         |
|-------|---------|---------|---------|
| C     | 1.517769| 1.894880| 0.339757|
| C     | 0.483131| 0.986600| 0.572516|
| C     | -0.001566| 0.075094| -0.416405|
| C     | -1.449836| -0.221597| -0.451633|
| C     | -2.387944| 0.482008| 0.191543|
| C     | -3.829912| 0.173609| 0.136415|
| O     | 2.161532| 2.089467| -0.727286|
| H     | 1.785772| 2.532005| 1.226139|
| H     | 0.036687| 0.948414| 1.571218|
| H     | 0.383659| 0.318985| -1.439739|
| H     | -1.729187| -1.091439| -1.074402|
| H     | -2.108310| 1.351003| 0.809698|
| H     | -4.043332| -0.711723| -0.511963|
| H     | -4.218216| -0.045082| 1.163176|
| H     | -4.399567| 1.048182| -0.267793|
| C     | 2.216609| -1.537084| 0.520421|
| H     | 2.377793| -0.463403| 0.791709|
| H     | 2.293674| -2.164657| 1.434965|
| H     | 3.000299| -1.853046| -0.202386|
| S     | 0.627436| -1.731627| -0.189876|
### 7_transtrans24hexadienal_9_am1_HEI

| Datum                                                      | Value          |
|------------------------------------------------------------|----------------|
| AM1 Energy                                                 | -0.082638      |
| AM1 Free Energy (Quasiharmonic)                           | 0.047454       |
| Number of Imaginary Frequencies                           | 0              |

#### Frequencies (Top 3 out of 54)

1. 39.3820 cm⁻¹  
2. 65.8771 cm⁻¹  
3. 67.5087 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|         |                  |                  |                  |
|---------|------------------|------------------|------------------|
| C       | 1.199160         | 2.028680         | -0.226344        |
| C       | 1.003522         | 0.929072         | -1.061860        |
| C       | 0.087429         | -0.156321        | -0.879605        |
| C       | -1.095432        | 0.100088         | -0.032953        |
| C       | -2.331773        | -0.311950        | -0.342600        |
| C       | -3.514057        | -0.053381        | 0.500649         |
| O       | 0.629976         | 2.323835         | 0.860235         |
| H       | 1.983421         | 2.745131         | -0.598264        |
| H       | 1.645949         | 0.859256         | -1.949124        |
| H       | -0.189386        | -0.644547        | -1.851093        |
| H       | -0.888965        | 0.691312         | 0.879686         |
| H       | -2.529304        | -0.885372        | -1.261553        |
| H       | -3.251360        | 0.547732         | 1.405809         |
| H       | -4.291114        | 0.507508         | -0.077786        |
| H       | -3.969028        | -1.017988        | 0.840926         |
| C       | 2.190318         | -1.092172        | 0.913147         |
| H       | 1.984266         | -1.257041        | 1.993307         |
| H       | 3.123398         | -1.630271        | 0.636816         |
| H       | 2.324908         | 0.003018         | 0.728111         |
| S       | 0.861400         | -1.698344        | -0.053208        |
Ester Structures (AM1)

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J. Chem. Inf. Model., 2018, 58 (3), pp 561564. 
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1_methylacrylate_1_am1

| Datum                          | Value     |
|--------------------------------|-----------|
| AM1 Energy                     | -0.111754 |
| AM1 Free Energy (Quasiharmonic)| -0.042739 |
| Number of Imaginary Frequencies| 0         |

Frequencies (Top 3 out of 30)

1. 64.7273 cm⁻¹
2. 105.8498 cm⁻¹
3. 156.2156 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|     | x          | y          | z           |
|-----|------------|------------|-------------|
| C   | 2.514027   | 0.004176   | -0.000243   |
| C   | 1.341801   | -0.630855  | 0.000000    |
| C   | 0.070446   | 0.101925   | 0.00162     |
| O   | -1.022280  | -0.726364  | 0.000452    |
| O   | -0.128107  | 1.320526   | 0.000217    |
| C   | -2.302045  | -0.093503  | -0.000243   |
| H   | -3.019472  | -0.950469  | -0.000758   |
| H   | -2.416005  | 0.536895   | 0.913941    |
| H   | -2.415065  | 0.536712   | -0.915028   |
| H   | 2.589027   | 1.102064   | -0.000315   |
| H   | 3.468471   | -0.540034  | -0.000387   |
| H   | 1.250761   | -1.728916  | 0.000086    |
**1_methylacrylate_1_reopt_am1_HEI**

| Datum                                      | Value    |
|--------------------------------------------|----------|
| AM1 Energy                                 | -0.18556 |
| AM1 Free Energy (Quasiharmonic)            | -0.082671|
| Number of Imaginary Frequencies            | 0        |

**Frequencies** (Top 3 out of 45)

1. 32.4607 cm⁻¹
2. 66.1314 cm⁻¹
3. 87.1139 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | 0.966286  | -0.850938  | -0.878882 |
|------------|-----------|------------|-----------|
| C          | 0.006820  | -1.186344  | 0.123217  |
| C          | -1.236957 | -0.573891  | 0.282595  |
| O          | -1.548541 | 0.431015   | -0.653645 |
| O          | -2.150404 | -0.777891  | 1.121036  |
| C          | -2.813348 | 1.042893   | -0.512121 |
| H          | -2.905309 | 1.535872   | 0.486622  |
| H          | -2.854778 | 1.800851   | -1.334037 |
| H          | -3.631742 | 0.290235   | -0.625361 |
| H          | 0.543991  | -0.242816  | -1.711556 |
| H          | 1.515476  | -1.736739  | -1.282021 |
| H          | 0.250755  | -1.969749  | 0.847202  |
| S          | 2.435938  | 0.145771   | -0.296063 |
| C          | 1.838430  | 1.065760   | 1.071433  |
| H          | 0.818334  | 0.700884   | 1.351354  |
| H          | 2.527947  | 0.932999   | 1.933282  |
| H          | 1.784493  | 2.146243   | 0.814938  |

**1_methylacrylate_2_am1_HEI**

| Datum                                      | Value    |
|--------------------------------------------|----------|
| AM1 Energy                                 | -0.185964|
| AM1 Free Energy (Quasiharmonic)            | -0.083141|
| Datum                          | Value          |
|-------------------------------|----------------|
| Number of Imaginary Frequencies | 0             |

**Frequencies (Top 3 out of 45)**

1. 37.1627 cm⁻¹  
2. 62.1105 cm⁻¹  
3. 83.6437 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C   1.158592   -1.218346   0.017424
C  -0.029832   -0.764707  -0.633377
C  -1.148472   -0.332589   0.080666
O  -2.210579    0.096011  -0.744486
O  -1.407421   -0.263520   1.307020
C  -3.383962    0.512003  -0.079213
H  -4.088562    0.800986  -0.898968
H  -3.809131   -0.321047   0.532668
H  -3.173283    1.384192   0.587206
H   1.646025   -2.081437  -0.498096
H   1.005775   -1.441893   1.098796
H  -0.061419   -0.733409  -1.724950
S   2.598530   -0.031182  -0.006115
C   1.860868    1.559196   0.020158
H   2.029585    2.047141  1.004824
H   2.314401    2.186974  -0.777344
H   0.760970    1.464133  -0.160516
```

**1-methylacrylate_2_am1**

| Datum                          | Value          |
|-------------------------------|----------------|
| AM1 Energy                    | -0.111084      |
| AM1 Free Energy (Quasiharmonic) | -0.042211     |
| Number of Imaginary Frequencies | 0             |

**Frequencies (Top 3 out of 30)**

1. 53.5318 cm⁻¹  
2. 109.5252 cm⁻¹  
3. 150.1631 cm⁻¹
AM1 Molecular Geometry in Cartesian Coordinates

C    -2.184665       -0.745815       -0.000034
C    -1.506473        0.400865       -0.000003
C    -0.042373        0.489976        0.000016
O     0.606468       -0.718736        0.000106
O     0.648891        1.512387       -0.000009
C     2.033678       -0.676146       -0.000057
H     2.399004       -0.150323       -0.914749
H     2.399145       -0.150130        0.914478
H     2.329894       -1.753868        0.000039
H    -1.688730       -1.727648       -0.000053
H    -3.283534       -0.768488       -0.000039
H    -1.999652        1.387969        0.000019

1_methylacrylate_3_reopt_am1_HEI

| Datum                                    | Value       |
|------------------------------------------|-------------|
| AM1 Energy                               | -0.18556    |
| AM1 Free Energy (Quasiharmonic)          | -0.082672   |
| Number of Imaginary Frequencies          | 0           |

Frequencies (Top 3 out of 45)

1. 32.4206 cm⁻¹
2. 66.0983 cm⁻¹
3. 87.0716 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

C     0.966359        0.851109        0.878887
C     0.006827        1.186533       -0.123115
C    -1.236894        0.573964       -0.282495
O    -1.548368       -0.431034        0.653679
O    -2.150397        0.777926       -1.120885
C    -2.813064       -1.043116        0.512032
H    -2.904625       -1.536560       -0.486516
H    -2.854669       -1.800707        1.334273
H    -3.631590       -0.290510        0.624655
H     0.544052        0.243219        1.711732
H     1.515720        1.736891        1.281816
### 1_methylacrylate_4_am1_HEI

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.185964   |
| AM1 Free Energy (Quasiharmonic)      | -0.083142   |
| Number of Imaginary Frequencies      | 0           |

#### Frequencies (Top 3 out of 45)

1. 37.1569 cm⁻¹
2. 62.0973 cm⁻¹
3. 83.6094 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

| C       | -1.158598 | -1.218340 | -0.016949 |
|---------|-----------|-----------|-----------|
| C       | 0.029803  | -0.764359 | 0.633659  |
| C       | 1.148487  | -0.332626 | -0.080550 |
| O       | 2.210529  | 0.096447  | 0.744440  |
| O       | 1.407525  | -0.264249 | -1.306921 |
| C       | 3.383971  | 0.512036  | 0.079019  |
| H       | 4.088539  | 0.801409  | 0.898657  |
| H       | 3.809136  | -0.321345 | -0.532407 |
| H       | 3.173374  | 1.383889  | -0.587859 |
| H       | -1.645997 | -2.081200 | 0.498980  |
| H       | -1.005760 | -1.442422 | -1.098202 |
| H       | 0.061347  | -0.732514 | 1.725217  |
| S       | -2.598549 | -0.031190 | 0.005945  |
| C       | -1.860877 | 1.559192  | -0.020463 |
| H       | -0.761051 | 1.464193  | 0.160667  |
| H       | -2.029195 | 2.046878  | -1.005321 |
| H       | -2.314753 | 2.187145  | 0.776699  |

### 1_methylacrylate_5_reopt3_am1_HEI
| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.181937     |
| AM1 Free Energy (Quasiharmonic)            | -0.078611     |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 45)

1. 25.6951 cm⁻¹  
2. 60.5611 cm⁻¹  
3. 81.9644 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|        |       |       |       |
|--------|-------|-------|-------|
| C      | -0.973005 | 0.501776 | -1.118016 |
| C      | 0.296965   | -0.066918 | -0.784496 |
| C      | 1.210722   | 0.602727  | 0.032707  |
| O      | 2.459395   | 0.024083  | 0.354581  |
| O      | 1.162433   | 1.726668  | 0.586388  |
| C      | 2.739852   | -1.251413 | -0.167008 |
| H      | 2.000764   | -2.008845 | 0.195561  |
| H      | 3.762323   | -1.503391 | 0.216186  |
| H      | 2.745948   | -1.238962 | -1.285575 |
| H      | -1.030508  | 1.593180  | -0.898060 |
| H      | -1.292200  | 0.294957  | -2.168741 |
| H      | 0.522781   | -1.061846 | -1.172603 |
| S      | -2.439138  | -0.232708 | -0.234213 |
| C      | -1.854035  | -0.541056 | 1.390385  |
| H      | -2.311945  | 0.174128  | 2.107992  |
| H      | -2.126498  | -1.576820 | 1.688218  |
| H      | -0.742077  | -0.425780 | 1.415237  |

**1_methylacrylate_6_am1_HEI**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.181676     |
| AM1 Free Energy (Quasiharmonic)            | -0.079574     |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 45)

1. 25.6951 cm⁻¹  
2. 60.5611 cm⁻¹  
3. 81.9644 cm⁻¹
1. 39.5511 cm⁻¹
2. 59.4888 cm⁻¹
3. 61.0891 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |             |
|---|---|---|-------------|
| C | -1.011505 | 0.096091 | 0.864191    |
| C | 0.241428  | -0.559519| 0.659366    |
| C | 1.364904  | 0.129065 | 0.196043    |
| O | 2.493500  | -0.697879| 0.011127    |
| O | 1.584937  | 1.339954 | -0.049205   |
| C | 3.669746  | -0.052880| -0.427568   |
| H | 3.501824  | 0.453741 | -1.409492   |
| H | 4.423747  | -0.873446| -0.528551   |
| H | 4.008542  | 0.704596 | 0.321371    |
| H | -1.547349 | -0.234031| 1.786760    |
| H | -0.943758 | 1.208498 | 0.841947    |
| H | 0.315614  | -1.636255| 0.826341    |
| S | -2.131986 | -0.402491| -0.512290   |
| C | -3.649183 | 0.388174 | -0.144889   |
| H | -3.539070 | 1.495815 | -0.135188   |
| H | -4.383373 | 0.106342 | -0.931707   |
| H | -4.044247 | 0.072405 | 0.846915    |

1_methylacrylate_7_am1_HEI

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.181188 |
| AM1 Free Energy (Quasiharmonic)           | -0.079046 |
| Number of Imaginary Frequencies            | 0       |

Frequencies (Top 3 out of 45)

1. 40.1008 cm⁻¹
2. 57.4743 cm⁻¹
3. 67.7840 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
### 1_methylacrylate_8_am1_HEI

| Datum                        | Value   |
|------------------------------|---------|
| AM1 Energy                   | -0.181937 |
| AM1 Free Energy (Quasiharmonic) | -0.078613 |
| Number of Imaginary Frequencies | 0 |

**Frequencies (Top 3 out of 45)**

1. 25.6653 cm⁻¹  
2. 60.5208 cm⁻¹  
3. 81.9234 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C | -0.860618 | -0.293920 | 0.831783 |
| C | 0.242580   | -1.085533 | 0.391821 |
| C | 1.498081   | -0.583179 | 0.043821 |
| O | 1.671764   | 0.803641  | 0.219021 |
| O | 2.530788   | -1.168740 | -0.366661|
| C | 2.936602   | 1.321398  | -0.135409|
| H | 2.851483   | 2.423158  | 0.040117 |
| H | 3.738035   | 0.879679  | 0.506521 |
| H | 3.166972   | 1.107365  | -1.207725|
| H | -0.588106  | 0.747704  | 1.118188 |
| H | -1.455230  | -0.766714 | 1.650873 |
| H | 0.185166   | -2.164032 | 0.270564 |
| S | -2.050943  | -0.165574 | -0.572055|
| C | -3.401314  | 0.733052  | 0.084289 |
| H | -3.097248  | 1.758351  | 0.393215 |
| H | -4.179513  | 0.811812  | -0.706772|
| H | -3.838865  | 0.221739  | 0.971192 |
### 2_tert-butylacrylate_1_am1

| Datum                                              | Value        |
|----------------------------------------------------|--------------|
| AM1 Energy                                         | -0.128603    |
| AM1 Free Energy (Quasiharmonic)                    | 0.019497     |
| Number of Imaginary Frequencies                    | 0            |

**Frequencies (Top 3 out of 57)**

1. 50.0712 cm⁻¹
2. 64.2355 cm⁻¹
3. 95.0063 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C        | 3.499667 | 0.174956 | -0.000001 |
|----------|----------|----------|-----------|
| C        | 2.289815 | 0.734049 | 0.000000  |
| C        | 1.064378 | -0.082790| -0.000000 |
| O        | -0.059596| 0.690086 | 0.000000  |
| O        | 0.976581 | -1.314219| -0.000002 |
| C        | -1.376447| 0.083455 | -0.000000 |
| C        | -2.312205| 1.291543 | 0.000111  |
| C        | -1.586020| -0.745610| -1.256449 |
| C        | -1.585952| -0.745792| 1.256339  |
| H        | 3.643380 | -0.916060| -0.000002 |
| H        | 4.417989 | 0.777979 | -0.000001 |
| H        | 2.128587 | 1.823763 | 0.000001  |
| H        | -2.656021| -1.054840| -1.322444 |
| H        | -1.324800| -0.144627| -2.159757 |
| H        | -0.944778| -1.659697| -1.233612 |
| H        | -3.368647| 0.934785 | 0.000121  |
| H        | -2.132804| 1.916309 | 0.906609  |
| H        | -2.132861| 1.916431 | -0.906314 |
| H        | -2.655936| -1.055083| 1.322317  |
| H        | -0.944664| -1.659844| 1.233359  |
| H        | -1.324738| -0.144921| 2.159724  |
2 tertbutylacrylate_1_reopt_am1_HEI_reopt

| Datum                                    | Value   |
|------------------------------------------|---------|
| AM1 Energy                               | -0.200538 |
| AM1 Free Energy (Quasiharmonic)          | -0.018109 |
| Number of Imaginary Frequencies          | 0       |

Frequencies (Top 3 out of 72)

1. 24.8114 cm$^{-1}$
2. 28.7396 cm$^{-1}$
3. 59.8356 cm$^{-1}$

AM1 Molecular Geometry in Cartesian Coordinates

| C       | 1.896407 | 0.486424 | -1.143991 |
| C       | 1.124029 | 1.344700 | -0.304913 |
| C       | -0.191688| 1.108759 | 0.104339  |
| O       | -0.759453| -0.071605| -0.400842 |
| O       | -0.938694| 1.800948 | 0.839512  |
| C       | -2.105984| -0.425628| -0.087549 |
| C       | -2.321025| -1.751289| -0.826689 |
| C       | -2.296970| -0.647169| 1.407616  |
| C       | -3.096264| 0.607917 | -0.609264 |
| H       | 1.285708 | -0.270734| -1.687277 |
| H       | 2.555982 | 1.039570 | -1.856742 |
| H       | 1.583160 | 2.261082 | 0.078638  |
| H       | -3.309750| -1.072219| 1.603046  |
| H       | -1.523495| -1.356656| 1.785532  |
| H       | -2.188676| 0.322501 | 1.951228  |
| H       | -3.355832| -2.121032| -0.639222 |
| H       | -1.585830| -2.509191| -0.468303 |
| H       | -2.173559| -1.604075| -1.922053 |
| H       | -4.139356| 0.232896 | -0.483257 |
| H       | -2.974203| 1.560015 | -0.048238 |
| H       | -2.905648| 0.801146 | -1.691260 |
| C       | 2.593788 | -0.763850| 1.343521  |
| H       | 2.318122 | -1.829502| 1.500250  |
| H       | 3.379703 | -0.482284| 2.077646  |
| H       | 1.691998 | -0.121504| 1.500161  |
| S       | 3.207125 | -0.528121| -0.281745 |
### 2_tern-butylacrylate_2_am1

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.127898     |
| AM1 Free Energy (Quasiharmonic)            | 0.020043      |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 57)

1. 36.1412 cm⁻¹  
2. 70.9276 cm⁻¹  
3. 83.1618 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -2.873458 | 1.138045 | -0.000000 |
|-----|-----------|----------|------------|
| C   | -2.485984 | -0.136136| 0.000001   |
| C   | -1.081137 | -0.575533| -0.000000  |
| O   | -0.184328 | 0.452685 | -0.000005  |
| O   | -0.686293 | -1.744841| 0.000001   |
| C   | 1.242180  | 0.192142 | 0.000000   |
| C   | 1.848884  | 1.594670 | -0.000093  |
| C   | 1.651115  | -0.558700| 1.256537   |
| C   | 1.651102  | -0.558863| -1.256443  |
| C   | -3.935599 | 1.420472 | 0.000001   |
| C   | -3.198913 | -0.978228| 0.000003   |
| C   | 2.764400  | -0.591233| 1.323190   |
| C   | 1.247649  | -0.042208| 2.159757   |
| H   | 1.258224  | -1.603903| 1.233259   |
| H   | 2.960841  | 1.511113 | -0.000100  |
| H   | 1.520576  | 2.155439 | -0.906714  |
| H   | 1.520597  | 2.155549 | 0.906468   |
| H   | 2.764387  | -0.591452| -1.323076  |
| H   | 1.258164  | -1.604046| -1.233047  |
| H   | 1.247671  | -0.042460| -2.159729  |

### 2_ternbutylacrylate_2_reopt_am1_HEI_reopt

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.201033     |
| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Free Energy (Quasiharmonic)            | -0.018611 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 72)

1. 25.8607 cm⁻¹
2. 33.2063 cm⁻¹
3. 61.1148 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|        | X          | Y          | Z          |
|--------|------------|------------|------------|
| C      | -2.262422  | -1.210975  | 0.147332   |
| C      | -1.025059  | -0.784787  | 0.721445   |
| C      | 0.104376   | -0.525978  | -0.061000  |
| O      | 1.198480   | -0.087199  | 0.707900   |
| O      | 0.310829   | -0.626865  | -1.294496  |
| C      | 2.462789   | 0.163242   | 0.097178   |
| C      | 3.034491   | -1.090575  | -0.552693  |
| C      | 2.385081   | 1.303238   | -0.910746  |
| C      | 3.362931   | 0.582269   | 1.265349   |
| H      | -2.156666  | -1.562165  | -0.905436  |
| H      | -2.799082  | -1.972371  | 0.764297   |
| H      | -0.961584  | -0.634272  | 1.801520   |
| H      | 3.409641   | 1.573570   | -1.259655  |
| H      | 1.762965   | 0.993197   | -1.785190  |
| H      | 1.913495   | 2.195731   | -0.435954  |
| H      | 2.409221   | -1.379416  | -1.432108  |
| H      | 4.082178   | -0.902509  | -0.886611  |
| H      | 3.029755   | -1.931562  | 0.180164   |
| H      | 4.387381   | 0.806408   | 0.887253   |
| H      | 2.944873   | 1.489483   | 1.760757   |
| H      | 3.417649   | -0.239564  | 2.016883   |
| C      | -2.750025  | 1.598083   | -0.135203  |
| H      | -2.983116  | 1.993630   | -1.162938  |
| H      | -3.136846  | 2.330834   | 0.598734   |
| H      | -1.656765  | 1.436965   | 0.038814   |
| S      | -3.605659  | 0.081265   | 0.067642   |

**2_tertbutylacrylate_3_am1_HEI**

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.200538 |
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Free Energy (Quasiharmonic)            | -0.018108   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 72)

1. 24.8366 cm⁻¹  
2. 28.7355 cm⁻¹  
3. 59.8376 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C   -1.896364  0.486231  -1.144049
C   -1.124005 1.344587  -0.305030
C    0.191705 1.108689   0.104264
O    0.759499 -0.071711  -0.400803
O    0.938691 1.800935   0.839404
C    2.106059 -0.425623  -0.826487
C    2.321159 -1.751359  -0.609373
C    3.096253  0.607928  -0.609373
C    2.297108 -0.646966   1.407682
H   -2.555860 1.039304  -1.856932
H   -1.285655 -0.271027  -1.687185
H    4.139379  0.233050  -0.483234
H    2.905674  0.800923  -1.691417
H    2.974049  1.566120  -0.048540
H    1.586064 -2.509281  -0.467941
H    2.173588 -1.604303  -1.921858
H    3.356016 -2.120982  -0.639059
H    3.309897 -1.071987   1.603128
H    2.188833  0.322776   1.951170
H    1.523650 -1.356401   1.785726
C   -2.594058 -0.763621   1.343614
H   -1.691510 -0.121096   1.500336
H   -3.380148 -0.482145   2.077585
H   -2.318214 -1.829207   1.500474
S   -3.207204 -0.528108  -0.281762
```

**2_tert-butylacrylate_3_am1**

| Datum          | Value     |
|----------------|-----------|
| AM1 Energy     | -0.117824 |
| Datum                          | Value        |
|-------------------------------|--------------|
| AM1 Free Energy (Quasiharmonic) | 0.030767     |
| Number of Imaginary Frequencies | 0            |

**Frequencies (Top 3 out of 57)**

1. 39.2989 cm⁻¹  
2. 48.4828 cm⁻¹  
3. 109.8983 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C         | -2.881558 | -0.931187 | -0.188380 |
| C         | -1.650562 | -0.663990 | 0.250243  |
| C         | -1.068126 | 0.679260  | 0.129335  |
| O         | 0.278750  | 0.926468  | 0.138748  |
| O         | -1.710063 | 1.733089  | 0.048771  |
| C         | 1.269023  | -0.108975 | -0.026874 |
| C         | 1.349536  | -0.995600 | 1.209627  |
| C         | 1.024003  | -0.912899 | -1.293756 |
| C         | 2.564692  | 0.695379  | -0.177793 |
| H         | -3.509987 | -0.169806 | -0.674667 |
| H         | -3.333475 | -1.927188 | -0.085347 |
| H         | -1.032091 | -1.423270 | 0.752467  |
| H         | 0.091442  | -1.520411 | -1.216205 |
| H         | 0.928979  | -0.224750 | -2.168138 |
| H         | 1.884468  | -1.602296 | -1.467397 |
| H         | 2.413596  | -1.122282 | 1.525096  |
| H         | 0.787982  | -0.529455 | 2.055199  |
| H         | 0.931299  | -2.011307 | 1.009672  |
| H         | 3.413821  | -0.004447 | -0.356411 |
| H         | 2.476817  | 1.400707  | -1.037764 |
| H         | 2.755606  | 1.286116  | 0.748935  |

**2_tertbutylacrylate_4_reopt_am1_HEI**

| Datum                          | Value        |
|-------------------------------|--------------|
| AM1 Energy                    | -0.201033    |
| AM1 Free Energy (Quasiharmonic) | -0.018611    |
| Number of Imaginary Frequencies | 0            |

**Frequencies (Top 3 out of 72)**
1. 25.8647 cm\(^{-1}\)
2. 33.2002 cm\(^{-1}\)
3. 61.1074 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C           2.262438       -1.210985        0.147318
C           1.025091       -0.784786        0.721456
C          -0.104391       -0.526077       -0.060957
O          -1.198479       -0.087255        0.707953
O          -0.310928       -0.627137       -1.294423
C          -2.462776        0.163276        0.097251
C          -3.362830        0.582503        1.265421
C          -2.384982        1.303184       -0.910766
C          -3.034652       -1.090527       -0.552492
H           2.799154       -1.972300        0.764336
H           2.156637       -1.562289       -0.905411
H           0.961670       -0.634174        1.801521
H          -3.409533        1.573635       -1.259614
H          -1.913230        2.195646       -0.436077
H          -1.762981         0.992996       -1.785241
H          -4.387271         0.806724        0.887344
H          -3.417611        -0.239263        2.017026
H          -2.944652        1.489713        1.760737
H          -2.409486        -1.379495       -1.431940
H          -3.029938        -1.931465        0.180424
H          -4.082351        -0.902381       -0.886337
C           2.750061        1.598144        -0.135207
H           1.656832        1.437132        0.091077
H           3.137149        2.338049        0.598639
H           2.902897        1.993705       -1.162977
S           3.605638         0.081282        0.067379
```

**2_tertbutylacrylate_5_am1_HEI**

| Datum                                           | Value     |
|-------------------------------------------------|-----------|
| AM1 Energy                                      | -0.200538 |
| AM1 Free Energy (Quasiharmonic)                 | -0.018108 |
| Number of Imaginary Frequencies                 | 0         |

**Frequencies** (Top 3 out of 72)
1. 24.8237 cm\(^{-1}\)  
2. 28.7549 cm\(^{-1}\)  
3. 59.8525 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | -1.896386 | 0.486194 | 1.144075 |
| C       | -1.124038 | 1.344597 | 0.305097 |
| C       | 0.191661  | 1.108715 | -0.104249 |
| O       | 0.759452  | -0.071715 | 0.400747 |
| O       | 0.938623  | 1.801002 | -0.839374 |
| C       | 2.106025  | -0.425616 | 0.087499 |
| C       | 2.321107  | -1.751335 | 0.826524 |
| C       | 2.297103  | -0.646999 | -1.407677 |
| C       | 3.096221  | 0.607932 | 0.609371 |
| H       | -1.285683 | -0.271086 | 1.687186 |
| H       | -2.555893 | 1.039243 | 1.856965 |
| H       | -1.583187 | 2.261034 | -0.078301 |
| H       | 3.309974  | -1.071830 | -1.603111 |
| H       | 1.523781  | -1.356610 | -1.785676 |
| H       | 2.188631  | 0.322696 | -1.951214 |
| H       | 3.355923  | -2.121035 | 0.639015 |
| H       | 1.585928  | -2.509226 | 0.468082 |
| H       | 2.173649  | -1.604216 | 1.921903 |
| H       | 4.139333  | 0.232904 | 0.483545 |
| H       | 2.974265  | 1.566029 | 0.048322 |
| H       | 2.905419  | 0.801170 | 1.691334 |
| C       | -2.593861 | -0.763557 | -1.343632 |
| H       | -1.691147 | -0.121220 | -1.500124 |
| H       | -2.318247 | -1.829186 | -1.500607 |
| H       | -3.379779 | -0.481777 | -2.077672 |
| S       | -3.207160 | -0.528174 | 0.281706 |

---

**2_tertbutylacrylate_6_am1.HEI**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.201033 |
| AM1 Free Energy (Quasiharmonic)            | -0.018611 |
| Number of Imaginary Frequencies            | 0       |

**Frequencies** (Top 3 out of 72)
1. 25.8432 cm⁻¹
2. 33.1992 cm⁻¹
3. 61.1080 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | X          | Y          | Z          |
|---|------------|------------|------------|
| C | -2.262423  | -1.210937  | 0.147190   |
| C | -1.025104  | -0.784705  | 0.721354   |
| C | 0.104364   | -0.525881  | -0.061031  |
| O | 1.198391   | -0.086954  | 0.707905   |
| O | 0.310898   | -0.626814  | -1.294509  |
| C | 2.462798   | 0.163225   | 0.097280   |
| C | 2.385325   | 1.303070   | -0.910833  |
| C | 3.362873   | 0.582327   | 1.265475   |
| C | 3.034419   | -1.090762  | -0.552334  |
| H | -2.156616  | -1.562130  | -0.905573  |
| H | -2.799060  | -1.972372  | 0.764131   |
| H | -0.961688  | -0.634190  | 1.801431   |
| H | 4.387356   | 0.806399   | 0.887433   |
| H | 2.944811   | 1.489598   | 1.760773   |
| H | 3.417512   | -0.239439  | 2.017085   |
| H | 3.40933    | 1.573095   | -1.259831  |
| H | 1.763094   | 0.993027   | -1.785194  |
| H | 1.913976   | 2.195758   | -0.436174  |
| H | 2.409328   | -1.379555  | -1.431890  |
| H | 4.082232   | -0.902935  | -0.885990  |
| H | 3.029321   | -1.931684  | 0.180594   |
| C | -2.750019  | 1.598056   | -0.135162  |
| H | -1.656723  | 1.436838   | 0.038538   |
| H | -2.903344  | 1.993905   | -1.162744  |
| H | -3.136618  | 2.337811   | 0.599087   |
| S | -3.605701  | 0.081228   | 0.067470   |

**2_tertbutylacrylate_7_am1_HEI**

| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| AM1 Energy                                 | -0.196262              |
| AM1 Free Energy (Quasiharmonic)            | -0.014577              |
| Number of Imaginary Frequencies            | 0                      |

**Frequencies** (Top 3 out of 72)
1. 26.1312 cm⁻¹
2. 37.7033 cm⁻¹
3. 48.6430 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   | C       | O       | C       | O       | C       | H       | C       | C       | C       | H       | H       | H       | H       | H       | H       | H       | H       | C       | H       | H       | H       | S       |
|---|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
|   | -1.828256 | 0.422325 | -0.848580 | -0.902934 | 1.405988 | -0.386672 | 0.439718 | 1.166025 | -0.076793 | 0.876188 | -0.142676 | -0.339237 | 1.316768 | 1.955139 | 0.352734 | 2.198946 | -0.551417 | 0.005798 | 2.236272 | -2.038119 | -0.366443 |
|   | 3.247748 | 0.196876 | -0.807754 | 2.465730 | -0.400250 | 1.497928 | -2.528209 | 0.797483 | -1.634295 | -1.353722 | -0.525963 | -1.190079 | -1.257640 | 2.426573 | -0.214626 | 4.256181 | -0.244856 | 0.4717234 | 3.006360 | 0.123716 | -1.894358 |
|   | 3.254453 | 1.274759 | -0.515013 | 3.241011 | -2.458737 | -0.129172 | 1.457244 | -2.592003 | 0.207760 | 2.031341 | -2.163071 | -1.455287 | 3.441937 | -0.872271 | 1.760141 | 2.490267 | 0.682678 | 1.770482 | 1.651086 | -0.894868 | 2.077837 |
|   | -4.080168 | -1.144288 | -0.111807 | -4.804276 | -1.418918 | 0.686827 | -4.637197 | -0.696855 | -0.965611 | -3.577485 | -2.068628 | -0.475149 | -2.929833 | -0.013223 | 0.565984 |

2_tertbutylacrylate_8_reopt_am1_HEI

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.196801 |
| AM1 Free Energy (Quasiharmonic)            | -0.01516 |
| Number of Imaginary Frequencies            | 0       |

Frequencies (Top 3 out of 72)
1. 27.3546 cm\(^{-1}\)
2. 39.1447 cm\(^{-1}\)
3. 46.5256 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -2.140516 | -0.398273 | 0.815280 |
| C | -0.864114 | 0.235867 | 0.919050 |
| C | 0.268421 | -0.285666 | 0.284043 |
| O | 1.406439 | 0.519526 | 0.475289 |
| O | 0.449949 | -1.339045 | -0.372323 |
| C | 2.662803 | 0.148236 | -0.088085 |
| C | 3.607877 | 1.279448 | 0.333622 |
| C | 3.170594 | -1.169304 | 0.484628 |
| C | 2.601845 | 0.085550 | -1.609107 |
| H | -2.095297 | -1.429244 | 0.393728 |
| H | -2.719807 | -0.402666 | 1.770075 |
| H | -0.775695 | 1.174593 | 1.469917 |
| H | 4.217198 | -1.354054 | 0.145340 |
| H | 3.149482 | -1.129922 | 1.599229 |
| H | 2.514893 | -2.007002 | 0.144147 |
| H | 4.629339 | 1.083663 | -0.067627 |
| H | 3.235024 | 2.252826 | -0.062335 |
| H | 3.653404 | 1.342308 | 1.445897 |
| H | 2.178970 | 1.037146 | -2.009191 |
| H | 3.625861 | -0.064037 | -2.025687 |
| H | 1.942543 | -0.758474 | -1.926687 |
| C | -4.721370 | -0.199816 | -0.349590 |
| H | -5.165842 | -0.248565 | 0.669974 |
| H | -5.403417 | 0.376578 | -1.013020 |
| H | -4.634773 | -1.239438 | -0.737877 |
| S | -3.169764 | 0.609136 | -0.334916 |

**3_methylcrotonate_1_am1_HEI**

| Datum                               | Value   |
|-------------------------------------|---------|
| AM1 Energy                          | -0.192289 |
| AM1 Free Energy (Quasiharmonic)     | -0.06335 |
| Number of Imaginary Frequencies     | 0       |

**Frequencies** (Top 3 out of 54)
1. 38.9290 cm⁻¹
2. 60.5975 cm⁻¹
3. 70.6560 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|       |          |          |          |
|-------|----------|----------|----------|
| C     | -1.096570| -0.810800| 0.274709 |
| C     | 0.123937 | -0.660346| -0.459531|
| C     | 1.308804 | -0.247632| 0.152275 |
| O     | 2.392673 | -0.132830| -0.744206|
| O     | 1.608774 | 0.025654 | 1.340121 |
| C     | 3.628335 | 0.247904 | -0.177477|
| H     | 3.960871 | -0.498114| 0.585397 |
| H     | 4.339988 | 0.276429 | -1.040405|
| H     | 3.549868 | 1.253310 | 0.304355 |
| H     | -0.932006| -0.802672| 1.380959 |
| C     | -1.953402| -1.974383| -0.149070|
| H     | 0.127237 | -0.853856| -1.534645|
| H     | -1.467242| -2.931446| 0.163906 |
| H     | -2.964719| -1.919834| 0.324339 |
| H     | -2.079779| -1.991009| -1.258204|
| S     | -2.331007| 0.616093 | 0.047414 |
| C     | -1.329317| 2.025876 | -0.234111|
| H     | -1.694960| 2.562792 | -1.136406|
| H     | -1.376660| 2.712384 | 0.639291 |
| H     | -0.268779| 1.708220 | -0.395309|

3_methylcrotonate_1_am1

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.128575|
| AM1 Free Energy (Quasiharmonic)    | -0.033628|
| Number of Imaginary Frequencies    | 0       |

**Frequencies** (Top 3 out of 39)

1. 59.4071 cm⁻¹
2. 99.5100 cm⁻¹
3. 112.7452 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
3_methylcrotonate_2_am1_HEI

| Datum                              | Value         |
|------------------------------------|---------------|
| AM1 Energy                         | -0.191898     |
| AM1 Free Energy (Quasiharmonic)    | -0.062883     |
| Number of Imaginary Frequencies    | 0             |

**Frequencies** (Top 3 out of 54)

1. 34.0248 cm⁻¹
2. 57.1702 cm⁻¹
3. 82.5991 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C     | 1.902525 | 0.794302 | -0.537398 | -1.549133 | -0.850799 | -2.881605 | -3.517521 | -3.053281 | -3.053091 | 1.830572 | 3.267256 | 0.813325 | 3.821351 | 3.266291 | 3.821322 |
|-------|----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|----------|----------|-----------|----------|-----------|----------|
|       | 0.303453 | -0.448878| 0.160697  | -0.765943 | 1.355777  | -0.254078 | -1.173306 | 0.363013  | 0.363171  | 1.407125  | -0.253866 | -1.549994 | 0.100260  | -1.371544 | 0.100229 |
| H     | 0.00017  | 0.00029  | 0.00076   | 0.00030   | 0.000077  | 0.00077   | -0.000230 | 0.914482  | -0.914568 | -0.00033 | -0.00028 | 0.00037  | 0.906285  | -0.00009  | -0.906370 |
| H     | -0.00015 | 0.00017  | 0.00030   | 0.000077  | 0.000077  | 0.00077   | -0.000230 | 0.914482  | -0.914568 | -0.00033 | -0.00028 | 0.00037  | 0.906285  | -0.00009  | -0.906370 |
3_methylcrotonate_2_am1

### Datum

|                | Value    |
|----------------|----------|
| AM1 Energy     | -0.127879 |
| AM1 Free Energy (Quasiharmonic) | -0.033089 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 39)

1. 53.0971 cm⁻¹
2. 99.4099 cm⁻¹
3. 114.0481 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

|    |        |        |        |
|----|--------|--------|--------|
| C  | 1.681962 | -0.405366 | -0.000021 |
| C  | 0.857360 | 0.648921  | 0.000030  |
| C  | -0.602627| 0.541447  | -0.000014 |
| O  | -1.086497| -0.743383 | -0.000090 |
| O  | -1.425428| 1.461883  | -0.000023 |
| C  | -2.506492| -0.889427 | 0.000069  |
| H  | -2.658429| -1.996757 | 0.000410  |
| H  | -2.938326| -0.416072 | 0.914491  |
| H  | -2.938374| -0.416615 | -0.914608 |
| H  | 1.281420 | -1.435687 | -0.000100 |
| C  | 3.152083 | -0.289028 | 0.000021  |
| H  | 1.219551 | 1.690737  | 0.000107  |
| H  | 3.572554 | -0.794451 | -0.906316 |
| H  | 3.490778 | 0.776134  | 0.000103  |
| H  | 3.572512 | -0.794576 | 0.906307  |

3_methylcrotonate_3_am1_HEI
### Datum Value

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.188816   |
| AM1 Free Energy (Quasiharmonic)            | -0.05945    |
| Number of Imaginary Frequencies            | 0           |

### Frequencies (Top 3 out of 54)

1. 33.5335 cm⁻¹  
2. 47.1911 cm⁻¹  
3. 83.8195 cm⁻¹  

### AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 0.979197 | 0.741333 | 0.778790 |
| C | -0.044867 | -0.179327 | 1.156489 |
| C | -1.305701 | -0.376980 | 0.589724 |
| O | -1.669842 | 0.459316 | -0.479986 |
| O | -2.203468 | -1.199686 | 0.903266 |
| C | -2.950129 | 0.238064 | -1.036335 |
| H | -3.747378 | 0.404729 | -0.271234 |
| H | -3.030813 | 0.986558 | -1.863891 |
| H | -3.034736 | -0.803098 | -1.433121 |
| H | 1.587005  | 1.064184 | 1.665770  |
| C | 0.584695  | 1.932098 | -0.046635 |
| H | 0.184381  | -0.857113 | 1.989031 |
| H | 1.453108  | 2.620456 | -0.189614 |
| H | 0.213383  | 1.612282 | -1.050601 |
| H | -0.239638 | 2.490328 | 0.462734  |
| S | 2.417204  | -0.061623 | -0.190799 |
| C | 1.752630  | -1.532012 | -0.873516 |
| H | 2.395883  | -2.393472 | -0.590037 |
| H | 0.717728  | -1.697411 | -0.481212 |
| H | 1.717342  | -1.457574 | -1.982383 |

### 3_methylcrotonate_3_am1

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.120201   |
| AM1 Free Energy (Quasiharmonic)            | -0.025379   |
| Number of Imaginary Frequencies            | 0           |
**Frequencies (Top 3 out of 39)**

1. 17.1486 cm⁻¹
2. 104.7923 cm⁻¹
3. 109.9726 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 1.760311 | 0.237067 |
| C | 0.521428 | -0.276064 |
| C | -0.653980 | 0.598720 |
| O | -1.932928 | 0.091934 |
| O | -0.657252 | 1.833757 |
| C | -2.107036 | -1.317291 |
| H | -3.219777 | -1.446734 |
| H | -1.662681 | -1.770835 |
| H | -1.662970 | -1.770844 |
| H | 1.909166 | 1.333724 |
| C | 2.986689 | -0.580329 |
| H | 0.347682 | -1.362314 |
| H | 3.600221 | -0.342576 |
| H | 2.765174 | -1.675765 |
| H | 3.600154 | -0.342796 |

**3_methylcrotonate_4_am1_HEI**

| Datum                                      | Value    |
|--------------------------------------------|----------|
| AM1 Energy                                 | -0.187792|
| AM1 Free Energy (Quasiharmonic)            | -0.059195|
| Number of Imaginary Frequencies            | 0        |

**Frequencies (Top 3 out of 54)**

1. 42.8879 cm⁻¹
2. 58.3373 cm⁻¹
3. 65.3842 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
### 3_methylcrotonate_5_reopt3_am1_HEI

| Datum                              | Value            |
|------------------------------------|------------------|
| AM1 Energy                         | -0.188816        |
| AM1 Free Energy (Quasiharmonic)    | -0.059455        |
| Number of Imaginary Frequencies    | 0                |

**Frequencies** (Top 3 out of 54)

1. 33.4622 cm\(^{-1}\)
2. 47.1639 cm\(^{-1}\)
3. 83.6736 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C       | 0.889370 | 0.607174 | 0.280483 |
|---------|----------|----------|----------|
| C       | -0.375817| 0.632187 | -0.396591|
| C       | -1.519058| 0.061678 | 0.167331 |
| O       | -2.652535| 0.132728 | -0.670296|
| O       | -1.751776| -0.462194| 1.283663 |
| C       | -3.846528| -0.405797| -0.144296|
| H       | -4.601873| -0.272687| -0.959014|
| H       | -3.718155| -1.487831| 0.104099 |
| H       | -4.157560| 0.146369 | 0.776488 |
| H       | 0.883350 | 0.292070 | 1.350696 |
| C       | 1.688894 | 1.878703 | 0.159888 |
| H       | -0.438822| 1.069468 | -1.395051|
| H       | 2.706707 | 1.755047 | 0.604907 |
| H       | 1.801840 | 2.175826 | -0.910219|
| H       | 1.164799 | 2.705263 | 0.700220 |
| S       | 1.843777 | -0.747311| -0.560709|
| C       | 3.349958 | -0.920280| 0.314067 |
| H       | 3.179447 | -0.923618| 1.413859 |
| H       | 3.808637 | -1.889184| 0.015757 |
| H       | 4.064768 | -0.100015| 0.077378 |

| Datum                              | Value            |
|------------------------------------|------------------|
| AM1 Energy                         | -0.188816        |
| AM1 Free Energy (Quasiharmonic)    | -0.059455        |
| Number of Imaginary Frequencies    | 0                |

**Frequencies** (Top 3 out of 54)

1. 33.4622 cm\(^{-1}\)
2. 47.1639 cm\(^{-1}\)
3. 83.6736 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C       | 0.979191 | -0.741325 | -0.778770 |
|---------|----------|----------|----------|
| C       | -0.044906| 0.179246 | -1.156589|
| C       | -1.385725| 0.376912 | -0.589819|
| O       | -1.669728| -0.459226| 0.480071 |
| O       | -2.203565| 1.199492 | -0.903469|
| C       | -2.950020| -0.238010| 1.036416 |
| H       | -3.030516| -0.986173| 1.864273 |
### 3_methylcrotonate_6_am1_HEI

| Datum                                    | Value         |
|------------------------------------------|---------------|
| AM1 Energy                               | -0.188281     |
| AM1 Free Energy (Quasiharmonic)          | -0.058835     |
| Number of Imaginary Frequencies          | 0             |

**Frequencies** (Top 3 out of 54)

1. 26.8692 cm\(^{-1}\)
2. 53.4528 cm\(^{-1}\)
3. 78.1351 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C  | 0.952951  | 0.793279  | 0.378084  |
|----|-----------|-----------|-----------|
| C  | -0.364266 | 0.582180  | -0.149321 |
| C  | -1.368450 | -0.024169 | 0.609384  |
| O  | -2.657408 | -0.237177 | 0.071240  |
| O  | -1.376553 | -0.449401 | 1.788892  |
| C  | -2.881979 | 0.161340  | -1.258746 |
| C  | -2.744943 | 1.265082  | -1.378744 |
| H  | -2.283107 | -0.379947 | -1.964071 |
| H  | -3.947697 | -0.114587 | -1.468149 |
| H  | 0.092827  | 0.648091  | 1.486516  |
| C  | 1.602862  | 2.087943  | -0.033819 |
| H  | -0.553008 | 0.893924  | -1.178174 |
| H  | 2.682258  | 2.104096  | 0.256864  |
| H  | 1.529623  | 2.236066  | -1.138027 |
| H  | 1.087536  | 2.942475  | 0.470437  |
### 3_methylcrotonate_7_am1_HEI

| Datum                                      | Value  |
|--------------------------------------------|--------|
| AM1 Energy                                 | -0.187286 |
| AM1 Free Energy (Quasiharmonic)            | -0.058627 |
| Number of Imaginary Frequencies            | 0      |

#### Frequencies (Top 3 out of 54)

1. 40.7085 cm⁻¹
2. 55.3036 cm⁻¹
3. 72.9681 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

| C   | 0.756276 | 0.521337 | 0.424525 |
|-----|----------|----------|----------|
| C   | -0.352130 | 0.997839 | -0.349808 |
| C   | -1.634509 | 0.446175 | -0.328265 |
| O   | -1.837011 | -0.598607 | 0.594291 |
| O   | -2.669065 | 0.754316 | -0.970567 |
| C   | -3.128277 | -1.169637 | 0.612831 |
| H   | -3.397800 | -1.574741 | -0.393109 |
| H   | -3.063578 | -1.992584 | 1.368135 |
| H   | -3.890608 | -0.411493 | 0.918729 |
| H   | 0.457776  | -0.192108 | 1.232291 |
| C   | 1.644672  | 1.606391 | 0.977061 |
| H   | -0.193136 | 1.827380 | -1.044694 |
| H   | 2.549936  | 1.171631 | 1.467688 |
| H   | 1.976678  | 2.297784 | 0.165923 |
| H   | 1.082191  | 2.202247 | 1.737580 |
| S   | 1.764526  | -0.485085 | -0.771224 |
| C   | 3.078016  | -1.192048 | 0.144503 |
| H   | 3.871825  | -0.446330 | 0.376014 |
| H   | 2.715499  | -1.620157 | 1.105723 |
| H   | 3.523126  | -2.006274 | -0.469573 |
### 3_methylcrotonate_8_reopt_am1_HEI_reopt

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.19044    |
| AM1 Free Energy (Quasiharmonic)            | -0.061359   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 54)**

1. 37.5280 cm⁻¹
2. 50.8567 cm⁻¹
3. 64.8926 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 1.129815 | 0.813030 | 0.645806 |
|-----|----------|----------|----------|
| C   | -0.129882| 0.201615 | 0.939120 |
| C   | -1.247765| 0.219298 | 0.103120 |
| O   | -2.342344| -0.495624| 0.639980 |
| O   | -1.497022| 0.738704 |-1.011713 |
| C   | -3.522417| -0.499307| -0.134333|
| H   | -3.340153| -0.969156| -1.131949|
| H   | -4.251137| -1.104427| 0.461318 |
| H   | -3.901478| 0.541365 |-0.284204 |
| H   | 1.654276 | 1.147320 | 1.579969 |
| C   | 1.134899 | 1.906805 |-0.384120 |
| H   | -0.213173| -0.355605| 1.878259 |
| H   | 2.177721 | 2.240311 |-0.604832 |
| H   | 0.653783 | 1.556465|-1.330525 |
| H   | 0.550789 | 2.782668 | 0.006170 |
| S   | 2.466113 | -0.419149| 0.071985 |
| C   | 1.589446 | -1.782628| -0.592945|
| H   | 1.948732 | -2.719818| -0.114557|
| H   | 0.494974 | -1.661013| -0.395141|
| H   | 1.758203 | -1.849244| -1.689952|

### 4_methylnmethacrylate_1_am1

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.122128   |
| AM1 Free Energy (Quasiharmonic)            | -0.027479   |
### datnum

| Datum                          | Value     |
|-------------------------------|-----------|
| Number of Imaginary Frequencies | 0         |

**Frequencies** (Top 3 out of 39)

1. 16.8333 cm\(^{-1}\)
2. 65.9829 cm\(^{-1}\)
3. 107.4095 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|        |          |          |          |
|--------|----------|----------|----------|
| C      | 1.408626 | 1.551213 | 0.075878 |
| C      | 1.160591 | 0.238666 | 0.006574 |
| C      | -0.212607| -0.299396| 0.029831 |
| O      | -1.194990| 0.653712 | -0.067255|
| O      | -0.568209| -1.477253| 0.124284 |
| C      | -2.543161| 0.183740 | -0.046825|
| H      | -3.149439| 1.118277 |-0.138292 |
| H      | -2.719617| -0.505448| -0.907353|
| H      | -2.747726| -0.345619| 0.914705 |
| H      | 0.605200 | 2.298385 | 0.144653 |
| H      | 2.432720 | 1.948981 | 0.067210 |
| C      | 2.220988 | -0.793219| -0.093482|
| H      | 2.183041 | -1.283133| -1.098918|
| H      | 3.233342 | -0.343620| 0.049196 |
| H      | 2.061445 | -1.585511| 0.680708 |

**4_methylmethacrylate_1_reopt_am1_HEI_reopt**

| Datum                          | Value     |
|-------------------------------|-----------|
| AM1 Energy                    | -0.19663  |
| AM1 Free Energy (Quasiharmonic) | -0.068012 |
| Number of Imaginary Frequencies | 0         |

**Frequencies** (Top 3 out of 54)

1. 20.2413 cm\(^{-1}\)
2. 45.2970 cm\(^{-1}\)
3. 59.1946 cm\(^{-1}\)
AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | 1.159949 | 0.491007 | -1.045466|
| C    | -0.031557| 0.794183 | -0.297182|
| C    | -1.126768| -0.079737| -0.362287|
| O    | -2.235569| 0.290284 | 0.423964 |
| O    | -1.309242| -1.138639| -1.011844|
| C    | -3.366259| -0.552252| 0.336448 |
| H    | -3.115220| -1.587353| 0.674752 |
| H    | -4.120211| -0.083864| 1.017585 |
| H    | -3.750057| -0.592561| -0.712294|
| H    | 0.975231 | -0.254201| -1.854373|
| H    | 1.662338 | 1.401407 | -1.454747|
| C    | -0.061208| 2.007079 | 0.532633 |
| H    | 0.398645 | 2.873614 | -0.010647|
| H    | -1.107136| 2.288141 | 0.810796 |
| H    | 0.519768 | 1.867510 | 1.482337 |
| C    | 1.840469 | -1.210432| 1.154111 |
| H    | 0.742093 | -1.004850| 1.188691 |
| H    | 2.004477 | -2.288990| 0.939564 |
| H    | 2.294214 | -0.963564| 2.138549 |
| S    | 2.585412 | -0.222972| -0.089170|

4_methylmethacrylate_2_am1_HEI_reopt

| Datum                                | Value      |
|--------------------------------------|------------|
| AM1 Energy                           | -0.196996  |
| AM1 Free Energy (Quasiharmonic)      | -0.068232  |
| Number of Imaginary Frequencies      | 0          |

Frequencies (Top 3 out of 54)

1. 19.1799 cm⁻¹
2. 65.9393 cm⁻¹
3. 76.1965 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | -0.935043| 0.214973 | -1.135635|
| C    | -0.001331| 0.938820 | -0.318900|
| C    | 1.256733 | 0.430276 | 0.037026 |
| O    | 1.557162 | -0.846290| -0.474270|
### 4_methylmethacrylate_2_am1

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| AM1 Energy                                 | -0.1223      |
| AM1 Free Energy (Quasiharmonic)            | -0.027164    |
| Number of Imaginary Frequencies            | 0            |

#### Frequencies (Top 3 out of 39)

1. 34.7745 cm⁻¹
2. 103.2036 cm⁻¹
3. 109.2900 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -2.163182 | -0.903750 | 0.000155 |
| C | -1.204730 | 0.031332  | 0.000012 |
| O | 0.210566  | -0.384471 | -0.000048 |
| O | 1.100867  | 0.658045  | 0.000094 |
| C | 0.670531  | -1.530662 | -0.000187 |
| C | 2.486301  | 0.310784  | 0.000078 |
| H | 3.005348  | 1.300680  | 0.000093 |
| H | 2.731143  | -0.280898 | 0.914689 |
| H | 2.731168  | -0.280864 | -0.914546 |
| H | -1.928767 | -1.978442 | 0.000225 |
| H | -3.229000 | -0.642613 | 0.000206 |
| C | -1.474896 | 1.487123  | -0.000107 |
### 4_methylmethacrylate_3_am1_HEI

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| AM1 Energy                                 | -0.196619    |
| AM1 Free Energy (Quasiharmonic)            | -0.068186    |
| Number of Imaginary Frequencies            | 0            |

#### Frequencies (Top 3 out of 54)

1. 20.4133 cm⁻¹
2. 30.8755 cm⁻¹
3. 60.5212 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|   |      |      |      |
|---|------|------|------|
| C | -1.164496 | 0.534608 | 1.012152 |
| C | 0.036488  | 0.813710 | 0.268472 |
| C | 1.119898  | -0.071896 | 0.351063 |
| O | 2.254385  | 0.293444  | -0.400029 |
| O | 1.271106  | -1.142867 | 0.989836 |
| C | 3.360632  | -0.581296 | -0.316708 |
| H | 3.088603  | -1.599994 | -0.687020 |
| H | 4.138378  | -0.115156 | -0.972184 |
| H | 3.724893  | -0.659670 | 0.736848 |
| H | -0.992714 | -0.193265 | 1.839326 |
| H | -1.662609 | 1.458779  | 1.394944 |
| C | 0.085857  | 2.032381  | -0.551758 |
| H | -0.808273 | 2.096750  | -1.225241 |
| H | 0.080586  | 2.952762  | 0.091121 |
| H | 1.004055  | 2.066193  | -1.187901 |
| C | -1.837221 | -1.320377 | -1.052900 |
| H | -2.226148 | -1.141205 | -2.078814 |
| H | -0.728605 | -1.178110 | -1.045166 |
| H | -2.074317 | -2.364412 | -0.752807 |
| S  | -2.584670 | -0.185630 | 0.056657 |

4_methylmethacrylate_3_am1
| Datum                              | Value            |
|-----------------------------------|------------------|
| AM1 Energy                        | -0.112769        |
| AM1 Free Energy (Quasiharmonic)   | -0.01791         |
| Number of Imaginary Frequencies   | 0                |

**Frequencies (Top 3 out of 39)**

1. 40.1635 cm⁻¹
2. 95.7542 cm⁻¹
3. 102.2911 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| X   | Y   | Z   |
|-----|-----|-----|
| C   | -1.313309 | -0.738686 | -1.232310 |
| C   | -0.908889 | -0.090703 | -0.137136 |
| C   | 0.340309  | 0.703759  | -0.124118 |
| O   | 1.553579  | 0.089796  | 0.082517  |
| O   | 0.447794  | 1.920629  | -0.268788 |
| C   | 1.544747  | -1.318469 | 0.283471  |
| H   | 2.623290  | -1.574985 | 0.436036  |
| H   | 0.942240  | -1.579022 | 1.187670  |
| H   | 1.135895  | -1.837773 | -0.617443 |
| H   | -0.734476 | -0.742898 | -2.165885 |
| H   | -2.257317 | -1.299900 | -1.260281 |
| C   | -1.678134 | -0.048079 | 1.129351  |
| H   | -1.919872 | 1.013062  | 1.392074  |
| H   | -2.633407 | -0.620528 | 1.039068  |
| H   | -1.075675 | -0.488294 | 1.963383  |

**4_methylmethacrylate_4_reopt_am1_HEI**

| Datum                              | Value            |
|-----------------------------------|------------------|
| AM1 Energy                        | -0.196996        |
| AM1 Free Energy (Quasiharmonic)   | -0.068231        |
| Number of Imaginary Frequencies   | 0                |

**Frequencies (Top 3 out of 54)**

1. 19.1912 cm⁻¹
2. 65.9432 cm⁻¹
3.  76.2419 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|  | x   | y   | z   |
|---|-----|-----|-----|
| C | 0.935023 | 0.214900 | 1.135661 |
| C | 0.001335  | 0.938791  | 0.318936  |
| C | -1.256734 | 0.430276  | -0.037018 |
| O | -1.557184 | -0.846304 | 0.474233  |
| O | -2.182502 | 0.920396  | -0.729418 |
| C | -2.828024 | -1.366162 | 0.141515  |
| H | -2.859074 | -2.370392 | 0.633625  |
| H | -3.640164 | -0.706354 | 0.533959  |
| H | -2.938129 | -1.463441 | -0.966301 |
| H | 0.458498  | -0.609067 | 1.715420  |
| H | 1.525267  | 0.878939  | 1.813903  |
| C | 0.377158  | 2.276296  | -0.169545 |
| H | 0.624164  | 2.961128  | 0.683801  |
| H | 1.285377  | 2.225014  | -0.825255 |
| H | -0.454166 | 2.737984  | -0.757961 |
| C | 1.718662  | -0.998378 | -1.345100 |
| H | 1.601085  | -2.097586 | -1.463953 |
| H | 0.725886  | -0.502990 | -1.486007 |
| H | 2.429676  | -0.625285 | -2.114045 |
| S | 2.342159  | -0.624689 | 0.250475  |

4_methylmethacrylate_5_am1_HEI

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.192043 |
| AM1 Free Energy (Quasiharmonic)      | -0.063896 |
| Number of Imaginary Frequencies      | 0         |

Frequencies (Top 3 out of 54)

1.  33.8345 cm⁻¹
2.  42.6979 cm⁻¹
3.  55.4077 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
### 4_methylmethacrylate_6_am1_HEI

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.192364   |
| AM1 Free Energy (Quasiharmonic)      | -0.064092   |
| Number of Imaginary Frequencies      | 0           |

#### Frequencies (Top 3 out of 54)

1. 35.6308 cm⁻¹
2. 56.7394 cm⁻¹
3. 69.2218 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

| C         | -0.866514 | 0.167550 | 0.779214 |
|-----------|-----------|----------|----------|
| C         | 0.267188  | 0.903195 | 0.295654 |
| C         | 1.497508  | 0.296047 | -0.00526 |
| O         | 1.568278  | -1.084273| 0.266039 |
| O         | 2.573486  | 0.775378 | -0.434540|
| C         | 2.793144  | -1.715014| -0.045791|
| H         | 3.622673  | -1.293871| 0.573789 |
| Datum                                      | Value |
|-------------------------------------------|-------|
| AM1 Energy                                | -0.201554 |
| AM1 Free Energy (Quasiharmonic)           | -0.046251 |
| Number of Imaginary Frequencies           | 0     |

**Frequencies** (Top 3 out of 63)

1. 28.4092 cm⁻¹  
2. 54.3013 cm⁻¹  
3. 71.6830 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -1.094249 | -0.527325 | 0.640770 |
|-----|-----------|-----------|----------|
| C   | 0.118997  | -0.663644 | -0.130527|
| C   | 1.289571  | -0.046585 | 0.336660 |
| O   | 2.428084  | -0.228256 | -0.472212|
| O   | 1.514610  | 0.638565  | 1.364936 |
| C   | 3.618793  | 0.376468  | -0.010682|
| H   | 3.495624  | 1.484437  | 0.067131 |
| H   | 3.907965  | -0.031260 | 0.988773 |
| H   | 4.384821  | 0.115165  | -0.783140|
| H   | -0.882518 | -0.128913 | 1.665747 |
| C   | -1.966413 | -1.753096 | 0.705549 |
| C   | 0.104303  | -1.440186 | -1.378423|
| H   | 1.029525  | -1.267723 | -1.981618|
| H   | 0.032684  | -2.541390 | -1.179060|
| H   | -0.780519 | -1.164116 | -2.009316|
5_methyltiglate_1_am1_reopt

**Datum** | **Value**
---|---
AM1 Energy | -0.137258
AM1 Free Energy (Quasiharmonic) | -0.016343
Number of Imaginary Frequencies | 0

**Frequencies** (Top 3 out of 48)

1. 33.8530 cm⁻¹
2. 49.3734 cm⁻¹
3. 81.7650 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 1.737310 | -0.682463 | -0.000079 |
| C   | 0.704516 | 0.180786  | 0.000003  |
| C   | -0.665525| -0.363081 | -0.000018 |
| O   | -1.648799| 0.593123  | 0.000071  |
| O   | -1.020128| -1.546764 | -0.000105 |
| C   | -2.995787| 0.118814  | 0.000055  |
| H   | -3.604650| 1.056137  | 0.000137  |
| H   | -3.184923| -0.493029 | -0.14507  |
| H   | -3.184895| -0.493170 | 0.14527   |
| H   | 1.533617 | -1.769879 | -0.000161 |
| C   | 3.157348 | -0.287238 | -0.000070 |
| C   | 0.831973 | 1.654839  | 0.000116  |
| H   | 0.328261 | 2.081291  | 0.904136  |
| H   | 1.902902 | 1.972713  | 0.000128  |
| H   | 0.328240 | 2.081431  | -0.903826 |
| H   | 3.820021 | -1.187259 | -0.000156 |
| H   | 3.396898 | 0.325826  | -0.905928 |
| H   | 3.396928 | 0.325675  | 0.905882  |
5_methyltiglate_2_am1_HEI

| Datum                                | Value    |
|--------------------------------------|----------|
| AM1 Energy                           | -0.201848|
| AM1 Free Energy (Quasiharmonic)      | -0.04645 |
| Number of Imaginary Frequencies      | 0        |

**Frequencies** (Top 3 out of 63)

1. 23.8674 cm⁻¹
2. 56.1355 cm⁻¹
3. 79.1135 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | C           | C           | C           | O           | O           |
|---|-------------|-------------|-------------|-------------|-------------|
|   | 0.906420    | 0.316693    | 0.771465    | -1.738696   | 0.761544    |
|   | -0.055146   | 0.858367    | -0.153343   | -0.550383   | 0.761544    |
|   | -1.391405   | 0.427761    | -0.188782   | 0.427761    | -0.188782   |
|   | -2.351034   | 0.773341    | -0.239288   | 0.773341    | -0.920977   |
|   | -3.084866   | -0.979482   | 0.749474    | -0.979482   | 0.749474    |
|   | -3.143114   | -1.745695   | 1.562550    | -1.745695   | 1.562550    |
|   | -3.773869   | -0.124872   | 0.958747    | -0.124872   | 0.958747    |
|   | -3.347876   | -1.428883   | -0.239288   | -1.428883   | -0.239288   |
|   | 0.415797    | -0.251195   | 1.601332    | -0.251195   | 1.601332    |
|   | 1.913750    | 1.295497    | 1.315308    | 1.295497    | 1.315308    |
|   | 0.357624    | 1.896038    | -1.113891   | 1.896038    | -1.113891   |
|   | -0.457886   | 2.108972    | -1.849115   | 2.108972    | -1.849115   |
|   | 0.609455    | 2.855929    | -0.589758   | 2.855929    | -0.589758   |
|   | 1.270949    | 1.577094    | -1.680061   | 1.577094    | -1.680061   |
|   | 1.389255    | 2.078692    | 1.916575    | 2.078692    | 1.916575    |
|   | 2.653889    | 0.777009    | 1.973302    | 0.777009    | 1.973302    |
|   | 2.466678    | 1.800479    | 0.486814    | 1.800479    | 0.486814    |
|   | 2.068602    | -0.995278   | 0.044069    | -0.995278   | 0.044069    |
|   | 1.139490    | -1.767190   | -1.225339   | -1.767190   | -1.225339   |
|   | 1.735732    | -1.778362   | -2.163745   | -1.778362   | -2.163745   |
|   | 0.895570    | -2.813792   | -0.939678   | -2.813792   | -0.939678   |
|   | 0.190425    | -1.200688   | -1.396678   | -1.200688   | -1.396678   |

5_methyltiglate_2_am1

| Datum   | Value   |
|---------|---------|
|         |         |

5_methyltiglate_2_am1

| Datum   | Value   |
|---------|---------|
|         |         |
| Datum                              | Value      |
|-----------------------------------|------------|
| AM1 Energy                        | -0.137423  |
| AM1 Free Energy (Quasiharmonic)   | -0.016722  |
| Number of Imaginary Frequencies   | 0          |

**Frequencies** (Top 3 out of 48)

1. 19.4043 cm⁻¹  
2. 32.6796 cm⁻¹  
3. 96.7783 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|          |          |          |          |
|----------|----------|----------|----------|
| C        | 1.364640 | -0.876664| 0.000011 |
| C        | 0.729531 | 0.308878 | 0.000001 |
| C        | -0.742585| 0.380451 | 0.000010 |
| O        | -1.372773| -0.839823| -0.000020|
| O        | -1.459273| 1.385871 | 0.000041 |
| C        | -2.800259| -0.819552| -0.000013|
| H        | -3.174268| -0.299627| 0.914551 |
| H        | -3.174275| -0.299609| -0.914564|
| H        | -3.079346| -1.901862| -0.000023|
| H        | -3.708062| -1.816058| 0.000027 |
| C        | 2.828141 | -1.049065| 0.000010 |
| C        | 1.423422 | 1.619851 | -0.000031|
| H        | 0.690066 | 2.465074 | -0.000031|
| H        | 2.071415 | 1.715134 | 0.907044 |
| H        | 2.071387 | 1.715113 | -0.907126|
| H        | 3.139903 | -1.628240| -0.906387|
| H        | 3.373371 | -0.073468| 0.000004 |
| H        | 3.139908 | -1.628231| 0.906412 |

5_methyltiglate_3_am1

| Datum                              | Value      |
|-----------------------------------|------------|
| AM1 Energy                        | -0.127248  |
| AM1 Free Energy (Quasiharmonic)   | -0.006773  |
| Number of Imaginary Frequencies   | 0          |

**Frequencies** (Top 3 out of 48)
1. 29.8969 cm⁻¹
2. 43.9998 cm⁻¹
3. 73.7279 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 1.303213 | 0.321701 | -0.707128 |
| C | 0.455774 | -0.345133 | 0.091259 |
| C | -0.956751 | -0.542711 | -0.305307 |
| O | -1.880204 | 0.460472 | -0.122191 |
| O | -1.455955 | -1.554893 | -0.795277 |
| C | -1.421782 | 1.667514 | 0.474356 |
| H | -2.344160 | 2.296465 | 0.551775 |
| H | -0.992290 | 1.465144 | 1.485779 |
| H | -0.659625 | 2.158375 | -0.178806 |
| H | 0.940053 | 0.751904 | -1.657388 |
| C | 2.736229 | 0.524782 | -0.421861 |
| C | 0.823205 | -0.987331 | 1.374499 |
| H | 0.425926 | -2.033517 | 1.407419 |
| H | 1.932508 | -1.024502 | 1.504690 |
| H | 0.383143 | -0.415688 | 2.230473 |
| H | 3.187024 | 1.243971 | -1.148980 |
| H | 2.889029 | 0.926832 | 0.611157 |
| H | 3.288338 | -0.446560 | -0.501276 |

5_methyltiglate_3_reopt_am1_HEI

| Datum | Value |
|-------|-------|
| AM1 Energy | -0.196861 |
| AM1 Free Energy (Quasiharmonic) | -0.0418 |

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 63)

1. 35.4307 cm⁻¹
2. 49.9067 cm⁻¹
3. 65.3242 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
### 5_methyltiglate_4_am1_HEI

| Datum                                    | Value       |
|------------------------------------------|-------------|
| AM1 Energy                               | -0.201554   |
| AM1 Free Energy (Quasiharmonic)          | -0.046244   |
| Number of Imaginary Frequencies          | 0           |

**Frequencies** (Top 3 out of 63)

1. 28.5346 cm⁻¹
2. 54.3709 cm⁻¹
3. 71.7317 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|          |         |         |
|----------|---------|---------|
| C        | 1.094263| 0.527201| 0.640782 |
| C        | -0.119003| 0.663678| -0.130474|
| C        | -1.289561| 0.046439| -0.336580|
| O        | -2.428230| 0.228706| -0.471931|
### 5_methyltiglate_4_am1_reopt

| Datum                              | Value       |
|------------------------------------|-------------|
| AM1 Energy                         | -0.127411   |
| AM1 Free Energy (Quasiharmonic)    | -0.006509   |
| Number of Imaginary Frequencies    | 0           |

**Frequencies** (Top 3 out of 48)

1. 33.5100 cm⁻¹
2. 49.9769 cm⁻¹
3. 85.2701 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.422894| 0.323270 | -0.671827|
| C | -0.465814| 0.143337 | 0.251445 |
| C | 0.890660 | 0.691545 | 0.029487 |
| O | 1.931363 | -0.144173| -0.304017|
| O | 1.245872 | 1.865884 | 0.123024 |
| C | 1.625428 | -1.517213| -0.513385|
| H | 2.609649 | -1.972689| -0.789750|
| H | 1.225071 | -1.975075| 0.424187 |
| H | 0.888320 | -1.630852| -1.344792|
| Datum                        | Value     |
|------------------------------|-----------|
| AM1 Energy                   | -0.201848 |
| AM1 Free Energy (Quasiharmonic) | -0.046452 |
| Number of Imaginary Frequencies | 0         |

**Frequencies** (Top 3 out of 63)

1. 23.8831 cm⁻¹
2. 56.1363 cm⁻¹
3. 79.0712 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |          |          |          |
|-----|----------|----------|----------|
| C   | 0.906471 | 0.316753 | 0.771372 |
| C   | -0.055176| 0.858469 | -0.153326|
| C   | -1.391420| 0.427812 | -0.188729|
| O   | -1.738630| -0.550415|  0.761535|
| O   | -2.351082|  0.773399| -0.920877|
| C   | -3.084774| -0.979599|  0.749452|
| H   | -3.142960| -1.745881|  1.562461|
| H   | -3.773826| -1.125054|  0.958809|
| H   | -3.347774| -1.428931| -0.239341|
| H   |  0.415910| -0.251154|  1.601254|
| C   |  1.913909|  1.295512|  1.315089|
| C   |  0.357466|  1.896350| -1.113704|
| H   | -0.458214|  2.109582| -1.848649|
| H   |  0.609545|  2.856048| -0.589341|
| H   |  1.270595|  1.577471| -1.680222|
| H   |  1.389481|  2.079686|  1.916068|
| H   |  2.653872|  0.777068|  1.973308|
| H   |  2.467031|  1.800160|  0.486518|
| S   |  2.068627| -0.995274|  0.043932|
5_methyltiglate_6_am1_HEI

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.197033 |
| AM1 Free Energy (Quasiharmonic)      | -0.041777 |
| Number of Imaginary Frequencies      | 0         |

**Frequencies** (Top 3 out of 63)

1. 36.8326 cm⁻¹
2. 50.6583 cm⁻¹
3. 74.9279 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C  | 0.766257 | 0.189549 | 0.583586 |
| C  | -0.366529 | 0.878841 | 0.017740 |
| C  | -1.627666 | 0.272612 | -0.104775 |
| O  | -1.733961 | -1.022023 | 0.437150 |
| O  | -2.704874 | 0.699906 | -0.587261 |
| C  | -2.990230 | -1.652748 | 0.297079 |
| H  | -2.847673 | -2.667797 | 0.745550 |
| H  | -3.780174 | -1.084222 | 0.846940 |
| H  | -3.277100 | -1.731042 | -0.779983 |
| H  | 0.469902 | -0.733460 | 1.143514 |
| C  | 1.673799 | 1.042851 | 1.432306 |
| C  | -0.214151 | 2.259275 | -0.472531 |
| H  | 0.677966 | 2.354078 | -1.143571 |
| H  | -1.120959 | 2.582975 | -1.041661 |
| H  | -0.066612 | 2.976790 | 0.378714 |
| H  | 2.532239 | 0.442806 | 1.822855 |
| H  | 2.077734 | 1.901246 | 0.843382 |
| H  | 1.101726 | 1.452338 | 2.301099 |
| S  | 1.773041 | -0.443194 | -0.852267 |
| C  | 3.011143 | -1.453333 | -0.137515 |
| H  | 3.821713 | -0.849293 | 0.329360 |
| H  | 2.585320 | -2.122692 | 0.643256 |
| H  | 3.452192 | -2.075756 | -0.947636 |
# 7_isobutylacrylate_10_reopt_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.212947   |
| AM1 Free Energy (Quasiharmonic)            | -0.029409   |
| Number of Imaginary Frequencies            | 0           |

## Frequencies (Top 3 out of 72)

1. 10.7078 cm⁻¹
2. 24.7508 cm⁻¹
3. 36.5580 cm⁻¹

## AM1 Molecular Geometry in Cartesian Coordinates

|   | x (Å)     | y (Å)     | z (Å)     |
|---|-----------|-----------|-----------|
| C | 0.142274  | 1.352974  | 0.304439  |
| C | 1.534312  | 1.354842  | 0.211394  |
| C | 2.293361  | 0.720926  | -0.819145 |
| O | -0.615785 | 1.862999  | 1.167196  |
| O | -0.528763 | 0.693945  | -0.744626 |
| C | -1.942045 | 0.652464  | -0.717724 |
| C | -2.425525 | -0.717968 | -0.232000 |
| C | -3.803255 | -1.011796 | -0.782869 |
| C | -2.425520 | -0.774102 | 1.279742  |
| H | 2.066199  | 1.871896  | 1.016003  |
| H | 1.687329  | 0.455021  | -1.715637 |
| H | 3.200778  | 1.299618  | -1.120376 |
| H | -2.371186 | 1.467935  | -0.079116 |
| H | -2.251083 | 0.805394  | -1.788561 |
| H | -1.704827 | -1.492183 | -0.619411 |
| H | -4.175086 | -1.991319 | -0.396651 |
| H | -3.778722 | -1.056733 | -1.898337 |
| H | -4.525296 | -0.216136 | -0.478020 |
| H | -2.555736 | -1.823788 | 1.635471  |
| H | -1.456276 | -0.365607 | 1.664836  |
| H | -3.253536 | -0.151862 | 1.696843  |
| S | 3.124782  | -0.879199 | -0.341481 |
| C | 2.078406  | -1.578951 | 0.879011  |
| H | 1.296576  | -0.835331 | 1.175633  |
| H | 2.684297  | -1.852519 | 1.770044  |
| H | 1.584397  | -2.493072 | 0.483333  |
**7_isobutylacrylate_11_am1_HEI**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.213929     |
| AM1 Free Energy (Quasiharmonic)            | -0.030259     |
| Number of Imaginary Frequencies            | 0             |

**Frequencies (Top 3 out of 72)**

1. 23.7348 cm⁻¹  
2. 29.4288 cm⁻¹  
3. 43.2580 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |     |     |     |
|-----|-----|-----|-----|
| C   | 0.118121 | -0.972085 | -0.049999 |
| C   | 1.346615 | -0.961780 | -0.711543 |
| C   | 2.587998 | -1.066685 | -0.010041 |
| O   | -0.199146 | -1.096411 | 1.158215 |
| O   | -0.983708 | -0.833638 | -0.922991 |
| C   | -2.275927 | -0.894132 | -0.352225 |
| C   | -2.705416 | 0.459067  | 0.217406  |
| C   | -4.024698 | 0.323030  | 0.943332  |
| C   | -2.794927 | 1.500038  | -0.875264 |
| H   | 1.356308  | -0.850154 | -1.798259 |
| H   | 3.348614  | -1.686173 | -0.545046 |
| H   | 2.465665  | -1.417680 | 1.041060  |
| H   | -2.944171 | -1.188594 | -1.206303 |
| H   | -2.318315 | -1.670631 | 0.456589  |
| H   | -1.907518 | 0.767969  | 0.952574  |
| H   | -4.821051 | -0.042052 | 0.250324  |
| H   | -3.929747 | -0.402526 | 1.786798  |
| H   | -4.344400 | 1.309543  | 1.357380  |
| H   | -1.833353 | 1.525726  | -1.444259 |
| H   | -3.621261 | 1.256938  | -1.586216 |
| H   | -2.988449 | 2.510204  | -0.441361 |
| S   | 3.566648  | 0.512061  | 0.141048  |
| C   | 2.355958  | 1.777537  | 0.225008  |
| H   | 2.314639  | 2.205443  | 1.250360  |
| H   | 2.618953  | 2.584034  | -0.493477 |
| H   | 1.354202  | 1.355427  | -0.038762 |

**7_isobutylacrylate_12_am1_HEI**
| Datum                                               | Value       |
|-----------------------------------------------------|-------------|
| AM1 Energy                                          | -0.211393   |
| AM1 Free Energy (Quasiharmonic)                     | -0.027833   |
| Number of Imaginary Frequencies                     | 0           |

**Frequencies (Top 3 out of 72)**

1. 18.5178 cm⁻¹
2. 27.8360 cm⁻¹
3. 34.1218 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C     -0.054539       1.041476       -0.198894
C     1.086301       0.804163       -0.966524
C     1.713529       -0.467621       -1.139033
O     -0.685386       2.106588        0.014899
O     -0.597505       -0.095303        0.433497
C     -1.792166       0.054510        1.174078
C     -3.009389       -0.448528        0.391432
C     -2.788027       -1.865265       -0.089305
C     -3.312878       0.476208        -0.766071
H     1.529933        1.681120        -1.447754
H     1.063701       -1.323661        -0.843436
H     2.118492       -0.624233        -2.168958
H     -1.645429       -0.589756        2.084469
H     -1.955659       1.120639        1.482829
H     -3.885830       -0.441031        1.099757
H     -1.861667       -1.910076        -0.713552
H     -2.658825       -2.553766         0.780014
H     -3.655036       -2.216941        -0.698194
H     -2.393905       0.611046        -1.389912
H     -4.133905       0.064237        -1.399724
H     -3.615589       1.481782        -0.386698
S     3.285991       -0.735043        -0.173581
C     3.093967        0.240610        1.270480
H     3.997327        0.873575        1.408815
H     2.193414        0.895825        1.163286
H     2.969461        -0.411673        2.162204
```
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.21279    |
| AM1 Free Energy (Quasiharmonic)            | -0.029863   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 72)

1. 17.7803 cm⁻¹  
2. 25.8102 cm⁻¹  
3. 38.7977 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -0.292293 | 1.409674  | 0.170120  |
| C | -1.570880 | 1.158595  | 0.669951  |
| C | -2.024988 | -0.096818 | 1.175732  |
| O | 0.213653  | 2.460279  | -0.297598 |
| O | 0.597623  | 0.318723  | 0.204653  |
| C | 1.911374  | 0.573714  | -0.270715 |
| C | 2.682207  | -0.743928 | -0.182188 |
| C | 2.935481  | -1.118434 | 1.261290  |
| C | 3.981620  | -0.628447 | -0.948207 |
| H | -2.268010 | 2.001651  | 0.644623  |
| H | -2.710341 | 0.000649  | 2.053058  |
| H | -1.197653 | -0.807027 | 1.406009  |
| H | 2.395218  | 1.366651  | 0.357348  |
| H | 1.866166  | 0.935783  | -1.331667 |
| H | 2.047940  | -1.547462 | -0.651818 |
| H | 3.604592  | -0.370441 | 1.750753  |
| H | 1.964163  | -1.141425 | 1.813689  |
| H | 3.418010  | -2.122884 | 1.328149  |
| H | 3.781830  | -0.411080 | -2.025027 |
| H | 4.609323  | 0.196767  | -0.533184 |
| H | 4.559484  | -1.581324 | -0.878396 |
| S | -3.150946 | -1.069365 | 0.047084  |
| C | -2.686126 | -0.587463 | -1.573171 |
| H | -3.593775 | -0.293335 | -2.143720 |
| H | -1.983121 | 0.281317  | -1.518808 |
| H | -2.187267 | -1.431385 | -2.097663 |
### Datum Value

**AM1 Energy**  
-0.21395

**AM1 Free Energy (Quasiharmonic)**  
-0.030183

**Number of Imaginary Frequencies**  
0

### Frequencies (Top 3 out of 72)

1. 24.3687 cm⁻¹  
2. 34.5569 cm⁻¹  
3. 47.1779 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

|         | x      | y      | z      |
|---------|--------|--------|--------|
| C       | -0.088828 | -0.098421 | -0.120196 |
| C       | -1.177591 | -0.899420 | 0.226086  |
| C       | -2.308012 | -1.058416 | -0.634829 |
| O       | 0.181328  | 0.578353  | -1.142402 |
| O       | 0.911362  | -0.060096 | 0.876584  |
| C       | 2.065172  | 0.712315  | 0.609616  |
| C       | 3.079162  | -0.060421 | -0.235851 |
| C       | 3.574902  | -1.283625 | 0.501413  |
| C       | 4.229839  | 0.841242  | -0.621720 |
| H       | -1.171386 | -1.402436 | 1.195853  |
| H       | -2.722780 | -2.095967 | -0.634716 |
| H       | -2.112880 | -0.714443 | -1.677234 |
| H       | 1.793055  | 1.667241  | 0.087042  |
| H       | 2.491631  | 0.935216  | 1.625038  |
| H       | 2.537211  | -0.390244 | -1.168536 |
| H       | 4.218198  | -1.909386 | -0.162590 |
| H       | 4.173154  | -0.989683 | 1.397555  |
| H       | 2.701320  | -1.891968 | 0.841712  |
| H       | 4.974794  | 0.280228  | -1.235865 |
| H       | 3.858706  | 1.709117  | -1.218332 |
| H       | 4.747269  | 1.232315  | 0.287697  |
| S       | -3.847105 | -0.139695 | -0.125555 |
| C       | -3.256287 | 1.312475  | 0.659680  |
| H       | -3.780257 | 1.442227  | 1.631498  |
| H       | -2.156018 | 1.219943  | 0.838834  |
| H       | -3.449998 | 2.202531  | 0.022175  |

### 7_isobutylacrylate_15_am1_HEI

| Datum | Value |
|-------|-------|
|       |       |
| Datum                                      | Value     |
|-------------------------------------------|-----------|
| AM1 Energy                                | -0.213477 |
| AM1 Free Energy (Quasiharmonic)           | -0.029461 |
| Number of Imaginary Frequencies           | 0         |

**Frequencies** *(Top 3 out of 72)*

1. 23.5176 cm⁻¹  
2. 32.8543 cm⁻¹  
3. 35.9108 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C  | -0.097914 | 0.158015 | -0.022999 |
| C  | -1.191710 | 0.397995 | -0.855417 |
| C  | -2.333413 | 1.138069 | -0.414930 |
| O  | 0.165472  | 0.504200 | 1.154777  |
| O  | 0.907571  | -0.614543| -0.644122 |
| C  | 2.081914  | -0.900923| 0.088541  |
| C  | 3.218202  | 0.039347 | -0.328684 |
| C  | 4.554996  | -0.652705| -0.178826 |
| C  | 3.177730  | 1.313850 | 0.485581  |
| H  | -1.180930 | -0.012467| -1.867810 |
| H  | -2.758941 | 1.806143 | -1.203109 |
| H  | -2.145298 | 1.710002 | 0.523477  |
| H  | 1.907378  | -0.837475| 1.194363  |
| H  | 2.340741  | -1.958527| -0.195025 |
| H  | 3.064107  | 0.301764 | -1.413202 |
| H  | 4.701884  | -0.998114| 0.873844  |
| H  | 4.615286  | -1.540938| -0.852835 |
| H  | 5.385836  | 0.046653 | -0.438733 |
| H  | 2.124503  | 1.693100 | 0.528284  |
| H  | 3.520615  | 1.123715 | 1.531145  |
| H  | 3.837090  | 2.092025 | 0.032661  |
| S  | -3.855692 | 0.130462 | -0.045811 |
| C  | -3.240283 | -1.400622| 0.547228  |
| H  | -3.430300 | -1.496725| 1.638463  |
| H  | -3.752983 | -2.231606| 0.015804  |
| H  | -2.139404 | -1.460345| 0.358246  |

7_isobutylacrylate_16_am1_HEI
| Datum                                      | Value            |
|--------------------------------------------|------------------|
| AM1 Energy                                 | -0.213534        |
| AM1 Free Energy (Quasiharmonic)            | -0.029605        |
| Number of Imaginary Frequencies            | 0                |

**Frequencies** (Top 3 out of 72)

1. 24.7370 cm⁻¹
2. 31.5078 cm⁻¹
3. 34.6348 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C              | -0.124568       | -0.987326       | 0.196901  |
|----------------|-----------------|-----------------|-----------|
| C              | -1.323215       | -1.160604       | -0.495896 |
| C              | -2.594531       | -1.061251       | 0.150653  |
| O              | 0.132388        | -0.758255       | 1.404359  |
| O              | 1.013207        | -1.117091       | -0.629480 |
| C              | 2.287818        | -0.932496       | -0.047502 |
| C              | 2.829847        | 0.460831        | -0.384035 |
| C              | 4.340914        | 0.463593        | -0.316794 |
| C              | 2.245640        | 1.496270        | 0.551374  |
| H              | -1.285361       | -1.350698       | -1.571038 |
| H              | -2.525898       | -1.140466       | 1.260615  |
| H              | -3.352117       | -1.778465       | -0.249172 |
| H              | 2.265754        | -1.085048       | 1.063142  |
| H              | 2.937358        | -1.716433       | -0.526094 |
| H              | 2.511179        | 0.707867        | -1.435678 |
| H              | 4.688361        | 0.148405        | 0.696753  |
| H              | 4.769013        | -0.240314       | -1.070554 |
| H              | 4.737157        | 1.487147        | -0.522248 |
| H              | 1.138147        | 1.345102        | 0.626545  |
| H              | 2.678685        | 1.390545        | 1.575091  |
| H              | 2.456946        | 2.527228        | 0.180156  |
| S              | -3.526480       | 0.525546        | -0.141481 |
| C              | -2.281682       | 1.759356        | -0.204617 |
| H              | -1.274102       | 1.275313        | -0.250093 |
| H              | -2.431473       | 2.386152        | -1.118438 |
| H              | -2.336067       | 2.407465        | 0.697183  |

**7_isobutylacrylate_17_reopt_am1_HEI**

| Datum                                      | Value            |
|--------------------------------------------|------------------|
|                                            |                  |
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.211393   |
| AM1 Free Energy (Quasiharmonic)            | -0.027833   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 72)**

1.  18.5304 cm\(^{-1}\)
2.  27.8448 cm\(^{-1}\)
3.  34.1081 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -0.054573 | 1.041468 | 0.198829 |
| C   | 1.086301  | 0.804286 | 0.966447 |
| C   | -0.685489 | 2.106522 | -0.015040|
| O   | -0.597500 | -0.095401| -0.433441|
| C   | -1.792135 | 0.054308 | -1.174084|
| C   | -3.009391 | -0.448598| -0.391405|
| C   | -3.312937 | 0.476353 | 0.765913 |
| C   | -2.788046 | -1.865250| 0.089594 |
| H   | 1.529905  | 1.681311 | 1.447577 |
| H   | 2.118547  | -0.623981| 2.169013 |
| H   | 1.063818  | -1.323549| 0.843518 |
| H   | -1.955613 | 1.120392 | -1.482996|
| H   | -1.645373 | -0.590096| -2.084373|
| H   | -3.885795 | -0.441233| -1.099773|
| H   | -2.393980 | 0.611356 | 1.389741 |
| H   | -3.615682 | 1.481839 | 0.386339 |
| H   | -4.133955 | 0.064474 | 1.399637 |
| H   | -1.861719 | -1.909950| 0.713898 |
| H   | -3.655084 | -2.216824| 0.698500 |
| H   | -2.658796 | -2.553903| -0.779595|
| S   | 3.286132  | -0.734823| 0.173725 |
| C   | 3.093833  | 0.240241 | -1.270703|
| H   | 3.997277  | 0.872963 | -1.409582|
| H   | 2.968908  | -0.412370| -2.162127|
| H   | 2.193437  | 0.895670 | -1.163483|

7_isobutylacrylate_18_reopt_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| Datum                              | Value     |
|-----------------------------------|-----------|
| AM1 Energy                        | -0.208569 |
| AM1 Free Energy (Quasiharmonic)   | -0.02636  |
| Number of Imaginary Frequencies   | 0         |

**Frequencies (Top 3 out of 72)**

1. 19.7007 cm⁻¹  
2. 25.9521 cm⁻¹  
3. 39.6052 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|     | X      | Y      | Z      |
|-----|--------|--------|--------|
| C   | -0.025621 | 1.620132 | -0.056012 |
| C   | 1.337837  | 1.561994 | 0.240370 |
| C   | 2.002847  | 0.436584 | 0.813550 |
| O   | -0.714867 | 2.537043 | -0.567340 |
| O   | -0.776023 | 0.488192 | 0.317361 |
| C   | -2.158103 | 0.524279 | -0.005819 |
| C   | -2.729705 | -0.856400| 0.319883 |
| C   | -2.221750 | -1.887382| -0.663568|
| C   | -4.241402 | -0.799008| 0.314376 |
| H   | 1.927016  | 2.442006 | -0.039349 |
| H   | 2.789381  | 0.710776 | 1.557862 |
| H   | 1.316462  | -0.322325| 1.254364 |
| H   | -2.662730 | 1.316076 | 0.608619 |
| H   | -2.95529  | 0.771279 | -1.090873 |
| H   | -2.376912 | -1.143435| 1.350086 |
| H   | -2.607573 | -1.675773| -1.689793|
| H   | -1.104529 | -1.854318| -0.691249|
| H   | -2.551523 | -2.911339| -0.365322|
| H   | -4.616822 | -0.465208| -0.683063|
| H   | -4.669127 | -1.806876| 0.533604 |
| H   | -4.608199 | -0.080781| 1.086592 |
| S   | 2.932968  | -0.410495| -0.535912|
| C   | 3.788192  | -1.705330| 0.272803 |
| H   | 3.083965  | -2.432841| 0.735307 |
| H   | 4.406455  | -2.235383| -0.485077|
| H   | 4.455528  | -1.315039| 1.073920 |

**7_isobutylacrylate_19_am1_HEI_reopt**

| Datum                              | Value     |
|-----------------------------------|-----------|
### AM1 Energy
-0.208959

### AM1 Free Energy (Quasiharmonic)
-0.026827

### Number of Imaginary Frequencies
0

### Frequencies (Top 3 out of 72)

1. 17.7746 cm⁻¹
2. 28.7232 cm⁻¹
3. 38.3194 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | -0.051803 | -0.644463 | 0.150248 |
| C    | -1.127178 | -0.148865 | 0.891126 |
| C    | -2.466671 | -0.590299 | 0.659579 |
| O    | 0.043414  | -1.537702 | -0.725798 |
| O    | 1.181464  | -0.049911 | 0.493321 |
| C    | 2.316579  | -0.530156 | -0.210508 |
| C    | 3.518836  | 0.285196  | 0.267906 |
| C    | 3.436602  | 1.706038  | -0.244515 |
| C    | 4.800704  | -0.379946 | -0.182709 |
| H    | -0.940925 | 0.627715  | 1.636034 |
| H    | -3.059157 | -0.740002 | 1.594354 |
| H    | -2.533622 | -1.499615 | 0.018258 |
| H    | 2.463812  | -1.619792 | 0.013465 |
| H    | 2.162443  | -0.410146 | -1.314708 |
| H    | 3.494185  | 0.310853  | 1.393479 |
| H    | 3.520155  | 1.728297  | -1.357755 |
| H    | 2.452085  | 2.148267  | 0.045770 |
| H    | 4.258476  | 2.327566  | 0.185031 |
| H    | 4.882333  | -1.405212 | 0.251863 |
| H    | 4.826408  | -0.466634 | -1.295838 |
| H    | 5.684938  | 0.217608  | 0.145729 |
| S    | -3.350708 | 0.761535  | -0.226994 |
| C    | -4.985506 | 0.164263  | -0.408238 |
| H    | -5.450756 | -0.057538 | 0.578563 |
| H    | -5.583714 | 0.949991  | -0.920425 |
| H    | -5.013731 | -0.765637 | -1.019430 |

### 7_isobutylacrylate_1_am1_HEI_reopt

| Datum                  | Value                  |
|------------------------|------------------------|
| AM1 Energy             | -0.208959              |
| AM1 Free Energy        | -0.026827              |
| Number of Imaginary    | 0                      |
| Frequencies (Top 3 out of 72) |                  |
| 1. 17.7746 cm^{-1}     |                        |
| 2. 28.7232 cm^{-1}     |                        |
| 3. 38.3194 cm^{-1}     |                        |
| AM1 Molecular Geometry |                        |
| in Cartesian Coordinates |                      |
### Datum

| Datum                                      | Value |
|--------------------------------------------|-------|
| AM1 Energy                                 | -0.212914 |
| AM1 Free Energy (Quasiharmonic)            | -0.029285 |
| Number of Imaginary Frequencies            | 0     |

### Frequencies (Top 3 out of 72)

1. 19.1516 cm

2. 38.7064 cm

3. 48.4052 cm

### AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -0.302540 | 1.561418 | 0.243327 |
| C | -1.653792 | 1.440819 | -0.084330 |
| C | -2.193224 | 0.509075 | -1.021224 |
| O | 0.283020 | 2.341397 | 1.034752 |
| O | 0.560299 | 0.676379 | -0.432970 |
| C | 1.933701 | 0.728370 | -0.083455 |
| C | 2.540317 | -0.632499 | -0.432580 |
| C | 2.046700 | -1.694318 | 0.525148 |
| O | 4.050019 | -0.541504 | -0.411736 |
| H | -2.336878 | 2.104312 | 0.454676 |
| H | -3.085377 | 0.899375 | -1.569084 |
| H | -1.436719 | 0.113540 | -1.737487 |
| H | 2.423993 | 1.540303 | -0.683794 |
| H | 2.064576 | 0.955656 | 1.007014 |
| H | 2.202683 | -0.906476 | -1.471405 |
| H | 2.423282 | -1.498744 | 1.557958 |
| H | 0.927624 | -1.684157 | 0.547334 |
| H | 2.396569 | -2.704960 | 0.205576 |
| H | 4.409291 | -0.220371 | 0.595779 |
| H | 4.502155 | -1.534774 | -0.647898 |
| H | 4.407445 | 0.200463 | -1.165702 |
| S | -2.967085 | -1.028765 | -0.295069 |
| C | -1.929429 | -1.435694 | 1.058570 |
| H | -1.229700 | -0.586707 | 1.261550 |
| H | -2.554221 | -1.623227 | 1.958606 |
| H | -1.338417 | -2.350207 | 0.831407 |
### AM1 Energy

- **AM1 Energy**: -0.1392

### AM1 Free Energy (Quasiharmonic)

- **AM1 Free Energy (Quasiharmonic)**: 0.010338

### Number of Imaginary Frequencies

- **Number of Imaginary Frequencies**: 0

#### Frequencies (Top 3 out of 57)

1. 41.4341 cm⁻¹
2. 49.6935 cm⁻¹
3. 61.1915 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|  | X     | Y     | Z     |
|---|-------|-------|-------|
| C | 1.324298 | -0.204028 | 0.154408 |
| C | 2.573738 | 0.565604  | 0.088372 |
| C | 3.664801 | 0.076184  | -0.500778 |
| O | 1.089224 | -1.335209 | -0.281121 |
| O | 0.325001 | 0.470380  | 0.804670 |
| C | -0.945028 | -0.180659 | 0.935797 |
| C | -1.783113 | -0.018178 | -0.327842 |
| C | -2.144610 | 1.433259  | -0.554056 |
| C | -3.026546 | -0.874354 | -0.224588 |
| H | 2.536731  | 1.562121  | 0.556913 |
| H | 4.601838  | 0.647467  | -0.553003 |
| H | 3.686090  | -0.921652 | -0.964358 |
| H | -0.795826 | -1.266479 | 1.172205 |
| H | -1.412213 | 0.353086  | 1.806373 |
| H | -1.162321 | -0.379109 | -1.197141 |
| H | -2.668342 | 1.553874  | -1.532402 |
| H | -2.818625 | 1.802070  | 0.256381 |
| H | -1.220961 | 2.061266  | -0.559055 |
| H | -3.651198 | -0.753353 | -1.142097 |
| H | -2.752114 | -1.951803 | -0.120933 |
| H | -3.638110 | -0.575819 | 0.660851 |

### 7_isobutylacrylate_20_am1_HEI

#### AM1 Energy

- **AM1 Energy**: -0.213477

#### AM1 Free Energy (Quasiharmonic)

- **AM1 Free Energy (Quasiharmonic)**: -0.029461

#### Number of Imaginary Frequencies

- **Number of Imaginary Frequencies**: 0
**Frequencies** (Top 3 out of 72)

1. 23.4908 cm⁻¹
2. 32.8467 cm⁻¹
3. 35.8887 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | C           | 0.097940 | 0.157968 | 0.023105 |
|---|-------------|----------|----------|----------|
| C | 1.191668    | 0.398277 | 0.855520 |
| C | 2.333411    | 1.138168 | 0.414830 |
| O | -0.165364   | 0.503710 | -1.154819|
| O | -0.907577   | -0.614383| 0.644427 |
| C | -2.081892   | -0.900979| -0.088198|
| C | -3.218151   | 0.039504 | 0.328613 |
| C | -4.554971   | -0.652533| 0.178938 |
| C | -3.177562   | 1.313694 | -0.486131|
| H | 1.180822    | -0.011821| 1.868060 |
| H | 2.759019    | 1.806376 | 1.202851 |
| H | 2.145309    | 1.709902 | -0.523700|
| H | -1.907294   | -0.837958| -1.194034|
| H | -2.340792   | -1.958457| 0.195771 |
| H | -3.064089   | 0.302317 | 1.413041 |
| H | -4.615334   | -1.540535| 0.853246 |
| H | -5.385786   | 0.046956 | 0.438575 |
| H | -4.701834   | -0.998292| -0.872821|
| H | -3.836703   | 2.092163 | -0.033396|
| H | -2.124262   | 1.692711 | -0.529141|
| H | -3.520643   | 1.123246 | -1.531572|
| S | 3.855512    | 0.130361 | 0.045904 |
| C | 3.240104    | -1.400542| -0.547473|
| H | 3.752619    | -2.231673| -0.016099|
| H | 2.139178    | -1.460118| -0.358642|
| H | 3.430246    | -1.496553| -1.638694|

**7_isobutylacrylate_21_am1_HEI_reopt**

| Datum                                | Value    |
|--------------------------------------|----------|
| AM1 Energy                           | -0.211853|
| AM1 Free Energy (Quasiharmonic)      | -0.028319|
| Number of Imaginary Frequencies      | 0        |

**Frequencies** (Top 3 out of 72)
1. 22.3017 cm⁻¹
2. 29.7033 cm⁻¹
3. 35.8978 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 0.006444  | -0.086753  | -0.183758  |
| C    | -0.985354 | -0.405664  | 0.744845   |
| C    | -2.135068 | -1.179439  | 0.392279   |
| O    | 0.163676  | 0.712840   | 0.363529   |
| C    | 2.12498   | 1.060544   | -0.466264  |
| C    | 3.356873  | 0.197503   | -0.178796  |
| C    | 3.120057  | -1.227876  | -0.625033  |
| C    | 3.720372  | 0.252832   | 1.288101   |
| H    | -0.888607 | -0.029864  | 1.766076   |
| H    | -2.450438 | -1.893337  | 1.191974   |
| H    | -2.020965 | -1.708620  | -0.582416  |
| H    | 1.855713  | 0.983181   | -1.553058  |
| H    | 2.352944  | 2.130445   | -0.204108  |
| H    | 4.209489  | 0.627235   | -0.777460  |
| H    | 2.185915  | -1.619797  | -0.150152  |
| H    | 2.978199  | -1.266183  | -1.731944  |
| H    | 3.980667  | -1.880528  | -0.344572  |
| H    | 3.976056  | 1.298178   | 1.585374   |
| H    | 2.851136  | -0.85689   | 1.903736   |
| H    | 4.596673  | -0.404317  | 1.503726   |
| S    | -3.727079 | -0.228017  | 0.218730   |
| C    | -3.238258 | 1.349896   | -0.369344  |
| H    | -3.727951 | 2.136922   | 0.244334   |
| H    | -2.127234 | 1.451953   | -0.288913  |
| H    | -3.541841 | 1.477508   | -1.431271  |

7_isobutylacrylate_22_am1_HEI

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.20925  |
| AM1 Free Energy (Quasiharmonic)            | -0.026027 |
| Number of Imaginary Frequencies            | 0         |

Frequencies (Top 3 out of 72)
1.  15.1042 cm⁻¹
2.  32.1771 cm⁻¹
3.  41.4179 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |        |        |        |
|-----|--------|--------|--------|
| C   | -0.251031 | 1.036795 | 0.102987 |
| C   | -0.955925 | 0.206458 | -0.770894 |
| C   | -2.325527 | 0.456049 | -1.104654 |
| O   | -0.590283 | 2.076655 | 0.716186  |
| O   | 1.100639  | 0.779868 | 0.427544  |
| C   | 1.711969  | -0.340792 | -0.180566 |
| C   | 3.160968  | -0.389426 | 0.312493  |
| C   | 3.959996  | 0.754373  | -0.271331 |
| C   | 3.780228  | -1.722333 | -0.044742 |
| H   | -0.484210 | -0.676733 | -1.205249 |
| H   | -2.570271 | 0.236780  | -2.172766 |
| H   | -2.657581 | 1.484248  | -0.829752 |
| H   | 1.175197  | -1.281227 | 0.117571  |
| H   | 1.685112  | -0.241756 | -1.298244 |
| H   | 3.146685  | -0.277985 | 1.433002  |
| H   | 4.987054  | 0.779660  | 0.165394  |
| H   | 4.048814  | 0.647693  | -1.379278 |
| H   | 3.442570  | 1.719518  | -0.047680 |
| H   | 4.842581  | -1.760881 | 0.296915  |
| H   | 3.219479  | -2.556610 | 0.441379  |
| H   | 3.758881  | -1.880951 | -1.150032 |
| S   | -3.566339 | -0.671666 | -0.297366 |
| C   | -2.945109 | -0.905372 | 1.326375  |
| H   | -2.949373 | -1.990409 | 1.568080  |
| H   | -1.899600 | -0.513587 | 1.386831  |
| H   | -3.580181 | -0.367796 | 2.063828  |

**7_isobutylacrylate_2_am1**

| Datum                               | Value  |
|-------------------------------------|--------|
| AM1 Energy                          | -0.1392|
| AM1 Free Energy (Quasiharmonic)     | 0.010338|
| Number of Imaginary Frequencies     | 0      |

**Frequencies** (Top 3 out of 57)
1. 41.4341 cm⁻¹
2. 49.6935 cm⁻¹
3. 61.1914 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C          -1.324298       -0.204028        0.154408
C          -2.573738        0.565605        0.088372
C          -3.664802        0.076184       -0.500778
O          -1.089225       -1.335209       -0.281121
O          -0.325001        0.470380        0.804670
C           0.945028       -0.180659        0.935797
C           1.783113       -0.018178       -0.327842
C           3.026546       -0.874355       -0.224588
C           2.144610       1.433259       -0.554056
H          -2.536731        1.562121        0.556913
H          -4.601838        0.647467       -0.553003
H          -3.686090       -0.921652       -0.964357
H           1.412213        0.353086        1.806373
H           0.795826       -1.266479       1.172205
H           1.162322       -0.379109       -1.197141
H           3.651198       -0.753353       -1.142097
H           3.638110       -0.575819        0.660852
H           2.752114       -1.951803       -0.120933
H           2.668342       1.553874       -1.532401
H           1.220961       2.061267       -0.559055
H           2.818625       1.802070        0.256382
```

**7_isobutylacrylate_2_reopt3_am1_HEI**

| Datum                                      | Value      |
|--------------------------------------------|------------|
| AM1 Energy                                 | -0.21279   |
| AM1 Free Energy (Quasiharmonic)            | -0.029863  |
| Number of Imaginary Frequencies            | 0          |

**Frequencies (Top 3 out of 72)**

1. 17.7782 cm⁻¹
2. 25.8091 cm⁻¹
3. 38.7969 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
### 7_isobutylacrylate_3_am1_HEI

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.213176   |
| AM1 Free Energy (Quasiharmonic)      | -0.030286   |
| Number of Imaginary Frequencies      | 0           |

**Frequencies** (Top 3 out of 72)

1. 17.6107 cm⁻¹
2. 26.6245 cm⁻¹
3. 41.6626 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
7_isobutylacrylate_3_am1

### Datum

|                    | Value    |
|--------------------|----------|
| AM1 Energy         | -0.1375  |
| AM1 Free Energy    | 0.01151  |
| (Quasiharmonic)    |          |
| Number of Imaginary Frequencies | 0       |

#### Frequencies (Top 3 out of 57)

| Rank | Frequency  |
|------|------------|
| 1.   | 30.1834 cm⁻¹ |
| 2.   | 44.3443 cm⁻¹ |
| 3.   | 71.1433 cm⁻¹ |

#### AM1 Molecular Geometry in Cartesian Coordinates
7_isobutylacrylate_4_am1_HEI

### Datum

|        | Value       |
|--------|-------------|
| AM1 Energy | -0.212829   |
| AM1 Free Energy (Quasiharmonic) | -0.029871   |

Number of Imaginary Frequencies 0

**Frequencies** (Top 3 out of 72)

1. 17.5501 cm⁻¹
2. 25.7708 cm⁻¹
3. 38.8576 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|        |        |        |        |
|--------|--------|--------|--------|
| C      | -0.265342 | 1.481332 | -0.097672 |
| C      | -1.572690 | 1.349611 | 0.373059 |
| C      | -2.052770 | 0.274022 | 1.179352 |
| O      | 0.262525  | 2.368880 | -0.813248 |
| O      | 0.628779  | 0.469615 | 0.302257 |
| C      | 1.963269  | 0.599952 | -0.166099 |
7_isobutylacrylate_4_am1

| Datum                                    | Value               |
|------------------------------------------|---------------------|
| AM1 Energy                               | -0.138514           |
| AM1 Free Energy (Quasiharmonic)          | 0.010869            |
| Number of Imaginary Frequencies          | 0                   |

**Frequencies** (Top 3 out of 57)

1. 34.1150 cm⁻¹
2. 44.8433 cm⁻¹
3. 70.8052 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C | 2.749762 | -0.588716 | 0.387655 |
|   | 4.231928 | -0.355744 | 0.193447 |
|   | 2.311343 | -1.875076 | -0.276483|
| H | -2.270339| 2.137178  | 0.072296 |
| H | -1.239622| -0.327647 | 1.646695 |
| H | -2.793349| 0.595222  | 1.952060 |
| H | 1.974696 | 0.603354  | -1.287319|
| H | 2.390873 | 1.567672  | 0.198974 |
| H | 2.530944 | -0.665263 | 1.489726 |
| H | 4.815614 | -1.225040 | 0.581263 |
| H | 4.469324 | -0.225866 | -0.890064|
| H | 4.557591 | 0.563273  | 0.737548 |
| H | 2.819177 | -2.752054 | 0.191732 |
| H | 1.204947 | -1.990827 | -0.166838|
| H | 2.560491 | -1.860916 | -1.364819|
| S | -3.099676| -0.998750 | 0.298520 |
| C | -2.566052| -0.944716 | -1.370457|
| H | -2.029814| -1.882544 | -1.633402|
| H | -1.880032| -0.835468 | -2.035723|
| H | -1.880032| -0.073028 | -1.517326|
### 7_isobutylacrylate_5_am1

| Datum                              | Value         |
|------------------------------------|---------------|
| AM1 Energy                         | -0.138514     |
| AM1 Free Energy (Quasiharmonic)    | 0.010869      |
| Number of Imaginary Frequencies    | 0             |

**Frequencies (Top 3 out of 57)**

1. 34.1146 cm⁻¹
2. 44.8429 cm⁻¹
3. 70.8071 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|        |        |        |
|--------|--------|--------|
| C      | 1.335129 | -0.624326 | -0.074588 |
| C      | 2.692614 | -0.122577 | -0.322420 |
| C      | 3.134135 | 1.068380  | 0.079066  |
| O      | 0.870210 | -1.714134 | -0.420390 |
| O      | 0.531622 | 0.236070  | 0.626663  |
| C      | -0.808535 | -0.184205 | 0.912677  |
| C      | -1.732406 | 0.065941  | -0.274469 |
| C      | -1.873440 | 1.547099  | -0.547832 |
| C      | -3.082006 | -0.564311 | -0.007488 |
| H      | 3.321439 | -0.836650 | -0.881175 |
| H      | 4.159557 | 1.405628  | -0.127716 |
| H      | 2.583676 | 1.777009  | 0.636096  |
| H      | -0.816778 | -1.269028 | 1.196068  |
| H      | -1.090596 | 0.456027  | 1.791046  |
| H      | -1.270212 | -0.428942 | -1.176073 |
### 7_isobutylacrylate_5_reopt2_am1_HEI_reopt

| Datum                                      | Value    |
|--------------------------------------------|----------|
| AM1 Energy                                 | -0.213827|
| AM1 Free Energy (Quasiharmonic)            | -0.029359|
| Number of Imaginary Frequencies            | 0        |

#### Frequencies (Top 3 out of 72)

1. 32.4226 cm\(^{-1}\)
2. 41.1468 cm\(^{-1}\)
3. 60.3505 cm\(^{-1}\)

#### AM1 Molecular Geometry in Cartesian Coordinates

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 0.09111 | -1.400213 | 0.272546 |
| C      | 1.485424 | -1.447612 | 0.259313 |
| C      | 2.321610 | -0.806519 | -0.704209 |
| O      | -0.739115 | -1.931980 | 1.051486 |
| O      | -0.496034 | -0.644900 | -0.762595 |
| C      | -1.908365 | -0.581225 | -0.803717 |
| C      | -2.458387 | 0.460485  | 0.171937 |
| C      | -3.970074 | 0.446957  | 0.146611 |
| C      | -1.923625 | 1.837562  | -0.149094 |
| H      | 1.952925  | -2.003119 | 1.078006 |
| H      | 3.250757  | -1.382562 | -0.935625 |
| H      | 1.786293  | -0.536010 | -1.643454 |
| H      | -2.140354 | -0.286389 | -1.862935 |
| H      | -2.358212 | -1.582890 | -0.573574 |
| H      | -2.101103 | 0.161631  | 1.199433 |
| H      | -4.350060 | 0.692594  | -0.874659 |
| H      | -4.354015 | -0.561508 | 0.433749 |
| H      | -4.377841 | 1.199688  | 0.863526 |
| H      | -2.262460 | 2.578450  | 0.614113 |
| H      | -0.804770 | 1.809543  | -0.158762 |
| H      | -2.278760 | 2.175598  | -1.152330 |
| S      | 3.114699  | 0.793695  | -0.161561 |
### 7_isobutylacrylate_6_am1

| Datum                               | Value  |
|-------------------------------------|--------|
| AM1 Energy                          | -0.136809 |
| AM1 Free Energy (Quasiharmonic)     | 0.011946  |
| Number of Imaginary Frequencies     | 0      |

**Frequencies** (Top 3 out of 57)

1. 21.2965 cm⁻¹
2. 43.8258 cm⁻¹
3. 63.0068 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|          |         |         |         |
|----------|---------|---------|---------|
| C        | -1.53515| -0.563535| -0.000019 |
| C        | -2.59792| 0.449159 | 0.000085  |
| C        | -2.37637| 1.762751 | -0.00103  |
| O        | -1.670939| -1.790672| 0.000004  |
| O        | -0.263649| -0.055035| -0.000140 |
| C        | 0.805465 | -1.017491| -0.000228 |
| C        | 2.120179 | -0.246360| 0.000066  |
| C        | 2.255390 | 0.600014 | 1.246775  |
| C        | 2.255852 | 0.600198 | -1.246469 |
| H        | -3.611298| 0.012566 | 0.00355   |
| H        | -3.200767| 2.489539 | 0.000012  |
| H        | -1.363371| 2.191809 | -0.000372 |
| H        | 0.709575 | -1.658120| 0.915056  |
| H        | 0.709750 | -1.657721| -0.915807 |
| H        | 2.937605 | -1.023721| 0.000155  |
| H        | 3.232703 | 1.139476 | 1.244400  |
| H        | 1.430712 | 1.351959 | 1.293237  |
| H        | 2.202233 | -0.040339| 2.159807  |
| H        | 3.233256 | 1.139495 | -1.243747 |
| H        | 2.202827 | -0.039996| -2.159621 |
| H        | 1.431317 | 1.352294 | -1.293029 |
### 7_isobutylacrylate_6_reopt2_am1_HEI

| Datum                          | Value     |
|--------------------------------|-----------|
| AM1 Energy                     | -0.213501 |
| AM1 Free Energy (Quasiharmonic)| -0.029693 |
| Number of Imaginary Frequencies| 0         |

#### Frequencies (Top 3 out of 72)

1. 25.1123 cm⁻¹  
2. 28.6981 cm⁻¹  
3. 44.6081 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

```
C   0.066229  0.692909  -0.708954  
C   1.287494  0.252276  -1.219690  
C   1.988262  -0.914851 -0.787951  
O  -0.628262  1.697554  -1.004606  
O  -0.500813  -0.121820  0.291452  
C  -1.740830  0.284615  0.837570  
C  -2.914621  -0.155093 -0.039277  
C  -4.207017  0.420016  0.494542  
C  -2.988404  -1.662761  0.291452  
H   1.733479  0.877480  -1.999269  
H   1.357071  -1.615839  -0.194576  
H   2.496697  -1.459322  -1.621105  
H  -1.784545  -0.227850  1.836539  
H  -1.770678  1.398007  0.972500  
H  -2.721410  0.260196  -1.070066  
H  -4.391394  0.073108  1.540183  
H  -4.163876  1.535822  0.494420  
H  -5.067665  0.097459  -0.139593  
H  -3.246603  -2.102303  0.869827  
H  -3.764593  -1.977948  -0.861703  
H  -1.996226  -2.066246  -0.443159  
S   3.473996  -0.613111  0.299764  
C   3.116584  0.882387  1.141985  
H   2.933813  0.682911  2.220402  
H   3.981005  1.574514  1.043928  
H   2.207409  1.356933  0.694684  
```
| Datum                              | Value       |
|-----------------------------------|------------|
| AM1 Energy                        | -0.138224  |
| AM1 Free Energy (Quasiharmonic)   | 0.010482   |
| Number of Imaginary Frequencies   | 0          |

**Frequencies** (Top 3 out of 57)

1. 25.2871 cm⁻¹  
2. 41.4666 cm⁻¹  
3. 58.4299 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C   -1.592057  -0.609504  0.103870
C   -2.819726  0.180990 -0.044615
C   -2.842688  1.468882 -0.384221
O   -1.502831 -1.801723  0.411897
O   -0.434273  0.082716 -0.133557
C    0.790667 -0.659843  0.001749
C    1.923170  0.318237 -0.292712
C    3.193461 -0.457241 -0.568823
C    2.115783  1.280500  0.859023
H   -3.735226 -0.401892  0.154582
H   -3.785601  2.024513 -0.484882
H   -1.927250  2.045747 -0.581922
H    0.853866 -1.070636  1.042385
H    0.777171 -1.507368 -0.732168
H    1.646421  0.908939 -1.211436
H    3.465024 -1.092688  0.308448
H    3.064639 -1.118251 -1.459444
H    4.035224  0.248737 -0.768269
H    2.435340  0.735068  1.779581
H    2.897849  2.035661  0.685494
H    1.157709  1.812087  1.075282
```

---

**7_isobutylacrylate_7_reopt_am1_HEI**

| Datum                              | Value       |
|-----------------------------------|------------|
| AM1 Energy                        | -0.213176  |
| AM1 Free Energy (Quasiharmonic)   | -0.030285  |
| Number of Imaginary Frequencies   | 0          |
Frequencies (Top 3 out of 72)

1. 17.6442 cm⁻¹
2. 26.6172 cm⁻¹
3. 41.6175 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 0.236542 | -0.768195 | 0.006851 |
| C | 1.305510 | -0.556803 | 0.878917 |
| C | 2.631779 | -0.993871 | 0.574353 |
| O | 0.139345 | -1.344360 | -1.104030 |
| O | -0.983680 | -0.241919 | 0.483309 |
| C | -2.115227 | -0.455529 | -0.346762 |
| C | -3.317155 | 0.168302 | 0.363823 |
| C | -4.598087 | -0.297973 | -0.292331 |
| C | -3.220619 | 1.677814 | 0.350659 |
| H | 1.121719 | -0.021727 | 1.813437 |
| H | 2.666893 | -1.729122 | -0.262909 |
| H | 3.186059 | -1.382904 | 1.463078 |
| H | -1.948450 | 0.020551 | -1.348289 |
| H | -2.271469 | -1.556517 | -0.496326 |
| H | -3.504937 | -0.179693 | 1.434804 |
| H | -4.612818 | -0.011084 | -1.371553 |
| H | -4.690649 | -1.408483 | -0.222358 |
| H | -5.482112 | 0.165946 | 0.208155 |
| H | -2.239529 | 1.990619 | 0.784731 |
| H | -3.286285 | 2.067272 | -0.693766 |
| H | -4.046725 | 2.130198 | 0.949987 |
| S | 3.826792 | 0.343508 | 0.063142 |
| C | 2.837504 | 1.522883 | -0.776294 |
| H | 3.060701 | 2.537193 | -0.379843 |
| H | 3.055426 | 1.504246 | -1.866383 |
| H | 1.756075 | 1.288303 | -0.612568 |

7_isobutylacrylate_8_am1_HEI_reopt

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.21395|
| AM1 Free Energy (Quasiharmonic)            | -0.030183|
| Number of Imaginary Frequencies            | 0       |

Frequencies (Top 3 out of 72)
1. 24.3809 cm⁻¹  
2. 34.5613 cm⁻¹  
3. 47.1808 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | X (Å)      | Y (Å)      | Z (Å)      |
|---|------------|------------|------------|
| C |  0.088814  |  0.098434  |  0.120166  |
| C |  1.177566  |  0.899439  | -0.226140  |
| C |  2.308010  |  1.058420  |  0.634746  |
| O | -0.181297  | -0.578364  |  1.142368  |
| O | -0.911412  |  0.060137  | -0.876577  |
| C | -2.065206  | -0.712297  | -0.609606  |
| C | -3.079189  |  0.060405  |  0.235901  |
| C | -4.229847  | -0.841828  |  0.621770  |
| C | -3.574960  |  1.283621  | -0.501325  |
| H |  1.171329  |  1.402475  | -1.195896  |
| H |  2.112905  |  0.714405  |  1.677142  |
| H |  2.722766  |  2.095980  |  0.634663  |
| H | -2.491683  | -0.935174  | -1.625026  |
| H | -1.793069  | -1.667235  | -0.087063  |
| H | -2.537225  |  0.390213  |  1.168584  |
| H | -4.747289  | -1.232340  | -0.287646  |
| H | -3.858691  | -1.709167  |  1.218355  |
| H | -4.974798  | -0.280292  |  1.235943  |
| H | -2.701391  |  1.891981  | -0.841628  |
| H | -4.173228  |  0.989693  | -1.397460  |
| H | -4.218247  |  1.909359  |  0.162618  |
| S |  3.847129  |  0.139801  |  0.125366  |
| C |  3.256403  | -1.312653  | -0.659405  |
| H |  2.156184  | -1.220123  | -0.838862  |
| H |  3.780605  | -1.442826  | -1.631042  |
| H |  3.449897  | -2.202476  | -0.021506  |

**7_isobutylacrylate_8_am1**

| Datum                                | Value  |
|--------------------------------------|--------|
| AM1 Energy                           | -0.137869 |
| AM1 Free Energy (Quasiharmonic)      | 0.011569 |
| Number of Imaginary Frequencies      | 0      |

**Frequencies** (Top 3 out of 57)
1.  23.8069 cm⁻¹
2.  43.7627 cm⁻¹
3.  77.9295 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| C  | -1.376338 | 0.471636 | -0.267850 |
| C  | -2.717759 | 0.122524 | 0.218286  |
| C  | -3.093882 | -1.110216 | 0.554943 |
| O  | -0.972519 | 1.593342 | -0.586827 |
| O  | -0.521651 | -0.593057 | -0.372266 |
| C  | 0.814723 | -0.359910 | -0.836287 |
| C  | 1.778418 | -0.321416 | 0.347375 |
| C  | 3.146414 | -0.796189 | -0.093581 |
| C  | 1.858870 | 1.071199 | 0.934197 |
| H  | -3.394078 | 0.992220 | 0.279253 |
| H  | -4.109272 | -1.327667 | 0.915097 |
| H  | -2.416205 | -1.974368 | 0.492396 |
| H  | 1.018963 | -1.252560 | -1.488204 |
| H  | 0.872932 | 0.582029 | -1.440028 |
| H  | 1.387616 | -1.024236 | 1.136969 |
| H  | 3.101011 | -1.854905 | -0.445455 |
| H  | 3.533386 | -0.161090 | -0.926680 |
| H  | 3.864811 | -0.735757 | 0.759084 |
| H  | 2.365957 | 1.768675 | 0.224472 |
| H  | 2.434617 | 1.056959 | 1.890106 |
| H  | 0.830953 | 1.462646 | 1.133236 |

7_isobutylacrylate_9_reopt_am1_HEI_reopt

| Datum                                                                 | Value     |
|-----------------------------------------------------------------------|-----------|
| AM1 Energy                                                            | -0.21186  |
| AM1 Free Energy (Quasiharmonic)                                       | -0.027182 |
| Number of Imaginary Frequencies                                       | 0         |

Frequencies (Top 3 out of 72)

1.  32.3257 cm⁻¹
2.  46.2902 cm⁻¹
3.  62.7763 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
8_ethylmethacrylate_10_reopt_am1_HEI_reopt

| Datum                              | Value      |
|------------------------------------|------------|
| AM1 Energy                         | -0.205588  |
| AM1 Free Energy (Quasiharmonic)    | -0.050228  |
| Number of Imaginary Frequencies    | 0          |

**Frequencies** (Top 3 out of 63)

1. 15.6004 cm⁻¹
2. 28.4583 cm⁻¹
3. 45.9895 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.201127   |
| AM1 Free Energy (Quasiharmonic)            | -0.04653    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 63)**

1. 31.9297 cm\(^{-1}\)
2. 36.0158 cm\(^{-1}\)
3. 55.6455 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 0.360071 | 0.821131 | -0.235393 |
| C   | 0.406150 | 2.070501 | 0.537895  |
| C   | 1.502048 | 0.484167 | -1.054030 |
| O   | -0.954918| -1.130735| -0.788839 |
| O   | -1.804392| 0.386405 | 0.614072  |
| C   | -2.945832| -0.450697| 0.679471  |
| C   | -3.873751| -0.214348| -0.492227 |
| H   | 1.344891 | 2.132427 | 1.147960  |
| H   | 0.394492 | 2.965415 | -0.139860 |
| H   | -0.465946| 2.156528 | 1.231335  |
| H   | 1.990721 | 1.380850 | -1.507881 |
| H   | 1.252420 | -0.268792| -1.837828 |
| H   | -2.644214| -1.530697| 0.721372  |
| H   | -3.441510| -0.157222| 1.645132  |
| H   | -4.796374| -0.831664| -0.383024 |
| H   | -4.162016| 0.861591 | -0.553523 |
| H   | -3.349595| -0.496680| -1.437765 |
| C   | 2.283822 | -1.313475| 1.022615  |
| H   | 1.180850 | -1.145535| 1.089634  |
| H   | 2.750146 | -1.107849| 2.010611  |
| H   | 2.476519 | -2.372628| 0.744491  |
| S   | 2.972100 | -0.236027| -0.178569 |
### 8_ethylmethacrylate_12_reopt2_am1_HEI

| Datum                          | Value         |
|-------------------------------|---------------|
| AM1 Energy                    | -0.205894     |
| AM1 Free Energy (Quasiharmonic) | -0.050127    |
| Number of Imaginary Frequencies | 0             |

**Frequencies (Top 3 out of 63)**

1. 17.7858 cm⁻¹
2. 40.4684 cm⁻¹
3. 64.8397 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| C     | 0.818398 | 0.847456 | -0.033231 |
| C     | -0.552633 | 1.088232 | -0.209687 |
| C     | -1.167030 | 2.200579 | 0.534807 |
| C     | -1.380300 | 0.302264 | -1.082021 |
| O     | 1.673147  | 1.434819 | 0.674831  |
| O     | 1.338729  | -0.221312 | -0.786560 |
| C     | 2.728490  | -0.476470 | -0.677852 |
| C     | 3.044101  | -1.313564 | 0.542475  |
| H     | -0.404150 | 2.749311  | 1.140908  |
### 8_ethylmethacrylate_1_am1_reopt

#### Datum               Value

| AM1 Energy                | -0.131525              |
| AM1 Free Energy (Quasiharmonic) | -0.010168              |

#### Number of Imaginary Frequencies

| Value                |
|----------------------|
| 0                    |

#### Frequencies (Top 3 out of 48)

| Value                |
|----------------------|
| 1. 28.3179 cm⁻¹      |
| 2. 55.2522 cm⁻¹      |
| 3. 98.8160 cm⁻¹      |

#### AM1 Molecular Geometry in Cartesian Coordinates

| Datum                | Value                |
|----------------------|----------------------|
| C                    | -0.367699            |
| C                    | -1.634983            |
| C                    | -1.533535            |
| C                    | -2.796385            |
| O                    | -0.213440            |
| O                    | 0.752275             |
| C                    | 2.015293             |
| C                    | 3.080279             |
| H                    | -2.544572            |
| H                    | -0.970866            |
| H                    | -0.970891            |
| H                    | -3.764252            |
| H                    | -2.837325            |
| H                    | 2.070208             |
8_ethylmethacrylate_1_reopt_am1_HEI

| Datum                                      | Value  |
|--------------------------------------------|--------|
| AM1 Energy                                 | -0.205365 |
| AM1 Free Energy (Quasiharmonic)           | -0.050376 |
| Number of Imaginary Frequencies           | 0      |

**Frequencies** (Top 3 out of 63)

1. 20.6391 cm$^{-1}$
2. 31.5845 cm$^{-1}$
3. 46.9909 cm$^{-1}$

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -0.651924 | -0.104553 | -0.556650 |
|-----|-----------|-----------|-----------|
| C   | 0.424402  | 0.780377  | -0.392495 |
| C   | 0.299235  | 2.005790  | 0.409499  |
| C   | 1.689547  | 0.475046  | -1.007058 |
| C   | 0.756350  | -1.174265 | -1.205827 |
| O   | -2.352249 | 0.269354  | -0.089092 |
| C   | -2.952249 | 0.057378  | 0.687473  |
| H   | 0.824832  | 2.862906  | -0.086875 |
| H   | -0.771769 | 2.928275  | 0.554505  |
| H   | 0.759785  | 1.879623  | 1.424858  |
| H   | 2.225151  | 1.382695  | -1.378605 |
| H   | 1.595519  | -0.285834 | -1.817025 |
| H   | -3.190489 | -0.655138 | -1.183613 |
| H   | -2.703534 | -1.619350 | 0.279407  |
| H   | -5.009523 | -0.638460 | 0.566000  |
| H   | -3.851441 | 0.076460  | 1.771339  |
| H   | -4.337843 | 1.032345  | 0.316497  |
| C   | 2.149069  | -1.174596 | 1.287567  |
| H   | 1.052881  | -0.974868 | 1.206179  |
| H   | 2.499650  | -0.904270 | 2.307357  |
| H   | 2.338081  | -2.256449 | 1.114119  |
| S   | 3.012663  | -0.209127 | 0.105297  |
8_ethylmethacrylate_2_am1_HEI

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.205745 |
| AM1 Free Energy (Quasiharmonic)      | -0.050626 |
| Number of Imaginary Frequencies      | 0         |

**Frequencies** (Top 3 out of 63)

1. 18.0684 cm⁻¹
2. 38.3243 cm⁻¹
3. 59.5883 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | x   | y   | z     |
|------|-----|-----|-------|
| C    | 0.699674 | 0.988181 | 0.063309 |
| C    | -0.624854 | 1.015353 | -0.399245 |
| C    | -1.445185 | 2.200181 | -0.095777 |
| C    | -1.213163 | -0.056666 | -1.152536 |
| O    | 1.362024 | 1.826650 | 0.722952 |
| O    | 1.428957 | -0.166167 | -0.274977 |
| C    | 2.778190 | -0.201273 | 0.171089 |
| C    | 3.359449 | -1.520009 | -0.289918 |
| H    | -0.852301 | 2.968740 | 0.459459 |
| H    | -1.834615 | 2.670986 | -1.036451 |
| H    | -2.335050 | 1.924534 | 0.528426 |
| H    | -0.455752 | -0.736723 | -1.606338 |
| H    | -1.931670 | 0.301788 | -1.930113 |
| H    | 3.341435 | 0.665847 | -0.264822 |
| H    | 2.807767 | -0.113336 | 1.289387 |
| H    | 4.420258 | -1.598284 | 0.046563 |
| H    | 3.322481 | -1.594044 | -1.402611 |
| H    | 2.776530 | -2.371358 | 0.134912 |
| C    | -1.759459 | -1.179833 | 1.432636 |
| H    | -0.992790 | -0.373586 | 1.546845 |
| H    | -1.305284 | -2.159246 | 1.698491 |
| H    | -2.611653 | -0.978338 | 2.117615 |
| S    | -2.340320 | -1.210403 | -0.221407 |

8_ethylmethacrylate_2_am1_reopt
| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.131638 |
| AM1 Free Energy (Quasiharmonic)            | -0.009679 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 48)

1. 30.9608 cm\(^{-1}\)
2. 66.2601 cm\(^{-1}\)
3. 94.7362 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| C | -0.211723 | -0.386726 | -0.167803 |
| C | -1.608458 | 0.033754  | 0.061462  |
| C | -1.870752 | 1.490133  | 0.109099  |
| C | -2.557371 | -0.898607 | 0.213300  |
| O | 0.229515  | -1.537854 | -0.315097 |
| O | 0.663738  | 0.655581  | -0.541110 |
| C | 2.044647  | 0.336745  | 0.754937  |
| C | 2.743866  | 0.008468  | 0.287874  |
| H | -2.953044 | 1.700466  | 0.927589  |
| H | -1.269668 | 1.960359  | -0.856154 |
| H | -1.563319 | 1.965681  | 0.385926  |
| H | -3.609316 | -0.634744 | 0.172364  |
| H | -2.329350 | -1.973876 | -1.269696 |
| H | 2.125466  | -0.511791 | 1.492607  |
| H | 2.443404  | 1.282347  | 0.563873  |
| H | 3.833156  | -0.140712 | 1.192486  |
| H | 2.615110  | 0.836090  |           |
| H | 2.320279  | -0.928235 |           |

**8_ethylmethacrylate_3_am1_reopt**

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.131485 |
| AM1 Free Energy (Quasiharmonic)            | -0.009882 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 48)
1. 19.3063 cm$^{-1}$
2. 64.6572 cm$^{-1}$
3. 69.4035 cm$^{-1}$

AM1 Molecular Geometry in Cartesian Coordinates

| Datum | Value |
|-------|-------|
| AM1 Energy | -0.205589 |
| AM1 Free Energy (Quasiharmonic) | -0.049979 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 63)

1. 22.9668 cm$^{-1}$
2. 35.7995 cm$^{-1}$
3. 41.8504 cm$^{-1}$

AM1 Molecular Geometry in Cartesian Coordinates
8_ethylmethacrylate_4_am1

| Datum                                      | Value      |
|--------------------------------------------|------------|
| AM1 Energy                                 | -0.122023  |
| AM1 Free Energy (Quasiharmonic)           | -0.000901  |
| Number of Imaginary Frequencies           | 0          |

**Frequencies (Top 3 out of 48)**

1. 42.7633 cm⁻¹  
2. 51.2104 cm⁻¹  
3. 93.9389 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 0.743580 | 0.340734 | 0.493238 |
| C   | -0.445043| 0.988677 | 0.128481 |
| C   | -0.492408| 1.977912 | -0.957642|
| C   | -1.660966| 0.690598 | 0.840198 |
| O   | 0.979799 | -0.513528| 1.383523 |
| O   | 1.878723 | 0.715174 | -0.251840|
| C   | 3.109752 | 0.184174 | 0.093384 |
| C   | 3.251644 | -1.257839| -0.550539|
| H   | -0.640326| 3.015297 | -0.554637|
| H   | 0.450024 | 1.977626 | -1.558453|
| H   | -1.348742| 1.768251 | -1.650120|
| H   | -2.326844| 1.580880 | 0.953111 |
| H   | -1.468163| 0.213508 | 1.829539 |
| H   | 3.885314 | 0.814834 | -0.303801|
| H   | 3.210873 | 0.017069 | 1.207518 |
| H   | 4.253718 | -1.690047| -0.319803|
| H   | 2.456591 | -1.935589| -0.154138|
| H   | 3.134954 | -1.182702| -1.657452|
| C   | -1.836041| -1.681097| -0.740736|
| H   | -0.766793| -1.358763| -0.694433|
| H   | -2.136810| -1.813683| -1.802731|
| H   | -1.949460| -2.650665| -0.208403|
| S   | -2.852851| -0.459259| 0.001377 |
8_ethylmethacrylate_4_reopt_am1_HEI

| Datum                                      | Value      |
|--------------------------------------------|------------|
| AM1 Energy                                 | -0.205605  |
| AM1 Free Energy (Quasiharmonic)           | -0.049898  |
| Number of Imaginary Frequencies           | 0          |

Frequencies (Top 3 out of 63)

1. 19.5074 cm⁻¹  
2. 45.5679 cm⁻¹  
3. 47.5816 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| C   | -0.745838 | -0.063138 | -0.221061 |
| C   | 0.363458  | 0.794830  | -0.263573 |
| C   | 0.410082  | 2.034339  | 0.525209  |
| C   | 1.494050  | 0.447470  | -1.084058 |
| O   | -0.982639 | -1.140414 | -0.821162 |
| O   | -1.785815 | 0.354799  | 0.631925  |
| C   | -2.946031 | -0.457056 | 0.684430  |
| C   | -3.881642 | -0.162214 | -0.467702 |
| H   | 0.863901  | 2.869178  | -0.070848 |
| H   | -0.612126 | 2.353721  | 0.847084  |
| H   | 1.035551  | 1.909110  | 1.448269  |
| H   | 1.978199  | 1.335547  | -1.559144 |
| H   | 1.241036  | -0.320749 | -1.851977 |
| H   | -2.669136 | -1.544492 | 0.688551  |
### AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 0.358645 | 0.891489 | -0.006354 |
| C | 1.130388 | -0.361685 | 0.154796 |
| C | 1.625731 | -0.946540 | -1.114450 |
| C | 1.416181 | -0.860770 | 1.360364 |
| O | 0.808514 | 1.970821 | -0.394425 |
| O | -0.978506 | 0.973070 | 0.295385 |
| C | -1.706203 | -0.218631 | 0.594386 |
| C | -2.212278 | -0.873439 | -0.668596 |
| H | 0.768881 | -1.282503 | -1.750782 |
| H | 2.204567 | -0.175660 | -1.684422 |
| H | 2.289751 | -1.823994 | -0.920908 |
| H | 2.033503 | -1.760814 | 1.485242 |
| H | 1.062528 | -0.398907 | 2.292215 |
| H | -1.083843 | -0.927396 | 1.200171 |
| H | -2.561406 | 0.158633 | 1.221019 |
| H | -2.781994 | -0.137945 | -1.286279 |
| H | -1.361948 | -1.260999 | -1.279832 |
| H | -2.884881 | -1.724086 | -0.404980 |
8_ethylmethacrylate_5_reopt_am1_HEI

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.205351 |
| AM1 Free Energy (Quasiharmonic)            | -0.050516 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 63)

1. 22.2570 cm⁻¹
2. 31.8113 cm⁻¹
3. 32.6136 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| C | -0.646962 | -0.083326 | 0.536383 |
| C | 0.418738  | 0.808379  | 0.349552 |
| C | 0.281439  | 2.030685  | -0.455604 |
| C | 1.689165  | 0.532214  | 0.968549 |
| O | -0.725672 | -1.158217 | 1.181757 |
| O | -1.851017 | 0.282679  | -0.095043 |
| C | -2.944151 | -0.605656 | 0.095470 |
| C | -4.120127 | -0.024814 | -0.659195 |
| H | -0.682795 | 2.048080  | -1.019830 |
| H | 0.315108  | 2.947318  | 0.192329 |
| H | 1.120620  | 2.118267  | -1.193377 |
| H | 1.604075  | -0.199963 | 1.805350 |
| H | 2.218508  | 1.457379  | 1.304150 |
| H | -2.675215 | -1.623323 | -0.293423 |
| H | -3.169745 | -0.696297 | 1.190932 |
| H | -5.006753 | -0.691220 | -0.538867 |
| H | -4.370178 | 0.990146  | -0.268975 |
| H | -3.878252 | 0.069220  | -1.744373 |
| C | 2.161647  | -1.312767 | -1.159735 |
| H | 1.058638  | -1.177235 | -1.040366 |
| H | 2.433653  | -2.356115 | -0.888201 |
| H | 2.444645  | -1.128636 | -2.218921 |
| S | 3.010170  | -0.176350 | -0.127244 |

8_ethylmethacrylate_6_am1_HEI
### Datum

| Datum                                      | Value  |
|--------------------------------------------|--------|
| AM1 Energy                                 | -0.205964 |
| AM1 Free Energy (Quasiharmonic)            | -0.050138 |
| Number of Imaginary Frequencies            | 0      |

**Frequencies** *(Top 3 out of 63)*

1. 18.7711 cm⁻¹  
2. 46.3003 cm⁻¹  
3. 58.0547 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

```plaintext
C  0.819077  0.602482  -0.187843  
C  -0.438231  0.955843  0.325179  
C  -0.984146  2.280313  -0.016529  
C  -1.213275  0.086623  1.166176  
O  1.614304  1.233965  -0.926604  
O  1.282687  -0.670502  0.193128  
C  2.550040  -1.073457  -0.296299  
C  3.673638  -0.511399  0.547199  
H  -0.263325  2.863809  -0.641356  
H  -1.945386  2.184724  -0.586032  
H  -1.206001  2.874387  0.908685  
H  -1.788262  0.639228  1.949395  
H  -0.606548  -0.725487  1.629316  
H  2.522352  -2.195267  -0.226612  
H  2.678398  -0.763048  -1.366939  
H  4.655891  -0.896930  0.185553  
H  3.542446  -0.799154  1.617019  
H  3.664813  0.603540  0.475005  
C  -2.138001  -1.008789  -1.320998  
H  -1.931356  -2.078243  -1.544120  
H  -1.216579  -0.405671  -1.516064  
H  -2.958415  -0.653317  -1.981754  
S  -2.621160  -0.821623  0.354025  
```

**8_ethylmethacrylate_6_am1**

| Datum                                      | Value  |
|--------------------------------------------|--------|
| AM1 Energy                                 | -0.122031 |
| AM1 Free Energy (Quasiharmonic)            | 2.3e-05 |
**Datum** | **Value**
---|---
Number of Imaginary Frequencies | 0

**Frequencies** (Top 3 out of 48)

1. 54.2624 cm⁻¹  
2. 64.5481 cm⁻¹  
3. 91.1780 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|  |  |
|---|---|
| C | -0.388705 | 0.863092 | -0.199515 |
| C | -1.082049 | -0.443231 | -0.118030 |
| C | -1.871183 | -0.647119 | 1.120807 |
| C | -1.046936 | -1.317770 | -1.126438 |
| O | -0.850765 | 1.908633 | -0.657290 |
| O | 0.880470 | 1.032358 | 0.296146 |
| C | 1.592529 | -0.107539 | 0.781008 |
| C | 2.341859 | -0.791156 | -0.337665 |
| H | -1.224963 | -0.519234 | 2.024989 |
| H | -2.696428 | 0.108122 | 1.171352 |
| H | -2.321998 | -1.669207 | 1.145913 |
| H | -1.591269 | -2.271246 | -1.087593 |
| H | -0.482708 | -1.134898 | -2.051173 |
| H | 2.305986 | 0.337531 | 1.528562 |
| H | 0.900333 | -0.818703 | 1.302614 |
| H | 1.627977 | -1.259629 | -1.058167 |
| H | 2.969583 | -0.053392 | -0.893121 |
| H | 3.002759 | -1.584929 | 0.084778 |

**8_ethylmethacrylate_7_reopt_am1_HEI_reopt**

| Datum | Value |
|---|---|
| AM1 Energy | -0.205745 |
| AM1 Free Energy (Quasiharmonic) | -0.050627 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

1. 18.0680 cm⁻¹  
2. 38.3065 cm⁻¹
8_ethylmethacrylate_8_am1_HEI

| Datum                                    | Value         |
|------------------------------------------|---------------|
| AM1 Energy                               | -0.200791     |
| AM1 Free Energy (Quasiharmonic)          | -0.046298     |
| Number of Imaginary Frequencies          | 0             |

Frequencies (Top 3 out of 63)

1. 29.3135 cm⁻¹  
2. 33.8012 cm⁻¹  
3. 43.7940 cm⁻¹  

AM1 Molecular Geometry in Cartesian Coordinates
### 8_ethylmethacrylate_9_reopt2_am1_HEI

| Datum                                      | Value               |
|--------------------------------------------|---------------------|
| AM1 Energy                                 | -0.205598           |
| AM1 Free Energy (Quasiharmonic)            | -0.049918           |
| Number of Imaginary Frequencies            | 0                   |

**Frequencies** (Top 3 out of 63)

1. 19.6338 cm⁻¹
2. 42.1230 cm⁻¹
3. 46.6461 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |     |     |
|---|-----|-----|
| C | 0.750853 | 0.349814 | -0.491983 |
| C | -0.450656 | 0.976364 | -0.128253 |
| C | -0.520859 | 1.912688 | 1.002709 |
| C | -1.651306 | 0.684001 | -0.866577 |
ethylocrotonate_10_reopt_am1_HEI

| Datum                              | Value    |
|------------------------------------|----------|
| AM1 Energy                         | -0.196854|
| AM1 Free Energy (Quasiharmonic)    | -0.041197|
| Number of Imaginary Frequencies    | 0        |

**Frequencies (Top 3 out of 63)**

1. 36.1406 cm⁻¹
2. 44.8047 cm⁻¹
3. 52.6454 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|  |  |  |  |
|---|---|---|---|
| O | 1.019601 | -0.448110 | -1.423487 |
| O | 1.859183 | 0.681430 | 0.311399 |
| C | 3.112410 | 0.131198 | -0.055734 |
| C | 3.279573 | -1.272558 | 0.483993 |
| H | 0.492287 | 2.294555 | 1.282222 |
| H | -1.167446 | 2.793737 | 0.751681 |
| H | -0.965026 | 1.425300 | 1.910530 |
| H | -1.437680 | 0.219004 | -1.857535 |
| H | -2.319129 | 1.572310 | -0.983626 |
| H | 3.235583 | 0.133198 | -1.171034 |
| H | 3.861615 | 0.828290 | 0.410213 |
| H | 4.298562 | -1.657943 | 0.244470 |
| H | 3.136866 | -1.287028 | 1.590310 |
| H | 2.513218 | -1.938664 | 0.017540 |
| C | -1.859932 | -1.607707 | 0.837930 |
| H | -0.808554 | -1.229537 | 0.877317 |
| H | -1.871044 | -2.690227 | 0.355163 |
| H | -2.259100 | -1.699081 | 1.871511 |
| S | -2.856307 | -0.484643 | -0.068410 |
### ethylcrotonate_11_am1_HEI

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.197016 |
| AM1 Free Energy (Quasiharmonic)      | -0.041493 |
| Number of Imaginary Frequencies      | 0         |

**Frequencies (Top 3 out of 63)**

1. 18.9487 cm\(^{-1}\)
2. 44.0715 cm\(^{-1}\)
3. 71.2223 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|                  |           |           |           |
|------------------|-----------|-----------|-----------|
| C                | -0.836709 | 0.074763  | -0.886008 |
| C                | 0.062944  | 0.602726  | 0.043390  |
| C                | 1.446721  | 0.800455  | 0.843690  |
| C                | 2.062288  | 2.048237  | 0.296353  |
| O                | -0.683740 | -0.279017 | -2.079328 |
| O                | -2.194446 | -0.129824 | -0.555439 |
| C                | -2.598613 | 0.193284  | 0.761318  |
| C                | -4.073377 | -0.137099 | 0.870089  |
| H                | 1.639986  | 0.717103  | -1.378900 |
| H                | 1.836320  | 2.136324  | 1.386186  |
| H                | 3.172132  | 2.045872  | 0.161840  |
| H                | 1.644609  | 2.945961  | -0.222935 |
| H                | -2.007150 | -0.405856 | 1.504948  |
| H                | -2.426969 | 1.285524  | 0.959722  |
ethylcrotonate_12_reopt_am1_HEI_reopt

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.197016   |
| AM1 Free Energy (Quasiharmonic)            | -0.041493   |
| Number of Imaginary Frequencies            | 0           |

Frequencies (Top 3 out of 63)

1. 18.9461 cm⁻¹
2. 44.0681 cm⁻¹
3. 71.2196 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|          |          |          |
|----------|----------|----------|
| C -0.836705 | 0.074718 | 0.886006 |
| C -0.062943 | 0.602727 | -0.043371 |
| C -1.446719 | 0.800454 | 0.280179 |
| C -2.062280 | 2.048253 | -0.296298 |
| O 0.683734  | -0.279111| 2.079310 |
| O 2.194439  | -0.129869| 0.555428 |
| C 2.598618  | 0.193317 | -0.761306 |
| C 4.073385  | -0.137051| -0.870083 |
| H -1.639984 | 0.717080 | 1.378812 |
| H -1.644621 | 2.945963 | 0.223033 |
| H -1.836287 | 2.136383 | -1.386122 |
| H -3.172127 | 2.045877 | -0.161813 |
| H 2.426969  | 1.285566 | -0.959651 |
| H 2.007166  | -0.405785| -1.504975 |
| H 4.658645  | 0.453191 | -0.125876 |
| H 4.243517  | -1.220710| -0.666326 |
| H 4.437308  | 0.104097 | -1.896585 |
| C -1.692694 | -2.001709| -0.343431 |
| H -0.630394 | -1.774477| -0.078202 |
ethylcrotonate_14_reopt_am1_HEI

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.200668 |
| AM1 Free Energy (Quasiharmonic)            | -0.045294 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 63)

1. 25.8539 cm⁻¹
2. 44.1519 cm⁻¹
3. 56.1580 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C     | 0.860656 | 0.864341 | -0.673359 |
|-------|----------|----------|-----------|
| C     | -0.498169| 1.100529 | -0.456660 |
| C     | -1.265206| 0.560248 | 0.623225  |
| C     | -2.314940| 1.485153 | 1.181161  |
| O     | 1.625654 | 1.271536 | -1.583199 |
| O     | 1.499196 | 0.054936 | 0.284392  |
| C     | 2.886514 | -0.173865| 0.079302  |
| C     | 3.356734 | -1.069980| 1.204258  |
| H     | -0.628368| 0.129853 | 1.434851  |
| H     | -2.997742| 0.940954 | 1.879281  |
| H     | -1.821800| 2.315863 | 1.744300  |
| H     | -2.926680| 1.931759 | 0.360968  |
| H     | 3.044908 | -0.659856| -0.919701 |
| H     | 3.434255 | 0.805537 | 0.084210  |
| H     | 2.789587 | -2.030900| 1.198509  |
| H     | 4.444239 | -1.285859| 1.080148  |
| H     | 3.192716 | -0.575128| 2.190734  |
| C     | -1.515721| -1.680381| -1.196159 |
| H     | -2.229149| -1.825669| -2.036423 |
| H     | -1.107585| -2.669757| -0.893985 |
| H     | -0.675873| -1.021850| -1.532701 |
| S     | -2.348662| -0.932454| 0.151480  |
| H     | -0.997924| 1.736081 | -1.194030 |
ethylcrotonate_1_am1_HEI

| Datum                              | Value       |
|------------------------------------|-------------|
| AM1 Energy                         | -0.200831   |
| AM1 Free Energy (Quasiharmonic)    | -0.044807   |
| Number of Imaginary Frequencies    | 0           |

**Frequencies** (Top 3 out of 63)

1. 29.4746 cm⁻¹  
2. 40.4139 cm⁻¹  
3. 59.1007 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 0.927833 | -0.771149 | -0.570216 |
| C      | -0.454114 | -0.944334 | -0.664874 |
| C      | -1.389225 | -0.697610 | 0.389801  |
| C      | -2.544078 | -1.662750 | 0.452008  |
| O      | 1.830850  | -0.948833 | -1.425783 |
| O      | 1.402825  | -0.351042 | 0.686719  |
| C      | 2.804098  | -0.207173 | 0.837069  |
| C      | 3.281359  | 1.133428  | 0.322425  |
| H      | -0.897452 | -0.586538 | 1.387546  |
| H      | -3.327585 | -1.304129 | 1.164222  |
| H      | -3.009494 | -1.789937 | -0.554775 |
| H      | -2.179997 | -2.661196 | 0.799731  |
| H      | 2.968089  | -0.288318 | 1.946486  |
| H      | 3.346346  | -1.037594 | 0.312114  |
| H      | 4.373073  | 1.253807  | 0.517191  |
| H      | 3.093438  | 1.192609  | -0.777351 |
| H      | 2.729291  | 1.964030  | 0.822299  |
| C      | -1.251633 | 2.000625  | -0.652483 |
| H      | -0.380093 | 1.411466  | -1.034014 |
| H      | -0.882421 | 2.816413  | 0.006738  |
| H      | -1.797129 | 2.449297  | -1.511129 |
| S      | -2.332538 | 0.946961  | 0.236731  |
| H      | -0.830297 | -1.278503 | -1.636622 |
| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.137799 |
| AM1 Free Energy (Quasiharmonic)            | -0.016604 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies (Top 3 out of 48)**

1. 41.5939 cm⁻¹
2. 62.6763 cm⁻¹
3. 93.7381 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C    0.018633  0.365276  -0.000004
C    1.254538 -0.422035  0.000001
C    2.455458  0.170958  -0.000002
C    3.730879 -0.568335  0.000004
O   -0.122838  1.592889 -0.000011
O   -1.108267 -0.413253  0.000001
C   -2.365953  0.285343 -0.000007
C   -3.438474 -0.776473  0.000017
H    1.122017 -1.515251  0.000008
H    2.535574  1.274044 -0.000008
H    4.328291 -0.293704  0.906341
H    3.576515 -1.675296  0.000011
H    4.328292 -0.293715 -0.906336
H   -2.416873  0.934247  0.913064
H   -2.416881  0.934213 -0.913102
H   -4.439044 -0.282044  0.000012
H   -3.349772 -1.424012 -0.904753
H   -3.349765 -1.423977  0.904811
```

**ethylcrotonate_2_am1**

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.137914 |
| AM1 Free Energy (Quasiharmonic)            | -0.016141 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies (Top 3 out of 48)**
1. 49.4426 cm⁻¹
2. 65.7857 cm⁻¹
3. 92.0254 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | 0.077044 | 0.135040 | -0.218328 |
| C    | -1.251320 | -0.453854 | -0.024012 |
| C    | -2.346009 | 0.313553  | 0.056748  |
| C    | -3.705672 | -0.221786 | 0.251596  |
| O    | 0.388432  | 1.325212  | -0.331476 |
| O    | 1.068359  | -0.808637 | -0.283752 |
| C    | 2.413888  | -0.348716 | -0.470532 |
| C    | 3.017052  | 0.105514  | 0.835900  |
| H    | -1.278528 | -1.552307 | 0.048996  |
| H    | -2.265989 | 1.413772  | -0.022718 |
| H    | -4.147083 | 0.197244  | 1.191445  |
| H    | -4.359331 | 0.082537  | -0.605069 |
| H    | -3.713262 | -1.337101 | 0.323697  |
| H    | 2.933529  | -1.260908 | -0.870876 |
| H    | 2.432947  | 0.474801  | -1.231437 |
| H    | 2.947815  | -0.701926 | 1.603323  |
| H    | 4.090657  | 0.367161  | 0.680558  |
| H    | 2.475009  | 1.005625  | 1.215674  |

**ethylcrotonate_2_reopt_am1_HEI_reopt**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.200668 |
| AM1 Free Energy (Quasiharmonic)            | -0.045294 |
| Number of Imaginary Frequencies            | 0       |

**Frequencies (Top 3 out of 63)**

1. 25.8691 cm⁻¹
2. 44.1632 cm⁻¹
3. 56.1652 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
| C       | 0.860710   | -0.864154 | 0.673508 |
|---------|------------|-----------|----------|
| C       | -0.498114  | -1.100350 | 0.456826 |
| C       | -1.265114  | -0.560284 | -0.623200|
| C       | -2.314708  | -1.485379 | -1.181098|
| O       | 1.625663   | -1.271139 | 1.583481 |
| O       | 1.499314   | -0.055026 | -0.284434|
| C       | 2.886608   | 0.173870  | -0.079292|
| C       | 3.356832   | 1.069920  | -1.204300|
| H       | -0.628241  | -0.129973 | -1.434847|
| H       | -2.997309  | -0.941417 | -1.879598|
| H       | -1.821415  | -2.316292 | -1.743802|
| H       | -2.926674  | -1.931678 | -0.360904|
| H       | 3.044934   | 0.659948  | 0.919681 |
| H       | 3.434397   | -0.805507 | -0.084102|
| H       | 2.789636   | 2.030813  | -1.198649|
| H       | 4.444323   | 1.285861  | -1.080161|
| H       | 3.192878   | 0.574982  | -2.190744|
| C       | -1.516214  | 1.680375  | 1.196082 |
| H       | -1.108053  | 2.669582  | 0.893974 |
| H       | -0.676421  | 1.021914  | 1.532899 |
| H       | -2.229888  | 1.825656  | 2.036141 |
| S       | -2.348755  | 0.932324  | -0.151733|
| H       | -0.997907  | -1.735749 | 1.194304 |

**ethylcrotonate_3_am1_HEI**

| Datum                              | Value       |
|------------------------------------|-------------|
| AM1 Energy                         | -0.200903   |
| AM1 Free Energy (Quasiharmonic)    | -0.04484    |
| Number of Imaginary Frequencies    | 0           |

**Frequencies** (Top 3 out of 63)

1. 30.8552 cm⁻¹
2. 44.0455 cm⁻¹
3. 54.8769 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C       | -0.950317  | 0.125730  | 0.759958 |
|---------|------------|-----------|----------|
| C       | 0.346307   | 0.634679  | 0.852813 |
| C       | 1.231593   | 0.838454  | -0.252652|
| C       | 2.104024   | 2.061981  | -0.149509|
| Datum                        | Value          |
|------------------------------|----------------|
| AM1 Energy                   | -0.137102      |
| AM1 Free Energy (Quasiharmonic) | -0.01605      |
| Number of Imaginary Frequencies | 0              |

**Frequencies (Top 3 out of 48)**

1. 44.6530 cm\(^{-1}\)
2. 59.7331 cm\(^{-1}\)
3. 93.7881 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C    | 0.012474 | 0.900161 | 0.000002 |
|------|----------|----------|----------|
| C    | -1.428876 | 0.639219 | 0.000002 |
| C    | -1.964377 | -0.587356 | -0.000002 |
| C    | -3.417133 | -0.841587 | -0.000002 |
| O    | 0.574113  | 2.000307  | 0.000003  |
| O    | 0.800007  | -0.221179  | -0.000001 |
| C    | 2.222072  | -0.002293  | -0.000001 |
| C    | 2.860268  | -1.369925  | -0.000000 |
| H    | -2.039379 | 1.557852  | 0.000005  |
## ethylcrotonate_4_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.196351   |
| AM1 Free Energy (Quasiharmonic)            | -0.040645   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 63)

1. 35.5541 cm\(^{-1}\)
2. 44.0472 cm\(^{-1}\)
3. 54.5815 cm\(^{-1}\)

## AM1 Molecular Geometry in Cartesian Coordinates

| C       | 1.177909 | 0.587743 | -0.539085 |
|---------|----------|----------|-----------|
| C       | -0.114718| 1.083338 | -0.356908 |
| C       | -1.118678| 0.470260 | 0.463021  |
| C       | -1.972093| 1.442472 | 1.236571  |
| O       | 2.122712 | 1.017511 | -1.246716 |
| O       | 1.504609 | -0.551052| 0.222339  |
| C       | 2.793124 | -1.108051| 0.035479  |
| C       | 3.829135 | -0.401212| 0.882998  |
| H       | -0.713725| -0.322535| 1.139871  |
| H       | -1.347280| 1.964615 | 2.002590  |
| H       | -2.409935| 2.212671 | 0.557384  |
| H       | -2.805847| 0.914137 | 1.760922  |
| H       | 2.678039 | -2.178477| 0.359780  |
| H       | 3.088925 | -1.069591| -1.046268 |
| H       | 3.533213 | -0.416487| 1.958487  |
| H       | 4.821337 | -0.898960| 0.773053  |
| H       | 3.910149 | 0.662576 | 0.551188  |
| C       | -3.404983| -1.293057| 0.214594  |
| H       | -4.189802| -0.615445| 0.620440  |
### ethylcrotonate_4_am1

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.137224   |
| AM1 Free Energy (Quasiharmonic)            | -0.015608   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 48)

1. 43.0055 cm⁻¹
2. 69.3824 cm⁻¹
3. 90.5986 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

|   |       |       |       |
|---|-------|-------|-------|
| C | 0.122711 | 0.688254 | -0.099292 |
| C | -1.331197 | 0.647946 | 0.078617  |
| C | -2.063130 | -0.468485 | -0.016178 |
| C | -3.526349 | -0.500682 | 0.165255  |
| O | 0.856804  | 1.677650 | -0.016863 |
| O | 0.695130  | -0.521638 | -0.396690 |
| C | 2.116806  | -0.557998 | -0.582772 |
| C | 2.835033  | -0.613867 | 0.743060  |
| H | -1.771933 | 1.634133 | 0.301381  |
| H | -1.585290 | -1.439605 | -0.240973 |
| H | -4.015332 | -0.888926 | -0.764146 |
| H | -3.788942 | -1.187969 | 1.009230  |
| H | -3.945735 | 0.510831  | 0.389358  |
| H | 2.265039  | -1.502040 | -1.173633 |
| H | 2.445226  | 0.331088  | -1.182156 |
| H | 2.467248  | -1.471977 | 1.354607  |
| H | 3.930593  | -0.735594 | 0.569332  |
| H | 2.660406  | 0.330958  | 1.313287  |

### ethylcrotonate_5_am1
### SI_sqm_esters.md

**Datum** | **Value**  
--- | ---  
AM1 Energy | -0.137799  
AM1 Free Energy (Quasiharmonic) | -0.016604  
Number of Imaginary Frequencies | 0  

**Frequencies (Top 3 out of 48)**

1. 41.5942 cm⁻¹  
2. 62.6763 cm⁻¹  
3. 93.7373 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 0.018633 | 0.365278 | -0.000029 |
|-----|----------|----------|-----------|
| C   | 1.254538 | -0.422034| 0.000013  |
| C   | 2.455459 | 0.170958 | 0.000003  |
| C   | 3.730878 | -0.568337| 0.000043  |
| O   | -0.122838| 1.592891 | -0.000072 |
| O   | -1.108267| -0.413251| -0.000016 |
| C   | -2.365953| 0.285342 | -0.000061 |
| C   | -3.438473| -0.776475| 0.000098  |
| H   | 1.122016 | -1.515250| 0.000051  |
| H   | 2.535576 | 1.274044 | -0.000036 |
| H   | 4.328300 | -0.293745| -0.906300 |
| H   | 4.328282 | -0.293679| 0.906377  |
| H   | 3.576513 | -1.675298| 0.000081  |
| H   | -2.416855| 0.934343 | 0.912942  |
| H   | -2.416903| 0.934117 | -0.913223 |
| H   | -4.439044| -0.282047| 0.000058  |
| H   | -3.349787| -1.424112| -0.904603 |
| H   | -3.349747| -1.423881| 0.904960  |

---

**ethylcrotonate_5_reopt_am1_HEI**

**Datum** | **Value**  
--- | ---  
AM1 Energy | -0.201313  
AM1 Free Energy (Quasiharmonic) | -0.045343  
Number of Imaginary Frequencies | 0  

**Frequencies (Top 3 out of 63)**

---
1.  32.2044 cm\(^{-1}\)  
2.  42.0531 cm\(^{-1}\)  
3.  59.4919 cm\(^{-1}\)  

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---|--------------|--------------|--------------|
| C | -0.885440    | -0.559895    | 0.159643     |
| C | 0.345614     | -0.787008    | -0.458500    |
| C | 1.577798     | -0.756438    | 0.271665     |
| C | 2.596386     | -1.778382    | -0.159534    |
| O | -1.212528    | -0.343717    | 1.352209     |
| O | -1.973738    | -0.604865    | -0.737464    |
| C | -3.269678    | -0.438819    | -0.191708    |
| C | -3.613214    | 1.024712     | -0.017139    |
| H | 1.417288     | -0.777918    | 1.378393     |
| H | 3.590131     | -1.575854    | 0.310897     |
| H | 2.258942     | -2.791812    | 0.151120     |
| H | 2.719679     | -1.772136    | -1.269119    |
| H | -3.948828    | -0.918755    | -0.948538    |
| H | -3.358384    | -0.975014    | 0.790145     |
| H | -4.661054    | 1.133146     | 0.349567     |
| H | -2.912790    | 1.479618     | 0.725158     |
| H | -3.509115    | 1.570342     | -0.984574    |
| C | 1.383104     | 2.083786     | -0.230876    |
| H | 1.328235     | 2.767815     | 0.644034     |
| H | 0.381615     | 1.612023     | -0.392518    |
| H | 1.664096     | 2.671141     | -1.132081    |
| S | 2.584079     | 0.838615     | 0.047058     |
| H | 0.367628     | -0.973195    | -1.534679    |

**ethylcrotonate_6_am1_HEI**

| Datum                                      | Value  |
|--------------------------------------------|--------|
| AM1 Energy                                 | -0.201058 |
| AM1 Free Energy (Quasiharmonic)            | -0.04578 |
| Number of Imaginary Frequencies            | 0      |

**Frequencies (Top 3 out of 63)**

1.  28.7430 cm\(^{-1}\)  
2.  41.0021 cm\(^{-1}\)  
3.  58.4175 cm\(^{-1}\)
AM1 Molecular Geometry in Cartesian Coordinates

| Element | x          | y          | z          |
|---------|------------|------------|------------|
| C       | -0.829318  | 0.310491   | 0.361087   |
| C       | 0.297026   | 0.667820   | -0.382552  |
| C       | 1.589700   | 0.806397   | 0.218625   |
| C       | 2.428210   | 1.930105   | -0.330859  |
| O       | -1.010851  | 0.086588   | 1.582856   |
| O       | -1.999346  | 0.197665   | -0.418564  |
| C       | -3.186195  | -0.128097  | 0.290201   |
| C       | -4.306291  | -0.187127  | -0.725653  |
| H       | 1.538738   | 0.839523   | 1.335443   |
| H       | 2.001137   | 2.910632   | -0.004610  |
| H       | 3.480844   | 1.861786   | 0.039475   |
| H       | 2.441069   | 1.906598   | -1.446969  |
| H       | -3.056865  | -1.115110  | 0.808445   |
| H       | -3.387002  | 0.653700   | 1.069865   |
| H       | -4.088985  | -0.960471  | -1.500032  |
| H       | -5.263228  | -0.443009  | -0.212355  |
| H       | -4.418837  | 0.797272   | -1.238694  |
| C       | 1.695814   | -2.050789  | -0.210329  |
| H       | 1.813849   | -2.709228  | 0.677867   |
| H       | 0.632934   | -1.707738  | -0.275299  |
| H       | 1.954032   | -2.627630  | -1.125034  |
| S       | 2.756963   | -0.662426  | -0.081721  |
| H       | 0.188811   | 0.825676   | -1.458020  |

ethylothiocrotonate_6_am1

| Datum                              | Value  |
|------------------------------------|--------|
| AM1 Energy                         | -0.129237 |
| AM1 Free Energy (Quasiharmonic)    | -0.007566 |
| Number of Imaginary Frequencies    | 0      |

**Frequencies** (Top 3 out of 48)

1. 23.9699 cm⁻¹
2. 72.6289 cm⁻¹
3. 98.5637 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
**ethylcrotonate_7_am1_HEI**

| Datum                        | Value     |
|------------------------------|-----------|
| AM1 Energy                   | -0.201318 |
| AM1 Free Energy (Quasiharmonic) | -0.04533 |
| Number of Imaginary Frequencies | 0        |

**Frequencies** (Top 3 out of 63)

1. 33.7312 cm⁻¹
2. 44.1270 cm⁻¹
3. 55.9031 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

C  -0.909618  0.075677  0.086898
C  0.252825  0.570626 -0.507164
C  1.434733  0.847185  0.253734
C  2.199725  2.068353 -0.183716
O  -1.212292 -0.187793  1.276403
O  -1.949570 -0.157427 -0.837989
C  -3.177981 -0.638037 -0.323408
C  -4.033118  0.489760  0.212546
H   1.239264  0.857285  1.354987
## ethylcrotonate_7_am1_reopt

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.129262   |
| AM1 Free Energy (Quasiharmonic)      | -0.008283   |
| Number of Imaginary Frequencies      | 0           |

### Frequencies (Top 3 out of 48)

1. 17.9374 cm⁻¹
2. 90.7399 cm⁻¹
3. 91.6844 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| C     | 0.015470 | 0.830349 | -0.048342 |
|-------|----------|----------|-----------|
| C     | -0.979582| -0.243884| -0.117883 |
| C     | -2.279735| 0.007784 | 0.091248  |
| C     | -3.334580| -1.019614| 0.028394  |
| O     | -0.211748| 2.043330 | 0.007508  |
| O     | 1.363911 | 0.568746 | -0.044963 |
| C     | 1.791909 | -0.796869| -0.041046 |
| C     | 3.296760 | -0.765831| 0.100088  |
| H     | -0.619557| -1.254151| -0.362641 |
| H     | -2.617793| 1.034789 | 0.326787  |
| H     | -4.085234| -0.743197| -0.755381 |
| H     | -2.926033| -2.031102| -0.214445 |
| H     | -3.866068| -1.078696| 1.012236  |
| H     | 1.317405 | -1.338662| 0.818850  |
### ethylcrotonate_8_am1_HEI

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.196858 |
| AM1 Free Energy (Quasiharmonic)            | -0.041232 |
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 63)

1. 37.0873 cm⁻¹
2. 44.9695 cm⁻¹
3. 50.7675 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 1.108514 | 0.409942 | 0.202439 |
|-----|----------|----------|----------|
| C   | -0.083828| 0.788423 | -0.419062|
| C   | -1.351696| 0.649357 | 0.239492 |
| C   | -2.302995| 1.795779 | 0.012949 |
| O   | 1.372254 | 0.001451 | 1.359460 |
| O   | 2.240271 | 0.569629 | -0.624942|
| C   | 3.499963 | 0.240984 | -0.068546|
| C   | 3.763491 | -1.247666| -0.136426|
| H   | -1.251730| 0.426199 | 1.331441 |
| H   | -2.427333| 1.997934 | -1.077854|
| H   | -3.307137| 1.574969 | 0.451372 |
| H   | -1.900991| 2.719574 | 0.497533 |
| H   | 4.235628 | 0.804772 | -0.705241|
| H   | 3.569333 | 0.596634 | 0.993630 |
| H   | 3.685927 | -1.612035| -1.187923|
| H   | 4.783236 | -1.476891| 0.253192 |
| H   | 3.001420 | -1.782414| 0.481758 |
| C   | -3.596607| -1.175573| 0.352744 |
| H   | -3.921547| -2.214062| 0.120121 |
| H   | -3.452348| -1.078811| 1.452041 |
| H   | -4.404133| -0.472706| 0.046675 |
| S   | -2.104914| -0.873602| -0.511787|
| H   | -0.052962| 1.158368 | -1.445844|
**ethylcrotonate_9_reopt_am1_HEI_reopt**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.196573 |
| AM1 Free Energy (Quasiharmonic)            | -0.04164   |
| Number of Imaginary Frequencies            | 0       |

**Frequencies (Top 3 out of 63)**

1. 29.5496 cm\(^{-1}\)
2. 41.8175 cm\(^{-1}\)
3. 57.4621 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| C | 1.025541 | 0.127897 | 0.369639 |
| C | -0.076021 | 0.633753 | -0.324584 |
| C | -1.392742 | 0.625082 | 0.246441 |
| C | -2.200921 | 1.867333 | -0.026027 |
| O | 1.170597  | -0.314393 | 1.535094 |
| O | 2.221499  | 0.169375  | -0.376956 |
| C | 3.381767  | -0.310083 | 0.286522 |
| C | 4.526908  | -0.213121 | -0.698168 |
| H | -1.390896 | 0.384199  | 1.339173 |
| H | -2.229169 | 2.089810  | -1.119589 |
| H | -3.250076 | 1.750579  | 0.341283 |
| H | -1.737919 | 2.739727  | 0.497794 |
| H | 3.578814  | 0.313619  | 1.198583 |
| H | 3.218581  | -1.370595 | 0.615257 |
| H | 5.464360  | -0.582503 | -0.219153 |
| H | 4.312898  | -0.827630 | -1.604557 |
| H | 4.674385  | 0.844544  | -1.021414 |
| C | -3.820396 | -0.952608 | 0.182998 |
| H | -3.741666 | -0.879389 | 1.290730 |
| H | -4.236067 | -1.949257 | -0.085449 |
| H | -4.527043 | -0.166178 | -0.166264 |
| S | -2.250037 | -0.803815 | -0.575651 |
| H | 0.062801  | 1.004740  | -1.342003 |

**n-propylacrylate_10_am1**
### AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -0.886165 | 0.513925 | -0.232791 |
| C    | -2.263487 | 0.378264 | 0.259177  |
| C    | -2.846651 | -0.786486 | 0.537956  |
| O    | -0.294122 | 1.563622 | -0.498875 |
| O    | -0.231985 | -0.675723 | -0.409979 |
| C    | 1.121033  | -0.650880 | -0.886000 |
| C    | 2.091748  | -0.779152 | 0.274852  |
| C    | 2.498048  | 0.561266  | 0.829238  |
| H    | -2.776342 | 1.347959  | 0.378195  |
| H    | -3.881048 | -0.842868 | 0.905175  |
| H    | -2.331452 | -1.750861 | 0.417731  |
| H    | 1.170424  | -1.557244 | -1.549134 |
| H    | 1.315347  | 0.276704  | -1.484239 |
| H    | 1.619464  | -1.399467 | 1.081749  |
| H    | 3.000054  | -1.330337 | -0.085311 |
| H    | 3.108378  | 1.127559  | 0.084593  |
| H    | 3.103738  | 0.431217  | 1.757814  |
| H    | 1.593140  | 1.172522  | 1.069803  |

### n-propylacrylate_10_reopt_am1_HEI

| Datum                        | Value  |
|------------------------------|--------|
| AM1 Energy                   | -0.200215 |
| AM1 Free Energy (Quasiharmonic) | -0.044669 |
| Number of Imaginary Frequencies | 0       |

**Frequencies (Top 3 out of 63)**

1. 26.4896 cm⁻¹
2. 52.1392 cm⁻¹
3. 84.3643 cm⁻¹
1. 20.8342 cm⁻¹  
2. 37.3115 cm⁻¹  
3. 42.5867 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 0.491749 | 1.432972 | 0.130566 |
| C | -0.823585 | 1.370282 | 0.595524 |
| C | -1.538536 | 0.164844 | 0.866456 |
| O | 1.213561 | 2.420684 | -0.154410 |
| O | 1.148456 | 0.194511 | -0.002913 |
| C | 2.485326 | 0.249229 | -0.479585 |
| C | 2.965970 | -1.184906 | -0.642326 |
| C | 3.211353 | -1.849597 | 0.686616 |
| H | -2.185756 | 0.220886 | 1.775304 |
| H | -0.895743 | -0.743739 | 0.918589 |
| H | 2.513651 | 0.789738 | -1.462635 |
| H | 3.123347 | 0.810138 | 0.253102 |
| H | 2.195343 | -1.764342 | -1.214801 |
| H | 3.910209 | -1.175065 | -1.246618 |
| H | 2.282467 | -1.804908 | 1.306639 |
| H | 3.501637 | -2.918641 | 0.546412 |
| H | 4.029281 | -1.331258 | 1.243052 |
| S | -2.727141 | -0.102819 | -0.518252 |
| C | -3.615986 | -1.537412 | -0.055908 |
| H | -4.124553 | -1.403456 | 0.925361 |
| H | -2.947588 | -2.424240 | 0.020906 |
| H | -4.384225 | -1.732697 | -0.836457 |
| H | -1.337707 | 2.328662 | 0.713701 |

**n-propylacrylate_11_am1_HEI**

| Datum                              | Value  |
|------------------------------------|--------|
| AM1 Energy                         | -0.204625 |
| AM1 Free Energy (Quasiharmonic)    | -0.047329 |
| Number of Imaginary Frequencies    | 0 |

**Frequencies** (Top 3 out of 63)

1. 25.4900 cm⁻¹  
2. 28.4538 cm⁻¹  
3. 60.3737 cm⁻¹
**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -0.383861  | -0.750677  | 0.242666   |
| C    | 0.810016   | -1.146503  | -0.361568  |
| C    | 1.623627   | -0.322904  | -1.197976  |
| O    | -1.164020  | -1.386797  | 0.995322   |
| O    | -0.795088  | 0.565353   | -0.042831  |
| C    | -1.998928  | 1.032572   | 0.536294   |
| C    | -3.152860  | 0.934830   | -0.454996  |
| C    | -3.869811  | -0.385534  | -0.348354  |
| H    | 2.084547   | -0.877705  | -2.051702  |
| H    | 1.099464   | 0.589153   | -1.565586  |
| H    | -2.241448  | 0.480484   | 1.481893   |
| H    | -1.792306  | 2.113449   | 0.770920   |
| H    | -3.870020  | 1.775153   | -0.263462  |
| H    | -2.748837  | 1.063634   | -1.493151  |
| H    | -3.120107  | -1.217883  | -0.316889  |
| H    | -4.554849  | -0.536307  | -1.216654  |
| H    | -4.473925  | -0.431046  | 0.589841   |
| S    | 3.183911   | 0.336059   | -0.415006  |
| C    | 2.808931   | 0.462473   | 1.292945   |
| H    | 3.611245   | -0.032081  | 1.882506   |
| H    | 2.744403   | 1.530499   | 1.595154   |
| H    | 1.831081   | -0.040075  | 1.500566   |
| H    | 1.138353   | -2.168208  | -0.147334  |

**n-propylacrylate_11_am1**

| Datum                                | Value  |
|--------------------------------------|--------|
| AM1 Energy                           | -0.122369 |
| AM1 Free Energy (Quasiharmonic)      | 0.000568 |
| Number of Imaginary Frequencies      | 0      |

**Frequencies (Top 3 out of 48)**

1. 26.8371 cm⁻¹
2. 48.8846 cm⁻¹
3. 75.8234 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
### AM1 Molecular Geometry in Cartesian Coordinates

|   |     |     |     |
|---|-----|-----|-----|
| C | -0.279415 | -0.938975 | 0.019257 |
| C | 0.892445 | -0.924017 | -0.738547 |
| C | 2.182601 | -1.089371 | -0.145660 |
| O | -0.501383 | -1.113973 | 1.242463 |
| O | -1.443578 | -0.736677 | -0.753705 |
| C | -2.686516 | -0.789319 | -0.079286 |
| C | -3.029426 | 0.536996 | 0.582997 |
| C | -3.260251 | 1.630211 | -0.425746 |
| H | 2.882741 | -1.697481 | -0.768920 |

### n-propylacrylate_12_am1_HEI

| Datum                          | Value  |
|-------------------------------|--------|
| AM1 Energy                    | -0.205481 |
| AM1 Free Energy (Quasiharmonic) | -0.048559 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 63)

1. 26.9471 cm⁻¹
2. 31.1441 cm⁻¹
3. 55.8602 cm⁻¹
n-propylacrylate_12_am1

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.122371 |
| AM1 Free Energy (Quasiharmonic)            | 6.6e-05   |
| Number of Imaginary Frequencies            | 0         |

Frequencies (Top 3 out of 48)

1. 27.4728 cm\(^{-1}\)
2. 48.4342 cm\(^{-1}\)
3. 80.6858 cm\(^{-1}\)

AM1 Molecular Geometry in Cartesian Coordinates

| C           | 1.097846 | 0.525998 | -0.158793 |
| C           | 1.816985 | -0.753874| -0.104235 |
| C           | 2.998733 | -0.864350|  0.504172 |
| O           | 1.585516 | 1.652733 | -0.033381 |
| O           | -0.256579|  0.576532| -0.378812 |
| C           | -0.974361| -0.660744| -0.446760 |
| C           | -2.451372| -0.303776| -0.454198 |
| C           | -2.944965|  0.085675|  0.914246 |
| H           | 1.342156 | -1.607393| -0.612696 |
| H           | 3.549511 | -1.814388|  0.540361 |
| H           | 3.484870 | -0.011145|  1.001456 |
| H           | -0.717245| -1.300632|  0.437192 |
| H           | -0.691467| -1.189133| -1.395649 |
| H           | -3.019533| -1.193890| -0.831594 |
n-propylacrylate_13_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.205496   |
| AM1 Free Energy (Quasiharmonic)            | -0.04848    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 63)

1. 26.8593 cm⁻¹
2. 36.8890 cm⁻¹
3. 51.5998 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C      | 0.299459 | -0.051795 | 0.186338 |
|--------|----------|-----------|----------|
| C      | -0.721745| -0.771283 | -0.435940|
| C      | -1.875480| -1.223608 | 0.276593 |
| O      | 0.482634 | 0.315484  | 1.372796 |
| O      | 1.335823 | 0.319558  | -0.697860|
| C      | 2.429460 | 1.032459  | -0.151843|
| C      | 3.444761 | 0.104443  | 0.498737 |
| C      | 4.116550 | -0.792713 | -0.506138|
| H      | -2.225359| -2.235717 | -0.042270|
| H      | -1.747333| -1.183495 | 1.383336 |
| H      | 2.883606 | 1.557873  | -1.035677|
| H      | 2.074275 | 1.785209  | 0.601043 |
| H      | 4.212002 | 0.722957  | 1.032505 |
| H      | 2.903591 | -0.513523 | 1.264168 |
| H      | 3.343495 | -1.352757 | -1.087714|
| H      | 4.785638 | -1.526654 | 0.004061 |
| H      | 4.730592 | -0.195903 | -1.223502|
| S      | -3.446521| -0.271021 | -0.040153|
| C      | -2.913928| 1.370647  | -0.349385|
| H      | -3.189217| 2.032629  | 0.500400 |
| H      | -1.803392| 1.384838  | -0.482943|
| H      | -3.403079| 1.746405  | -1.274237|
| H      | -0.642609| -0.974750 | -1.506382|
n-propylacrylate_13_am1_reopt

| Datum                                         | Value     |
|-----------------------------------------------|-----------|
| AM1 Energy                                    | -0.123305 |
| AM1 Free Energy (Quasiharmonic)               | -0.000501 |
| Number of Imaginary Frequencies               | 0         |

**Frequencies** (Top 3 out of 48)

1. 33.3563 cm\(^{-1}\)
2. 40.2945 cm\(^{-1}\)
3. 64.0806 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | C      | C      | C      | O      | O      | C      | C      | C      | O      | O      | H      | H      | H      | H      | H      | H      | H      | H      | H      | H      | H      |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|      | 1.21535| -0.517948| -0.066200| 2.473772| 1.571515| 0.106503| 2.126754| -1.296942| -0.360542| 0.055724| -1.189492| 0.234961| -1.093705| -0.459581| 0.659221| -1.923727| -0.12866| -0.531045| -3.186166| 0.670157| -0.076144| 0.355729| 1.502678| -0.122003| 2.551609| 2.667223| 0.130381| 3.424155| 1.022972| 0.193124| -0.808533| 0.403944| 1.313113| -1.661183| -1.213798| 1.272810| -1.322055| 0.678905| -1.176909| -2.173385| -0.909602| -1.157776| -3.791218| 0.988113| -0.959349| -3.806789| -0.019760| 0.545733| -2.950070| 1.575679| 0.533840 |

n-propylacrylate_14_am1_HEI

| Datum                                         | Value     |
|-----------------------------------------------|-----------|
| AM1 Energy                                    | -0.204959 |
| AM1 Free Energy (Quasiharmonic)               | -0.048694 |
| Datum                                      | Value  |
|-------------------------------------------|--------|
| Number of Imaginary Frequencies           | 0      |

**Frequencies** (Top 3 out of 63)

1. 19.7896 cm⁻¹
2. 33.9470 cm⁻¹
3. 45.8985 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |    |    |    |
|---|----|----|----|
| C | 0.172349 | -0.805023 | 0.057155 |
| C | -0.869577 | -0.597258 | -0.848139 |
| C | -2.214801 | -0.983776 | -0.559531 |
| O | 0.225931  | -1.340297 | 1.191341  |
| O | 1.418324  | -0.333648 | -0.408655 |
| C | 2.523303  | -0.546261 | 0.457405  |
| C | 3.755741  | 0.017126  | -0.233947 |
| C | 3.751792  | 1.523079  | -0.249226 |
| H | -2.759821 | -1.391038 | -1.445793 |
| H | -2.291491 | -1.684039 | 0.304490  |
| H | 2.339358  | -0.034929 | 1.438799  |
| H | 2.644961  | -1.645668 | 0.647516  |
| H | 3.792781  | -0.368273 | -1.286180 |
| H | 4.665193  | -0.359013 | 0.303014  |
| H | 4.629581  | 1.914890  | -0.817302 |
| H | 2.813681  | 1.892369  | -0.731780 |
| H | 3.793717  | 1.928722  | 0.790462  |
| S | -3.381692 | 0.406654  | -0.129308 |
| C | -2.376701 | 1.591697  | 0.683022  |
| H | -2.618470 | 1.624906  | 1.767723  |
| H | -2.561579 | 2.594409  | 0.240082  |
| H | -1.299318 | 1.319894  | 0.553718  |
| H | -0.648216 | -0.104631 | -1.797742 |

**n-propylacrylate_14_am1**

| Datum                                      | Value  |
|-------------------------------------------|--------|
| AM1 Energy                                 | -0.123248 |
| AM1 Free Energy (Quasiharmonic)            | -0.001099 |
| Number of Imaginary Frequencies            | 0      |
Frequencies (Top 3 out of 48)

1. 30.4558 cm⁻¹  
2. 46.2206 cm⁻¹  
3. 87.9001 cm⁻¹  

AM1 Molecular Geometry in Cartesian Coordinates

|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| C   | -1.271601 | -0.522852 | -0.074265 |
| C   | -1.726152 |  0.868347 | -0.200186 |
| C   | -2.940609 |  1.243878 |  0.203683 |
| O   | -1.983032 | -1.524970 |  0.037679 |
| O   |  0.063889 | -0.842949 | -0.081306 |
| C   |  1.012566 |  0.228182 | -0.113151 |
| C   |  2.372773 | -0.408717 |  0.117569 |
| C   |  3.457554 |  0.634553 |  0.074113 |
| H   | -1.023501 |  1.576311 | -0.666560 |
| H   | -3.294089 |  2.279404 |  0.103765 |
| H   | -3.652611 |  0.537734 |  0.657597 |
| H   |  0.776371 |  0.973045 |  0.690915 |
| H   |  0.969447 |  0.727081 | -1.117114 |
| H   |  2.371672 | -0.930761 |  1.110016 |
| H   |  2.550484 | -1.190671 | -0.666487 |
| H   |  4.452800 |  0.157593 |  0.245721 |
| H   |  3.478428 |  1.145146 | -0.919165 |
| H   |  3.296952 |  1.408124 |  0.863746 |

n-propylacrylate_15_am1_HEI

| Datum                        | Value     |
|-------------------------------|-----------|
| AM1 Energy                    | -0.205101 |
| AM1 Free Energy (Quasiharmonic) | -0.048061 |
| Number of Imaginary Frequencies | 0        |

Frequencies (Top 3 out of 63)

1. 20.0890 cm⁻¹  
2. 34.6396 cm⁻¹  
3. 48.6326 cm⁻¹  

AM1 Molecular Geometry in Cartesian Coordinates
### n-propylacrylate_15_am1

| Datum                                      | Value  |
|--------------------------------------------|--------|
| AM1 Energy                                 | -0.121381 |
| AM1 Free Energy (Quasiharmonic)            | 0.001935 |
| Number of Imaginary Frequencies            | 0      |

**Frequencies** (Top 3 out of 48)

1. 38.3873 cm\(^{-1}\)
2. 54.7171 cm\(^{-1}\)
3. 80.3617 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | X    | Y    | Z    |
|---|------|------|------|
| C | -1.013821 | -0.556856 | -0.191527 |
| C | -1.247569  | 0.868892  | 0.078358  |
| C | -2.461963  | 1.341273  | 0.358754  |
| O | -1.793461  | -1.335722 | -0.746960 |
n-propylacrylate_16_reopt_am1_HEI

| Datum                                 | Value       |
|---------------------------------------|-------------|
| AM1 Energy                            | -0.206377   |
| AM1 Free Energy (Quasiharmonic)       | -0.049595   |
| Number of Imaginary Frequencies       | 0           |

**Frequencies** (Top 3 out of 63)

1. 27.1800 cm⁻¹
2. 36.2781 cm⁻¹
3. 55.6342 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C         |          |          |          |
|-----------|----------|----------|----------|
| 0.188203  | -0.823799| 0.092752 |
| -1.056596 | -1.060541| -0.492117|
| -2.266495 | -1.056928| 0.269179 |
| 0.547725  | -0.613106| 1.276943 |
| 1.251849  | -0.846895| -0.835667|
| 2.560925  | -0.682550| -0.325582|
| 2.894453  | 0.789033 | -0.132614|
| 4.330547  | 0.977045 | 0.275668 |
| -2.995962 | -1.839459| -0.053283|
| -2.089682 | -1.114708| 1.368403 |
| 2.685119  | -1.233772| 0.643569 |
| 3.223752  | -1.137727| -1.11175 |
| 2.687855  | 1.344033 | -1.083953|
| 2.205431  | 1.198913 | 0.653409 |
| Datum                              | Value          |
|-----------------------------------|----------------|
| AM1 Energy                        | -0.204961      |
| AM1 Free Energy (Quasiharmonic)   | -0.048655      |
| Number of Imaginary Frequencies   | 0              |

**Frequencies** (Top 3 out of 63)

1. 19.7366 cm⁻¹  
2. 36.4652 cm⁻¹  
3. 43.1163 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -0.192358 | -0.370834 | 0.432619 |
| C | 0.795820 | -0.809810 | -0.450882 |
| C | 2.089665 | -1.216966 | 0.000044 |
| O | -0.235524 | -0.261445 | 1.682389 |
| O | -1.388441 | 0.008838 | -0.213053 |
| C | -2.446305 | 0.423806 | 0.638413 |
| C | -3.633580 | 0.767073 | -0.248613 |
| C | -4.272278 | -0.465122 | -0.833358 |
| H | 2.500393 | -2.091295 | -0.561397 |
| H | 2.131036 | -1.401298 | 1.098726 |
| H | -2.121582 | 1.321674 | 1.228417 |
| H | -2.700890 | -0.399339 | 1.356707 |
| H | -3.288592 | 1.439408 | -1.076908 |
| H | -4.381759 | 1.332815 | 0.365422 |
| H | -3.506517 | -1.056772 | -1.392668 |
| H | -5.097785 | -0.188581 | -1.532499 |
| H | -4.693949 | -1.112152 | -0.026634 |
| S | 3.474184 | -0.007218 | -0.315451 |
| C | 2.715100 | 1.570123 | -0.215062 |
### n-propylacrylate_18_am1_HEI

| Datum                                           | Value       |
|-------------------------------------------------|-------------|
| AM1 Energy                                      | -0.205809   |
| AM1 Free Energy (Quasiharmonic)                 | -0.049817   |
| Number of Imaginary Frequencies                 | 0           |

**Frequencies** (Top 3 out of 63)

1. 23.0521 cm⁻¹
2. 32.9976 cm⁻¹
3. 45.7298 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |     |     |     |
|-----|-----|-----|-----|
| C   | -0.100384 | -0.610575 | 0.139020 |
| C   | 1.001071  | -0.732510  | -0.709595 |
| C   | 2.289894  | -1.121189  | -0.229773 |
| O   | -0.260272 | -0.812228  | 1.367580 |
| O   | -1.273365 | -0.193776  | -0.526116 |
| C   | -2.437102 | -0.088247  | 0.279727 |
| C   | -3.566073 | 0.355068   | -0.638231 |
| C   | -4.854523 | 0.499632   | 0.127365 |
| H   | 2.841214  | -1.792899  | -0.932060 |
| H   | 2.259325  | -1.562901  | 0.793334 |
| H   | -2.665785 | -1.080618  | 0.750308 |
| H   | -2.265806 | 0.659412   | 1.098449 |
| H   | -3.289289 | 1.329379   | -1.118236 |
| H   | -3.687045 | -0.395256  | -1.462031 |
| H   | -4.746800 | 1.258350   | 0.940097 |
| H   | -5.678743 | 0.825202   | -0.552199 |
| H   | -5.145934 | -0.471951  | 0.595224 |
| S   | 3.552337  | 0.246253   | -0.102417 |
| C   | 2.616134  | 1.678625   | 0.279732 |
| H   | 1.527127  | 1.460222   | 0.146562 |
| H   | 2.914490  | 2.504191   | -0.402348 |
| H   | 2.801121  | 1.992182   | 1.330249 |
| H   | 0.873726  | -0.502146  | -1.769852 |
n-propylacrylate_19_reopt_am1_HEI

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.206383 |
| AM1 Free Energy (Quasiharmonic)            | -0.049541 |
| Number of Imaginary Frequencies            | 0       |

**Frequencies** (Top 3 out of 63)

1. 27.7128 cm\(^{-1}\)
2. 39.1012 cm\(^{-1}\)
3. 48.9275 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|    |        |        |        |
|----|--------|--------|--------|
| C  | -0.222492 | -0.242093 | 0.044719 |
| C  | 0.921582 | -0.708033 | 0.694020 |
| C  | 2.045743 | -1.222815 | -0.023410 |
| O  | -0.551884 | -0.183343 | -1.165260 |
| O  | -1.206963 | 0.242897 | 0.933261 |
| C  | -2.411457 | 0.722131 | 0.367304 |
| C  | -3.368939 | -0.420421 | 0.064235 |
| C  | -4.702266 | 0.092016 | -0.409107 |
| H  | 2.527914 | -2.098243 | 0.476176 |
| H  | 1.812578 | -1.458004 | -1.087937 |
| H  | -2.839510 | 1.396865 | 1.157935 |
| H  | -2.208774 | 1.310180 | -0.566362 |
| H  | -2.895508 | -1.068234 | -0.721041 |
| H  | -3.500618 | -1.047738 | 0.983402 |
| H  | -5.180326 | 0.734640 | 0.369862 |
| H  | -5.391213 | -0.757762 | -0.633799 |
| H  | -4.581081 | 0.701189 | -1.337633 |
| S  | 3.530619 | -0.098996 | -0.114472 |
| C  | 2.859483 | 1.520780 | -0.129472 |
| H  | 3.389931 | 2.144056 | 0.622832 |
| H  | 2.983892 | 1.981294 | -1.133754 |
| H  | 1.770736 | 1.476998 | 0.123599 |
| H  | 0.962925 | -0.657139 | 1.784531 |

n-propylacrylate_1_am1
### AM1 Energy
- **Value**: -0.131141

### AM1 Free Energy (Quasiharmonic)
- **Value**: -0.008325

### Number of Imaginary Frequencies
- **Value**: 0

### Frequencies (Top 3 out of 48)

1. 44.6269 cm\(^{-1}\)
2. 59.5380 cm\(^{-1}\)
3. 72.8066 cm\(^{-1}\)

### AM1 Molecular Geometry in Cartesian Coordinates

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | -0.950036 | -0.224406 | 0.118118 |
| C       | -2.096068 | 0.688721  | 0.220301 |
| C       | -3.251770 | 0.429768  | -0.391523|
| O       | -0.865518 | -1.293726 | -0.493621|
| O       | 0.138722  | 0.216178  | 0.822495 |
| C       | 1.321670  | -0.594271 | 0.797718 |
| C       | 2.131943  | -0.357016 | -0.462317|
| C       | 2.725771  | 1.026099  | -0.505719|
| H       | -1.926096 | 1.588792  | 0.832614 |
| H       | -4.112024 | 1.109290  | -0.318478|
| H       | -3.406177 | -0.474204 | -0.999814|
| H       | 1.875218  | -0.252692 | 1.713572 |
| H       | 1.041399  | -1.676369 | 0.888191 |
| H       | 2.948508  | -1.124953 | -0.503439|
| H       | 1.468722  | -0.518945 | -1.353412|
| H       | 1.922449  | 1.796107  | -0.485631|
| H       | 3.259204  | 1.189659  | -1.472789|
| H       | 3.454101  | 1.170332  | 0.328729 |

### n-propylacrylate_1_reopt_am1_HEI

### AM1 Energy
- **Value**: -0.205351

### AM1 Free Energy (Quasiharmonic)
- **Value**: -0.047634

### Number of Imaginary Frequencies
- **Value**: 0

### Frequencies (Top 3 out of 63)
1. 36.6906 cm\(^{-1}\)
2. 47.2792 cm\(^{-1}\)
3. 65.2763 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C           0.374854       -1.346332       -0.275244
C          -1.012997       -1.488235       -0.243078
C          -1.878357       -0.894255        0.724459
O           1.229169       -1.829185       -1.060089
O           0.922306       -0.543225        0.744859
C           2.326923       -0.368176        0.753061
C           2.774905        0.693148       -0.240822
C           2.201117        2.047445        0.079447
H          -2.766637       -1.526108        0.970052
H          -1.351952        0.581718       1.655621
H           2.846554       -1.336661       0.526665
H           2.554891       -0.045617       1.805425
H           2.441499        0.369334      -1.263045
H           3.894714        0.739920      -0.239305
H           1.083707        1.985676       0.109752
H           2.499796        2.795625      -0.693606
H           2.559720        2.405738       1.074607
S          -2.778741        0.648327       0.179093
C          -1.614557        1.497974      -0.819670
H          -1.245358        2.406719      -0.295268
H          -0.748994        0.824081     -1.040397
H          -2.099315        1.801949      -1.772652
H          -1.451902        2.082298      -1.050427
```

**n-propylacrylate_20_reopt_am1_HEI**

| Datum                               | Value    |
|-------------------------------------|----------|
| AM1 Energy                          | -0.19481 |
| AM1 Free Energy (Quasiharmonic)     | -0.037956|
| Number of Imaginary Frequencies     | 0        |

**Frequencies (Top 3 out of 63)**

1. 38.9388 cm\(^{-1}\)
2. 43.6855 cm\(^{-1}\)
3. 56.6971 cm\(^{-1}\)
AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | 0.960653 | 1.387609 | -0.051589 |
| C | -0.394354 | 1.622412 | 0.196781 |
| C | -1.482627 | 0.992651 | -0.473356 |
| O | 1.972410 | 1.945555 | 0.431435 |
| O | 1.356202 | 0.468391 | -1.062089 |
| C | 1.027047 | -0.886144 | -0.814156 |
| C | 2.258146 | -1.660441 | -0.359091 |
| C | 2.652105 | -1.304817 | 1.049870 |
| H | -2.356234 | 1.664660 | -0.646243 |
| H | -1.201648 | 0.482364 | -1.424261 |
| H | 0.677925 | -1.292879 | -1.803777 |
| H | 0.194421 | -0.979616 | -0.062122 |
| H | 3.108084 | -1.431463 | -1.053581 |
| H | 2.039211 | -2.757425 | -0.434715 |
| H | 2.759951 | -0.191892 | 1.136858 |
| H | 3.619843 | -1.789279 | 1.323661 |
| H | 1.870857 | -1.639152 | 1.774246 |
| S | -2.138379 | -0.331147 | 0.644366 |
| C | -3.523280 | -0.987777 | -0.201011 |
| H | -4.276075 | -0.197739 | -0.420431 |
| H | -3.226762 | -1.459894 | -1.164364 |
| H | -3.989524 | -1.760074 | 0.449900 |
| H | -0.621028 | 2.358211 | 0.975522 |

**n-propylacrylate_22_am1_HEI**

| Datum                                | Value    |
|--------------------------------------|----------|
| AM1 Energy                           | -0.194728|
| AM1 Free Energy (Quasiharmonic)      | -0.038536|
| Number of Imaginary Frequencies      | 0        |

**Frequencies (Top 3 out of 63)**

1. 36.9086 cm⁻¹
2. 46.4624 cm⁻¹
3. 49.4458 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
n-propylacrylate_23_am1_HEI

| Datum                                | Value    |
|--------------------------------------|----------|
| AM1 Energy                           | -0.195563|
| AM1 Free Energy (Quasiharmonic)      | -0.03955 |
| Number of Imaginary Frequencies      | 0        |

**Frequencies** (Top 3 out of 63)

1. 36.4425 cm⁻¹
2. 46.2210 cm⁻¹
3. 46.7766 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -0.725133 | 1.455893 | 0.035134 |
| C   | 0.656464  | 1.638719 | -0.057051|
| C   | 1.631030  | 0.841026 | 0.610925 |
| O   | -1.664614 | 2.108355 | -0.472660|
| O   | -1.231944 | 0.437401 | 0.895111 |
| C   | -1.148233 | -0.866996| 0.348925 |
| C   | -2.288985 | -1.138503| -0.622353|
| C   | -3.589176 | -1.395506| 0.092041 |
| H   | 2.536745  | 1.407352 | 0.931781 |
| H   | 1.227860  | 0.249091 | 1.465420 |
| H   | -1.215149 | -1.552266| 1.237048 |
| H   | -0.155506 | -1.012213| -0.165669|
| H   | -2.023580 | -2.019378| -1.261811|
| H   | -2.398513 | -0.239678| -1.287943|
| H   | -3.526517 | -2.321672| 0.713574 |
| H   | -4.424108 | -1.518905| -0.639088|
| H   | -3.824644 | -0.534282| 0.764231 |
| S   | 2.269550  | -0.399403| -0.607982|
| C   | 3.513122  | -1.277270| 0.256161 |
| H   | 3.959368  | -2.019307| -0.442217|
| H   | 4.314375  | -0.594616| 0.618086 |
| H   | 3.094878  | -1.816205| 1.135654 |
| H   | 0.999928  | 2.452293 | -0.703650|

| Datum                                | Value    |
|--------------------------------------|----------|
| AM1 Energy                           | -0.195563|
| AM1 Free Energy (Quasiharmonic)      | -0.03955 |
| Number of Imaginary Frequencies      | 0        |

**Frequencies** (Top 3 out of 63)

1. 36.4425 cm⁻¹
2. 46.2210 cm⁻¹
3. 46.7766 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | 0.798367 | -1.607760 | -0.066741 |
| C   | -0.572812| -1.698292 | -0.315802|
| C   | -1.581187| -1.001056 | 0.411963 |
| O   | 1.762123 | -2.189983 | -0.612739|
n-propylacrylate_24_am1_HEI

| Datum                               | Value       |
|-------------------------------------|-------------|
| AM1 Energy                          | -0.205054   |
| AM1 Free Energy (Quasiharmonic)     | -0.048004   |
| Number of Imaginary Frequencies     | 0           |

**Frequencies (Top 3 out of 63)**

1. 25.7886 cm⁻¹  
2. 34.5827 cm⁻¹  
3. 53.2019 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | -0.324806 | 0.829712 | 0.537339 |
| C | 0.852328  | 0.418688 | 1.164016 |
| C | 1.520030  | -0.821685 | 0.930539 |
| O | -0.986379 | 1.891276  | 0.658578 |
| O | -0.881874 | -0.092579 | -0.370129 |
| C | -2.080219 | 0.281794  | -1.024463 |
| C | -3.304487 | 0.020815  | -0.159464 |
| C | -3.521849 | -1.448715 | 0.084009 |
| H | 1.967540  | -1.264649 | 1.853847 |
### n-propylacrylate_25_am1_HEI

| Datum                                           | Value       |
|------------------------------------------------|-------------|
| AM1 Energy                                     | -0.205083   |
| AM1 Free Energy (Quasiharmonic)                | -0.047855   |
| Number of Imaginary Frequencies                | 0           |

**Frequencies** (Top 3 out of 63)

1. 24.0656 cm⁻¹  
2. 38.4797 cm⁻¹  
3. 48.5997 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C     | 0.337617 | -0.074825 | -0.061511 |
|-------|----------|-----------|-----------|
| C     | 0.759496 | -0.395449 | -0.862263 |
| C     | 1.847519 | -1.186951 | -0.378377 |
| O     | -0.645292| -0.376765 | 1.117787  |
| O     | -1.284901| 0.735610  | -0.723205 |
| C     | -2.454906| 1.106591  | -0.020166 |
| C     | -3.624460| 0.203315  | -0.394812 |
| C     | -3.716430| -0.994615 | 0.513665  |
| H     | 2.253496 | -1.895609 | -1.140955 |
| H     | 1.607137 | -1.725017 | 0.568042  |
| H     | -2.664359| 2.157671  | -0.363056 |
| H     | -2.288096| 1.098040  | 1.088984  |
| H     | -3.493872| -0.135323 | -1.455848 |
| H     | -4.574685| 0.796145  | -0.342331 |
### n-propylacrylate_26_am1_HEI

| Datum                                    | Value          |
|------------------------------------------|----------------|
| AM1 Energy                               | -0.194728      |
| AM1 Free Energy (Quasiharmonic)          | -0.038542      |
| Number of Imaginary Frequencies          | 0              |

#### Frequencies (Top 3 out of 63)

1. 36.8434 cm⁻¹
2. 46.3863 cm⁻¹
3. 49.3490 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| C         | 0.724920 | 1.455874 | 0.035129 |
|-----------|----------|----------|----------|
| C         | -0.656657| 1.638752 | -0.057199|
| C         | -1.631337| 0.841228 | 0.610862 |
| O         | 1.664442 | 2.108348 | -0.472567|
| O         | 1.231635 | 0.437281 | 0.895042 |
| C         | 1.148339 | -0.866974| 0.348349 |
| C         | 2.289547 | -1.138096| -0.622403|
| C         | 3.589402 | -1.395404| 0.092498 |
| H         | -2.537201| 1.407606 | 0.931184 |
| H         | -1.228399| 0.249707 | 1.465735 |
| H         | 0.155849 | -1.012169| -0.166594|
| H         | 1.214963 | -1.552491| 1.236391 |
| H         | 2.399401 | -0.239023| -1.287593|
| H         | 2.024441 | -2.018732| -1.262308|
| H         | 4.424683 | -1.518460| -0.638283 |
| H         | 3.526460 | -2.321855| 0.713573 |
| H         | 3.824559 | -0.534506| 0.765196 |
| S         | -2.269259| -0.399814| -0.607745|
| C         | -3.513428| -1.277169| 0.256007 |
### n-propylacrylate_27_reopt_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.205054   |
| AM1 Free Energy (Quasiharmonic)            | -0.048004   |
| Number of Imaginary Frequencies            | 0           |

#### Frequencies (Top 3 out of 63)

1. 25.7450 cm⁻¹
2. 34.5727 cm⁻¹
3. 53.2109 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|   |        |        |        |
|---|--------|--------|--------|
| C | -0.324827 | 0.829628 | -0.537327 |
| C | 0.852269  | 0.418564 | -1.164016 |
| C | 1.520007  | -0.821776 | -0.930477 |
| O | -0.986505 | 1.891111  | -0.658770 |
| O | -0.881758 | -0.092470 | 0.370423  |
| C | -2.080235 | 0.281910  | 1.024529  |
| C | -3.304355 | 0.020828  | 0.159355  |
| C | -3.521710 | -1.448734 | -0.083948 |
| H | 1.967584  | -1.264703 | -1.853780 |
| H | 0.886491  | -1.574085 | -0.406620 |
| H | -2.101605 | -0.361999 | 1.945513  |
| H | -2.050331 | 1.365701  | 1.314056  |
| H | -4.203994 | 0.462694  | 0.660922  |
| H | -3.514739 | 0.554124  | -0.817251 |
| H | -2.593909 | -1.901289 | -0.512824 |
| H | -4.365057 | -1.610951 | -0.797456 |
| H | -3.760736 | -1.978154 | 0.870187  |
| S | 3.065006  | -0.727964 | 0.113261  |
| C | 2.811846  | 0.651405  | 1.165281  |
| H | 2.669220  | 0.314136  | 2.215078  |
| H | 3.700413  | 1.317751  | 1.117350  |
| H | 1.905091  | 1.215864  | 0.832000  |
| H | 1.289611  | 1.128250  | -1.872947 |
## n-propylacrylate_2_am1_HEI

| Datum                                      | Value      |
|--------------------------------------------|------------|
| AM1 Energy                                 | -0.200821  |
| AM1 Free Energy (Quasiharmonic)            | -0.044523  |
| Number of Imaginary Frequencies            | 0          |

**Frequencies** (Top 3 out of 63)

1. 26.2695 cm⁻¹  
2. 42.2035 cm⁻¹  
3. 44.6195 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| C | -0.703078 | -1.316367 | -0.091847 |
| C | 0.674199  | -1.546585 | -0.105909 |
| C | 1.639062  | -0.779698 | 0.614638  |
| O | -1.635657 | -1.910435 | -0.687997 |
| O | -1.135003 | -0.283765 | 0.763535  |
| C | -2.523669 | -0.011569 | 0.804652  |
| C | -2.966309 | 0.861174  | -0.360119 |
| C | -3.47153  | 2.232157  | -0.305953 |
| H | 2.465080  | -1.392495 | 1.050623  |
| H | 1.202898  | -0.122828 | 1.401804  |
| H | -2.667064 | 0.527806  | 1.780399  |
| H | -3.113500 | -0.966295 | 0.804200  |
| H | -2.666183 | 0.343205  | -1.310152 |
| H | -4.084034 | 0.943435  | -0.347463 |
| H | -2.616818 | 2.823214  | -1.213960 |
| H | -1.233930 | 2.140033  | -0.252316 |
| H | -2.697978 | 2.791328  | 0.595194  |
| S | 2.485948  | 0.327622  | -0.592913 |
| C | 3.702882  | 1.153375  | 0.355403  |
| H | 3.243303  | 1.774838  | 1.156446  |
| H | 4.402608  | 0.433510  | 0.836669  |
| H | 4.280009  | 1.815666  | -0.327146 |
| H | 1.020112  | -2.354694 | -0.757179 |
| Datum                                    | Value     |
|------------------------------------------|-----------|
| AM1 Energy                               | -0.130945 |
| AM1 Free Energy (Quasiharmonic)          | -0.008672 |
| Number of Imaginary Frequencies          | 0         |

**Frequencies (Top 3 out of 48)**

1. 33.5849 cm\(^{-1}\)
2. 46.0600 cm\(^{-1}\)
3. 70.4542 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C   1.090837   0.238738   0.003208
C   2.104540  -0.810011  -0.165290
C   3.394761  -0.579485   0.078230
O   1.237878   1.410517   0.364937
O  -0.173783  -0.192297  -0.295171
C  -1.227805   0.777459  -0.154913
C  -2.519743   0.066844  -0.511504
C  -2.992266  -0.840262   0.594123
H   1.719321  -1.785369  -0.503280
H   4.157316  -1.360596  -0.046231
H   3.764192   0.400747   0.415433
H  -1.232983   1.156653   0.899943
H  -1.020154   1.629950  -0.853242
H  -2.367367  -0.528254  -1.450226
H  -3.294112   0.850328  -0.723377
H  -3.926513  -1.369738   0.288289
H  -2.210131  -1.602569   0.828926
H  -3.204278  -0.256620   1.522508
```

**n-propylacrylate_3_am1_HEI_reopt**

| Datum                                    | Value     |
|------------------------------------------|-----------|
| AM1 Energy                               | -0.204623 |
| AM1 Free Energy (Quasiharmonic)          | -0.047672 |
| Number of Imaginary Frequencies          | 0         |

**Frequencies (Top 3 out of 63)**

```
1. 23.4579 cm⁻¹
2. 40.3786 cm⁻¹
3. 51.4430 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 0.223539 | 1.500911 | 0.230199 |
| C | -1.146149 | 1.511133 | -0.038062 |
| C | -1.810217 | 0.645143 | -0.957579 |
| O | 0.914487  | 2.215003 | 0.998716  |
| O | 0.968739  | 0.543877 | -0.485809 |
| C | 2.355041  | 0.465301 | -0.193794 |
| C | 2.832623  | -0.912667 | -0.629827 |
| C | 2.326234  | -1.993193 | 0.289270  |
| H | -2.690046 | 1.120530 | -1.455849 |
| H | -1.126866 | 0.196111 | -1.714678 |
| H | 2.541717  | 0.628521 | 0.900412  |
| H | 2.888234  | 1.266178 | -0.772231 |
| H | 3.953472  | -0.911590 | -0.644527 |
| H | 2.474328  | -1.110961 | -1.673547 |
| H | 2.605236  | -3.002898 | -0.096682 |
| H | 1.211188  | -1.929667 | 0.367402  |
| H | 2.756121  | -1.874316 | 1.313101  |
| S | -2.681484 | -0.831413 | -0.213487 |
| C | -1.601798 | -1.371014 | 1.058576  |
| H | -0.814673 | -0.595828 | 1.234318  |
| H | -2.182548 | -1.527339 | 1.993371  |
| H | -1.113577 | -2.328313 | 0.771350  |
| H | -1.740298 | 2.227453  | 0.537404  |

**n-propylacrylate_3_am1**

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.132055     |
| AM1 Free Energy (Quasiharmonic)            | -0.00936      |
| Number of Imaginary Frequencies            | 0             |

**Frequencies (Top 3 out of 48)**

1. 49.9859 cm⁻¹
2. 54.7140 cm⁻¹
3. 67.3563 cm⁻¹
AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 1.046244 | 0.027881 | -0.167577 |
| C | 2.355936 | -0.496513 | 0.241323 |
| C | 3.429022 | 0.290358 | 0.321135 |
| O | 0.738392 | 1.181834 | -0.480804 |
| O | 0.076877 | -0.939461 | -0.193875 |
| C | -1.246455 | -0.547528 | -0.580851 |
| C | -1.989253 | 0.067737 | 0.589937 |
| C | -3.425273 | 0.339622 | 0.228354 |
| H | 2.379047 | -1.573520 | 0.472622 |
| H | 4.410947 | -0.096648 | 0.626521 |
| H | 3.389910 | 1.364818 | 0.086548 |
| H | -1.712582 | -1.518853 | -0.898548 |
| H | -1.199775 | 0.164434 | -1.445475 |
| H | -1.936906 | -0.625911 | 1.469475 |
| H | -1.475849 | 1.021987 | 0.882868 |
| H | -3.959977 | 0.796493 | 1.095793 |
| H | -3.488220 | 1.045056 | -0.635513 |
| H | -3.950034 | -0.606146 | -0.050783 |

**n-propylacrylate_4_am1**

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| AM1 Energy                                 | -0.131813      |
| AM1 Free Energy (Quasiharmonic)            | -0.009744      |
| Number of Imaginary Frequencies            | 0              |
| Frequencies (Top 3 out of 48)              |                |
| 1. 36.0398 cm⁻¹                           |                |
| 2. 46.0196 cm⁻¹                           |                |
| 3. 71.0388 cm⁻¹                           |                |

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | 1.185643 | 0.187932 | 0.000001 |
| C | 2.346513 | -0.710999 | -0.000001 |
| C | 3.593769 | -0.240424 | -0.000003 |
| O | 1.158494 | 1.422642 | -0.000001 |
| O | -0.006605 | -0.485181 | 0.000004 |
| C | -1.195671 | 0.324050 | 0.000006 |
## n-propylacrylate_4_reopt_am1_HEI

| Datum                                | Value       |
|--------------------------------------|-------------|
| AM1 Energy                           | -0.204563   |
| AM1 Free Energy (Quasiharmonic)      | -0.048245   |
| Number of Imaginary Frequencies      | 0           |

### Frequencies (Top 3 out of 63)

1. 18.8754 cm⁻¹
2. 32.9022 cm⁻¹
3. 44.8952 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

| C          | 0.178178 | 1.316783 | -0.241137 |
|------------|----------|----------|-----------|
| C          | -1.059661| 1.068637 | -0.836327 |
| C          | -1.546530| -0.217936| -1.217465 |
| O          | 0.704600 | 2.393511 | 0.136278  |
| O          | 0.992526 | 0.186382 | -0.038498 |
| C          | 2.266441 | 0.434169 | 0.539462  |
| C          | 2.962525 | -0.909899| 0.690277  |
| C          | 3.399052 | -1.468345| -0.638518 |
| H          | -2.134682| -0.205903| -2.167606 |
| H          | -0.751423| -0.997372| -1.262256 |
| H          | 2.853668 | 1.124200 | -0.121759 |
| H          | 2.135557 | 0.926275 | 1.539525  |
| H          | 3.850746 | -0.774416| 1.360770  |
| H          | 2.261343 | -1.630216| 1.187061  |
| H          | 2.517254 | -1.547881| -1.320842 |
| H          | 3.851092 | -2.481406| -0.511922 |
n-propylacrylate_5_am1

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.130516   |
| AM1 Free Energy (Quasiharmonic)            | -0.007686   |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 48)**

1. 32.3001 cm⁻¹
2. 52.8609 cm⁻¹
3. 80.9206 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|       |          |          |          |
|-------|----------|----------|----------|
| C     | -0.889901| -0.082400| 0.220465 |
| C     | -2.170546| -0.392716| -0.429989|
| C     | -3.221019| 0.421387 | -0.326513|
| O     | -0.594617| 0.896134 | 0.912971 |
| O     | 0.054470 | -1.048202| -0.000040|
| C     | 1.358027 | -0.877132| 0.573541 |
| C     | 2.317308 | -0.306808| -0.456445|
| C     | 2.353032 | 1.198890 | -0.430313|
| H     | -2.191598| -1.335485| -0.999778|
| H     | -4.180760| 0.194610 | -0.810873|
| H     | -3.184206| 1.359975 | 0.246829 |
| H     | 1.649500 | -1.926642| 0.851556 |
| H     | 1.308314 | -0.234049| 1.490040 |
| H     | 3.341687 | -0.712937| -0.246183|
| H     | 2.016001 | -0.664676| -1.476331|
| H     | 2.962691 | 1.588765 | -1.280224|
| H     | 1.317344 | 1.613231 | -0.507687|
| H     | 2.800799 | 1.566435 | 0.524725 |
### n-propylacrylate_6_am1

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.13046  |
| AM1 Free Energy (Quasiharmonic)      | -0.007794 |
| Number of Imaginary Frequencies      | 0         |

**Frequencies (Top 3 out of 48)**

1. 38.5759 cm⁻¹  
2. 53.5204 cm⁻¹  
3. 75.4435 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | C          | C          | O          | O          | C           | C           | C           | O          | O          | C           | C           | C           | C           | H           | H           | H           | H           | H           | H           | H           | H           | H           | H           | H           | H           |
|---|------------|------------|------------|------------|-------------|-------------|-------------|------------|------------|-------------|-------------|-------------|-------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|   | -0.999925  | -0.584231  | -0.071074  | -0.663615  | -0.105184   | 1.309106    | 0.060929    | -0.395592  | 0.925018   | -0.284491   | -0.257318   | -0.547866   | 0.617728    | 1.794494    | 1.228686    | -1.156569   | -0.888898   | -0.031132   | -1.459511   | -0.719021   | 0.308810    |

### n-propylacrylate_6_reopt_am1_HEI

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.205054 |
| AM1 Free Energy (Quasiharmonic)      | -0.048001 |
| Number of Imaginary Frequencies      | 0         |
**Frequencies (Top 3 out of 63)**

1. 25.7749 cm⁻¹
2. 34.5970 cm⁻¹
3. 53.2374 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atomic Number | X       | Y       | Z       |
|---------------|---------|---------|---------|
| C             | -0.324812 | 0.829676 | -0.537381 |
| C             | 0.852248  | 0.418542 | -1.164128 |
| C             | 1.519948  | -0.821793 | -0.930525 |
| O             | -0.986414 | 1.891213 | -0.658722 |
| O             | -0.881783 | -0.092458 | 0.370299 |
| C             | -2.080184 | 0.281924 | 1.024526 |
| C             | -3.304379 | 0.020779 | 1.59477 |
| C             | -3.521537 | -1.448779 | -0.083983 |
| H             | 1.967513  | -1.264781 | -1.853802 |
| H             | 0.886489  | -1.547050 | -0.406513 |
| H             | -2.101456 | -0.361963 | 1.945538 |
| H             | -2.050270 | 1.365738 | 1.314027 |
| H             | -4.204025 | 0.462434 | 0.661234 |
| H             | -3.154960 | 0.554220 | -0.817090 |
| H             | -4.364918 | -1.611028 | -0.797454 |
| H             | -3.760418 | -1.978349 | 0.870111 |
| H             | -2.593693 | -1.901148 | -0.512983 |
| S             | 3.064952  | -0.727996 | 0.113348 |
| C             | 2.811746  | 0.651440 | 1.165260 |
| H             | 1.904855  | 1.215749 | 0.832039 |
| H             | 3.700198  | 1.317944 | 1.117235 |
| H             | 2.669276  | 0.314208 | 2.215096 |
| H             | 1.289591  | 1.128196 | -1.873092 |

**n-propylacrylate_7_am1**

| Datum                              | Value         |
|------------------------------------|---------------|
| AM1 Energy                         | -0.130254     |
| AM1 Free Energy (Quasiharmonic)    | -0.008157     |
| Number of Imaginary Frequencies    | 0             |

**Frequencies (Top 3 out of 48)**
1. 29.9373 cm⁻¹
2. 49.0840 cm⁻¹
3. 59.6302 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| C       | 1.219650 | -0.569462 | 0.079674 |
| C       | 2.376107 | 0.333944  | 0.101348 |
| C       | 2.307112 | 1.641857  | -0.141838 |
| O       | 1.216678 | -1.785805 | 0.291602 |
| O       | 0.026266 | 0.035706  | -0.212259 |
| C       | -1.131328 | -0.818997 | -0.242687 |
| C       | -2.318941 | 0.071083  | -0.556418 |
| C       | -2.753696 | 0.879465  | 0.637750 |
| H       | 3.321930 | -0.181123 | 0.341534 |
| H       | 3.198987 | 2.283586  | -0.115606 |
| H       | 1.361786 | 2.150830  | -0.380975 |
| H       | -0.977238 | -1.595507 | -1.036940 |
| H       | -1.234773 | -1.323810 | 0.752810 |
| H       | -3.158986 | -0.587987 | -0.900567 |
| H       | -2.053126 | 0.758070  | -1.402488 |
| H       | -3.607577 | 1.545245  | 0.365115 |
| H       | -3.078558 | 0.211285  | 1.471730 |
| H       | -1.909422 | 1.512872  | 1.003663 |

n-propylacrylate_8_am1_HEI

| Datum                                      | Value      |
|--------------------------------------------|------------|
| AM1 Energy                                 | -0.20541   |
| AM1 Free Energy (Quasiharmonic)            | -0.049359  |
| Number of Imaginary Frequencies            | 0          |

Frequencies (Top 3 out of 63)

1. 22.5118 cm⁻¹
2. 38.8966 cm⁻¹
3. 41.4007 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
C  -0.053856  1.321536  0.025128
C   1.264812  1.268653 -0.428935
C   1.838585  0.190748 -1.168194
O  -0.659406  2.205146  0.681881
O  -0.858966  0.217976 -0.316162
C  -2.207296  0.272679  0.126400
C  -2.869711 -1.016764 -0.333866
C  -4.312492 -1.060980  0.094557
H   2.559669  0.525772 -1.953461
H   1.081329  0.525772 -1.953461
H  -2.715959  1.168959 -0.316731
H  -2.37503  0.365747  1.243921
H  -2.794388 -1.091676 -1.449659
H  -2.311144 -1.889838  0.092955
H  -4.395019 -1.004781  1.207134
H  -4.792632 -2.009547 -0.247323
H  -4.879358 -0.202101 -0.339942
S   2.975819 -0.938694 -0.208278
C   2.392813 -0.862996  1.443329
H   1.932106 -1.832251  1.733923
H   3.245026 -0.649389  2.124483
H   1.630409 -0.049144  1.534802
H   1.894199  2.125249 -0.169007

**n-propylacrylate_8_am1**

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.131387 |
| AM1 Free Energy (Quasiharmonic)      | -0.008852 |
| Number of Imaginary Frequencies      | 0         |

**Frequencies (Top 3 out of 48)**

1. 40.6913 cm⁻¹
2. 55.8677 cm⁻¹
3. 74.5144 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

C  -1.063782  0.541398  0.080150
C  -2.467504  0.241224 -0.228135
C  -2.985416 -0.986084 -0.233279
O  -0.524847  1.651705  0.091434
### n-propylacrylate_9_am1_HEI

| Datum                                | Value          |
|--------------------------------------|----------------|
| AM1 Energy                           | -0.205947      |
| AM1 Free Energy (Quasiharmonic)      | -0.04905       |
| Number of Imaginary Frequencies      | 0              |

**Frequencies** (Top 3 out of 63)

1. 27.6090 cm⁻¹
2. 36.7615 cm⁻¹
3. 50.9911 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|    |    |    |    |
|----|----|----|----|
| C  | 0.238211 | 0.878711 | 0.213438 |
| C  | -1.019517 | 1.203666 | -0.296085 |
| C  | -1.797128 | 0.375200 | -1.160937 |
| O  | 0.998780  | 1.520026 | 0.981189  |
| O  | 0.760278  | -0.360527 | -0.206449 |
| C  | 2.032226  | -0.732129 | 0.290270  |
| C  | 3.147564  | -0.086642 | -0.517958 |
| C  | 4.499096  | -0.585776 | -0.083522 |
| H  | -2.355939 | 0.949250  | -1.940144 |
| H  | -1.211282 | -0.448123 | -1.630553 |
| H  | 2.056764  | -1.850012 | 0.175666  |
| H  | 2.134611  | -0.457264 | 1.372992  |
| H  | 3.075770  | 1.025109  | -0.379256 |
| H  | 2.988474  | -0.301033 | -1.606298 |
n-propylacrylate_9_am1

| Datum                              | Value      |
|------------------------------------|------------|
| AM1 Energy                         | -0.131132  |
| AM1 Free Energy (Quasiharmonic)    | -0.009217  |
| Number of Imaginary Frequencies    | 0          |

**Frequencies** (Top 3 out of 48)

1. 41.1743 cm⁻¹
2. 44.8987 cm⁻¹
3. 61.0097 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C      | 1.274591 | 0.592567 | 0.000017 |
|--------|----------|----------|----------|
| C      | 2.571881 | -0.093840| 0.000009 |
| C      | 2.716700 | -1.418101| -0.000028|
| O      | 1.073300 | 1.810776 | 0.000047 |
| O      | 0.187182 | -0.239615| -0.000013|
| C      | -1.102947| 0.396702 | -0.000009|
| C      | -2.124418| -0.725187| -0.000008|
| C      | -3.521300| -0.161605| -0.000008|
| H      | 3.428295 | 0.602022 | 0.000036 |
| H      | 3.708320 | -1.892194| -0.000033|
| H      | 1.859826 | -2.107847| -0.000055|
| H      | -1.189184| 1.040695 | -0.913489|
| H      | -1.189184| 1.040694 | 0.913472 |
| H      | -1.966224| -1.371599| -0.902517|
| H      | -1.966223| -1.371599| 0.902501 |
| H      | -4.268666| -0.991431| -0.000006|
| H      | -3.693929| 0.469381 | 0.905470 |
| H      | -3.693930| 0.469380 | -0.905486|
Ketone Structures (AM1)

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1_pentene-3-one_trunc_1_am1_HEI

| Datum                                | Value  |
|--------------------------------------|--------|
| AM1 Energy                           | -0.107567 |
| AM1 Free Energy (Quasiharmonic)      | -0.008916 |
| Number of Imaginary Frequencies      | 0      |

Frequencies (Top 3 out of 42)

1. 32.4007 cm⁻¹  
2. 62.2793 cm⁻¹  
3. 86.1511 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

```
C  -1.616430  -0.068980  0.147056
C  -0.570036  -0.728070  -0.505451
C   0.598501  -1.208081  0.162576
O  -1.703099   0.185953  1.383681
H  -0.631803  -0.866667  -1.589517
H   0.474504  -1.251983  1.269344
H   0.981424  -2.179784   0.233699
H   1.570740   1.468948  -0.063517
H   1.909136   1.981123   0.863456
H   0.452899   1.473890  -0.100371
H   1.974114   2.013324  -0.944842
S   2.145614  -0.187842  -0.088248
```
**1_pentene-3-one_trunc_2_am1_HEI_reopt**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.107838 |
| AM1 Free Energy (Quasiharmonic)            | -0.008631 |
| Number of Imaginary Frequencies            | 0       |

**Frequencies** (Top 3 out of 42)

1. 29.7432 cm⁻¹  
2. 63.8808 cm⁻¹  
3. 98.0853 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C  | 0.360323 | -0.741923 |
|----|----------|-----------|
| H  | -0.528946 | -1.251697  |
| H  | 0.862561  | -0.141621  |
| H  | 1.069484  | -1.520983  |

**1_pentene-3-one_trunc_3_am1_HEI**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| Datum                                      | Value   |

**Value**
| Datum                              | Value      |
|-----------------------------------|------------|
| AM1 Energy                        | -0.107567  |
| AM1 Free Energy (Quasiharmonic)   | -0.008918  |
| Number of Imaginary Frequencies   | 0          |

**Frequencies** (Top 3 out of 42)

1. 32.3700 cm^-1  
2. 62.1027 cm^-1  
3. 86.0803 cm^-1  

**AM1 Molecular Geometry in Cartesian Coordinates**

|          | X            | Y            | Z            |
|----------|--------------|--------------|--------------|
| C        | -1.616560    | -0.069176    | -0.146961    |
| C        | -0.569948    | -0.727128    | 0.506351     |
| C        | 0.598446     | -1.208171    | -0.161149    |
| O        | -1.703653    | 0.183642     | -1.383983    |
| H        | -0.631521    | -0.864109    | 1.590633     |
| H        | 0.981307     | -2.179369    | 0.236423     |
| H        | 0.474313     | -1.253630    | -1.267832    |
| C        | 1.570973     | 1.469014     | 0.062149     |
| H        | 1.975149     | 2.014147     | 0.942632     |
| H        | 0.453165     | 1.474162     | 0.099882     |
| H        | 1.908662     | 1.980253     | -0.865595    |
| S        | 2.145716     | -0.187799    | 0.088141     |
| C        | -2.765888    | 0.361542     | 0.741654     |
| H        | -2.398569    | 1.071045     | 1.520214     |
| H        | -3.560399    | 0.863781     | 0.140956     |
| H        | -3.206473    | -0.527116    | 1.252027     |

**1_pentene-3-one_trunc_4_am1_HEI**

| Datum                              | Value      |
|-----------------------------------|------------|
| AM1 Energy                        | -0.107838  |
| AM1 Free Energy (Quasiharmonic)   | -0.008635  |
| Number of Imaginary Frequencies   | 0          |

**Frequencies** (Top 3 out of 42)
1. 29.6658 cm\(^{-1}\)
2. 63.8543 cm\(^{-1}\)
3. 98.0570 cm\(^{-1}\)

### AM1 Molecular Geometry in Cartesian Coordinates

C           1.672606        0.007506        0.148707
C           0.588556       -0.561799        0.832319
C           -0.506863       -1.237015        0.224387
O           2.646108        0.593160        0.706128
H            0.580099       -0.460421        1.923890
H           -0.290252       -1.660931       -0.783654
H           -0.967391       -2.015003        0.878581
C           -1.533080       1.463709        0.053957
H           -0.467653       1.492936        0.397735
H           -2.176910       1.971027        0.804836
H           -1.620991       1.998215       -0.917082
S           -2.045431       -0.201634       -0.132367
C           1.685749       -0.088531       -1.360295
H           1.776596       -1.155869       -1.673100
H           0.735751       0.325396       -1.775252
H           2.546976       0.482293       -1.781555

**1_pentene-3-one_trunc_5_am1_HEI**

| Datum                                | Value   |
|--------------------------------------|---------|
| AM1 Energy                           | -0.103359 |
| AM1 Free Energy (Quasiharmonic)      | -0.005383 |
| Number of Imaginary Frequencies      | 0       |

**Frequencies** (Top 3 out of 42)

1. 41.0630 cm\(^{-1}\)
2. 57.9909 cm\(^{-1}\)
3. 63.2968 cm\(^{-1}\)

### AM1 Molecular Geometry in Cartesian Coordinates

C           1.870114        0.191019        0.005622
C           0.764806       -0.452331        0.574273
### 1_pentene-3-one_trunc_6_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.103484   |
| AM1 Free Energy (Quasiharmonic)           | -0.004987   |
| Number of Imaginary Frequencies           | 0           |

**Frequencies (Top 3 out of 42)**

1. 44.0599 cm⁻¹  
2. 58.1489 cm⁻¹  
3. 68.7773 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| C | -1.925115 | -0.078648 | -0.010929 |
| C | -0.827496  | -0.859016  | 0.383214  |
| C | 0.412499   | -0.349941  | 0.861087  |
| O | -3.032108  | -0.545064  | -0.407465 |
| H | -0.922782  | -1.945529  | 0.275332  |
| H | 0.367869   | 0.673947   | 1.300538  |
| H | 0.938187   | -1.035085  | 1.567950  |
| C | 3.076940   | 0.372633   | 0.101999  |
| H | 3.468458   | -0.325524  | 0.875744  |
| H | 2.951624   | 1.373327   | 0.573359  |
| H | 3.822344   | 0.453562   | -0.719803 |
| S | 1.573813   | -0.207140  | -0.580389 |
| C | -1.787071  | 1.425171   | 0.065929  |
| H | -1.682214  | 1.743873   | 1.130439  |
**1pentene-3-one_truncated_1_am1**

| Datum                              | Value       |
|------------------------------------|-------------|
| AM1 Energy                         | -0.036892   |
| AM1 Free Energy (Quasiharmonic)    | 0.028009    |
| Number of Imaginary Frequencies    | 0           |

**Frequencies (Top 3 out of 27)**

1. 41.9253 cm⁻¹  
2. 133.5319 cm⁻¹  
3. 291.5239 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|       |       |       |       |
|-------|-------|-------|-------|
| C     | 0.763983 | 1.306900 | 0.000001 |
| H     | 0.296234 | 1.758732 | -0.908307 |
| H     | 1.855888 | 1.543992 | -0.000032 |
| C     | 0.549061 | -0.173380 | -0.000000 |
| H     | 0.296293 | 1.758720 | 0.908346  |
| C     | -0.842608 | -0.663936 | 0.000002  |
| O     | 1.499809 | -0.966019 | -0.000002 |
| C     | -1.921469 | 0.116608  | -0.000002 |
| H     | -2.938795 | -0.299623 | 0.000000  |
| H     | -1.871040 | 1.214527  | -0.000006 |
| H     | -0.930852 | -1.765349 | 0.000007  |

**1pentene-3-one_truncated_2_am1**

| Datum                              | Value       |
|------------------------------------|-------------|
| AM1 Energy                         | -0.038392   |
| AM1 Free Energy (Quasiharmonic)    | 0.026408    |
| Number of Imaginary Frequencies    | 0           |

**Frequencies (Top 3 out of 27)**


1. 61.4137 cm⁻¹
2. 97.6091 cm⁻¹
3. 268.2836 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | 1.716368 | -0.620130| 0.000000 |
| H    | 1.758423 | -1.270485| 0.907535 |
| H    | 2.600296 | 0.062476 | 0.000029 |
| C    | 0.441693 | 0.162629 | 0.000000 |
| H    | 1.758448 | -1.270441| -0.907564|
| C    | -0.790273| -0.646001| 0.000000 |
| O    | 0.432545 | 1.400584 | 0.000000 |
| C    | -2.009741| -0.105925| 0.000000 |
| H    | -2.923026| -0.716141| 0.000001 |
| H    | -2.164034| 0.983886 | 0.000000 |
| H    | -0.638750| -1.737405| 0.000000 |

**2_2cyclopentene1one_1_am1_HEI**

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.100657 |
| AM1 Free Energy (Quasiharmonic)            | 0.008225  |
| Number of Imaginary Frequencies            | 0         |

**Frequencies** (Top 3 out of 45)

1. 55.2692 cm⁻¹
2. 83.1112 cm⁻¹
3. 118.9315 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | 1.619492 | 0.855764 | 0.723714 |
| C    | 0.366788 | 1.586648 | 0.246688 |
| C    | -0.325765| 0.648907 | -0.749059|
| C    | 0.561136 | -0.475746| -0.946068|
| C    | 1.688011 | -0.430424| -0.110190|
| H    | 2.538424 | 1.467698 | 0.562430 |
| H    | 1.558002 | 0.602002 | 1.808783 |
### 2_2-cyclopentene-1-one_1_am1

| Datum                                           | Value            |
|-------------------------------------------------|------------------|
| AM1 Energy                                      | -0.034795        |
| AM1 Free Energy (Quasiharmonic)                | 0.040428         |
| Number of Imaginary Frequencies                | 0                |

**Frequencies** (Top 3 out of 30)

1. 127.7337 cm⁻¹
2. 306.6302 cm⁻¹
3. 477.1257 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |     |     |     |
|-----|-----|-----|-----|
| C   | -0.041540 | -1.190483 | -0.000000 |
| C   | -1.464463 | -0.618833 | 0.000000  |
| C   | -1.284748 | 0.872058  | -0.000000 |
| C   | 0.014630  | 1.227361  | -0.000000 |
| C   | 0.879040  | 0.018810  | 0.000000  |
| H   | 0.150883  | -1.816894 | 0.905044  |
| H   | 0.150882  | -1.816892 | -0.905045 |
| H   | -2.034751 | -0.946417 | 0.904887  |
| H   | -2.034752 | -0.946418 | -0.904886 |
| O   | 2.107655  | -0.011860 | -0.000000 |
| H   | 0.440764  | 2.231702  | 0.000001  |
| H   | -2.151784 | 1.536317  | 0.000000  |

---

### 2_2cyclopentene1one_2_am1.HEI
| Datum                                           | Value         |
|-------------------------------------------------|---------------|
| AM1 Energy                                      | -0.100657     |
| AM1 Free Energy (Quasiharmonic)                 | 0.008227      |
| Number of Imaginary Frequencies                 | 0             |

**Frequencies (Top 3 out of 45)**

1. 55.3106 cm⁻¹  
2. 83.1191 cm⁻¹  
3. 118.9355 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C       | -1.619315 | 0.855731 | -0.723828 |
|---------|-----------|----------|-----------|
| C       | -0.366713 | 1.586681 | -0.246628 |
| C       | 0.325859  | 0.648880 | 0.749053  |
| C       | -0.561120 | -0.475741| 0.946083  |
| C       | -1.687979 | -0.430372| 0.110206  |
| H       | -2.538285 | 1.467685 | -0.562834 |
| H       | -1.557571 | 0.601820 | -1.808850 |
| H       | -0.640137 | 2.545193 | 0.261826  |
| H       | 0.310160  | 1.834589 | -1.099931 |
| O       | -2.651549 | -1.229784| -0.005874 |
| H       | -0.372356 | -1.256300| 1.673957  |
| H       | 0.653494  | 1.175266 | 1.677432  |
| C       | 1.837742  | -1.343147| -0.683637 |
| H       | 2.587918  | -2.052584| -0.271347 |
| H       | 1.998532  | -1.245200| -1.779424 |
| H       | 0.808318  | -1.738461| -0.493622 |
| S       | 2.024467  | 0.215879 | 0.096393  |

**2_2cyclopentene1one_3_am1_HEI**

| Datum                                           | Value         |
|-------------------------------------------------|---------------|
| AM1 Energy                                      | -0.096283     |
| AM1 Free Energy (Quasiharmonic)                 | 0.011941      |
| Number of Imaginary Frequencies                 | 0             |

**Frequencies (Top 3 out of 45)**
1.  57.7568 cm⁻¹  
2.  73.0557 cm⁻¹  
3.  85.1042 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Atom | x    | y    | z     |
|------|------|------|-------|
| C    | -1.588592 | 1.183259 | -0.335832 |
| C    | -0.180337   | 1.384743   | 0.217895  |
| C    | 0.288319    | 0.008809    | 0.704892  |
| C    | -0.842951   | -0.885324   | 0.587973  |
| C    | -1.948921   | -0.276705   | -0.026899 |
| H    | -2.321212   | 1.872984    | 0.146182  |
| H    | -1.622285   | 1.354093    | -1.438158 |
| H    | -0.192324   | 2.108662    | 1.071138  |
| H    | 0.508546    | 1.789845    | -0.562732 |
| O    | -3.089793   | -0.732015   | -0.294079 |
| H    | -0.816620   | -1.917153   | 0.917693  |
| H    | 0.771468    | 0.060382    | 1.708868  |
| C    | 3.038430    | 0.268817    | -0.052567 |
| H    | 2.903338    | 1.331166    | -0.357212 |
| H    | 3.879656    | -0.167815   | -0.635154 |
| H    | 3.300644    | 0.251194    | 1.029171  |
| S    | 1.606965    | -0.683052   | -0.381246 |

3_3methyl3pentene2one_1_am1_HEI_reopt

| Datum                                    | Value       |
|------------------------------------------|-------------|
| AM1 Energy                               | -0.123756   |
| AM1 Free Energy (Quasiharmonic)          | 0.027973    |
| Number of Imaginary Frequencies          | 0           |

Frequencies (Top 3 out of 60)

1.  30.9094 cm⁻¹  
2.  69.3381 cm⁻¹  
3.  78.5955 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates
### 3_3methyl3pentene2one_2_reopt_am1_HEI

| Datum                              | Value     |
|------------------------------------|-----------|
| AM1 Energy                         | -0.124587 |
| AM1 Free Energy (Quasiharmonic)    | 0.02787   |
| Number of Imaginary Frequencies    | 0         |

#### Frequencies (Top 3 out of 60)

1. 34.5395 cm⁻¹  
2. 55.6552 cm⁻¹  
3. 85.3637 cm⁻¹  

#### AM1 Molecular Geometry in Cartesian Coordinates

| C       | -1.729752 | 0.168570 | 0.172735 |
|---------|-----------|----------|----------|
| C       | -0.606189 | -0.651825| -0.072488|
| C       | 0.600604  | -0.559192| 0.698282 |
| O       | -2.822926 | 0.107210 | -0.459038|
| H       | 0.439992  | -0.139964| 1.723390 |
### 3_methyl3pentene2one_3_am1.HEI

#### Datum

|          | Value   |
|----------|---------|
| AM1 Energy | -0.119269 |
| AM1 Free Energy (Quasiharmonic) | 0.032372 |
| Number of Imaginary Frequencies | 0 |

#### Frequencies (Top 3 out of 60)

1. 37.6852 cm$^{-1}$
2. 59.1108 cm$^{-1}$
3. 74.5371 cm$^{-1}$

#### AM1 Molecular Geometry in Cartesian Coordinates

|     |          |          |          |
|-----|----------|----------|----------|
| C   | 1.088769 | 1.618957 | -1.203592 |
| H   | 1.676564 | 1.548520 | -2.144596 |
| H   | 0.064479 | 1.200690 | -1.374061 |
| H   | 1.003580 | 2.688099 | -0.909557 |
| S   | 1.893826 | 0.716710 | 0.063572  |
| C   | -1.623070| 1.203557 | 1.269236  |
| H   | -2.522405| 1.864403 | 1.267763  |
| H   | -1.551923| 0.701884 | 2.263500  |
| H   | -0.709860| 1.827969 | 1.113947  |
| C   | 1.441019 | -1.805052| 0.770319  |
| H   | 0.861318 | -2.624816| 1.263498  |
| H   | 1.735097 | -2.148416| -0.250636 |
| H   | 2.370633 | -1.619856| 1.362729  |
| C   | -0.673719| -1.629629| -1.174077 |
| H   | -1.647165| -1.544450| -1.718549 |
| H   | 0.156309 | -1.470235| -1.911178 |
| H   | -0.580383| -2.681185| -0.793587 |
3_3methyl3pentene2one_4_am1_HEI

| Datum                                | Value      |
|--------------------------------------|------------|
| AM1 Energy                           | -0.120395  |
| AM1 Free Energy (Quasiharmonic)      | 0.032087   |
| Number of Imaginary Frequencies      | 0          |

**Frequencies (Top 3 out of 60)**

1. 34.0990 cm⁻¹
2. 60.3615 cm⁻¹
3. 80.8549 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -1.593844 | -0.137567 | -0.351845 |
| C          | -0.677463 | 0.249769  | 0.647839  |
| C          | 0.583980  | -0.375748 | 0.939338  |
| O          | -2.722198 | 0.405425  | -0.536825 |
| H          | 1.004661  | 0.029736  | 1.897865  |
| C          | 1.437726  | 1.417664  | -1.195631 |
| H          | 1.620166  | 1.209977  | -2.272574 |
| H          | 0.340414  | 1.557096  | -1.024525 |
| H          | 1.974767  | 2.348432  | -0.910289 |
| S          | 2.018543  | 0.065979  | -0.243473 |
| C          | -1.214564 | -1.254270 | -1.294491 |
| H          | -1.886643 | -1.251192 | -2.185945 |
| H          | -0.156535 | -1.127191 | -1.630670 |
| H          | -1.319153 | -2.237730 | -0.777236 |
| C          | 0.665253  | -1.879027 | 0.963318  |
| H          | -0.272898 | -2.305373 | 1.395980  |
| H          | 0.809296  | -2.303472 | -0.059578 |
| H     | 1.527581 | -2.210827 | 1.593723 |
| C    | -1.011438 | 1.433126  | 1.470244 |
| H    | -0.234211 | 2.234949  | 1.363190 |
| H    | -1.999234 | 1.861047  | 1.167857 |
| H    | -1.065218 | 1.171800  | 2.559729 |

3_3methyl3pentene2one_5_am1_HEI

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.124587   |
| AM1 Free Energy (Quasiharmonic)           | 0.027863    |
| Number of Imaginary Frequencies           | 0           |

**Frequencies** (Top 3 out of 60)

1. 34.4574 cm⁻¹
2. 55.6426 cm⁻¹
3. 85.3394 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C    | 1.729817 | -0.168913 | 0.172735 |
| C    | 0.606453 | 0.651792  | -0.072430|
| C    | -0.600330| 0.559366  | 0.698331 |
| O    | 2.823131 | -0.107540 | -0.458779|
| H    | -0.439822| 0.140062  | 1.723409 |
| C    | -1.089655| -1.618554 | -1.203950|
| H    | -1.004772| -2.687817 | -0.910281|
| H    | -1.677757| -1.547593 | -2.144720|
| H    | -0.065285| -1.200629 | -1.374673|
| S    | -1.893950| -0.716461 | 0.063818 |
| C    | 1.622646 | -1.204302 | 1.268812 |
| H    | 2.521174 | -1.866233 | 1.266410 |
| H    | 1.552902 | -0.702930 | 2.263330 |
| H    | 0.708556 | -1.827522 | 1.113977 |
| C    | -1.440547| 1.805355  | 0.770316 |
| H    | -0.860661| 2.625109  | 1.263284 |
| H    | -1.734672| 2.148603  | -0.250660|
| H    | -2.370105| 1.620403  | 1.362877 |
| C    | 0.674225 | 1.629642  | -1.173956|
| H    | 0.580487 | 2.681171  | -0.793518|
| H    | 1.647907 | 1.544663  | -1.718023|
| H    | -0.155457| 1.470100  | -1.911407|
### 3_3methyl3pentene2one_6_am1_HEI

| Datum                          | Value  |
|--------------------------------|--------|
| AM1 Energy                     | -0.124587 |
| AM1 Free Energy (Quasiharmonic)| 0.027873 |
| Number of Imaginary Frequencies| 0      |

**Frequencies** (Top 3 out of 60)

1. 34.6264 cm⁻¹  
2. 55.7980 cm⁻¹  
3. 85.3654 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -1.729712 | -0.168819 | -0.172867 |
| C | -0.606376 | 0.651946  | 0.072302  |
| C | 0.600480  | 0.559438  | -0.698332 |
| O | -2.823208 | -0.107125 | 0.458293  |
| H | 0.439996  | 0.140218  | -1.723470 |
| C | 1.089061  | -1.618621 | 1.203937  |
| H | 1.004035  | -2.687854 | 0.910181  |
| H | 1.676905  | -1.547862 | 2.144893  |
| H | 0.064708  | -1.200442 | 1.374398  |
| S | 1.893793  | -0.716621 | -0.063593 |
| C | -1.622262 | -1.204632 | -1.268501 |
| H | -1.552383 | -0.703575 | -2.263190 |
| H | -0.708137 | -1.827733 | -1.113320 |
| H | -2.520742 | -1.866644 | -1.265976 |
| C | 1.440906  | 1.805274  | -0.770241 |
| H | 0.861307  | 2.625020  | -1.263591 |
| H | 1.734779  | 2.148710  | 0.250753  |
| H | 2.370644  | 1.620039  | -1.362454 |
| C | -0.674263 | 1.629838  | 1.173787  |
| H | -0.580854 | 2.681390  | 0.793304  |
| H | -1.647867 | 1.544642  | 1.717984  |
| H | 0.155578  | 1.470482  | 1.911120  |

### 3_3methyl3pentene2one_7_reopt_am1_HEI

| Datum          | Value  |
|----------------|--------|
| Datum          | Value  |
| Datum                                      | Value               |
|-------------------------------------------|---------------------|
| AM1 Energy                                | -0.122068           |
| AM1 Free Energy (Quasiharmonic)           | 0.029907            |
| Number of Imaginary Frequencies           | 0                   |

**Frequencies (Top 3 out of 60)**

1. 27.1684 cm⁻¹
2. 55.9809 cm⁻¹
3. 65.3658 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| Atom | C    | C    | C    | O    | H    | C    | H    | H    | S    | C    | H    | H    | H    | C    | H    | H    | H    | C    | H    | H    | H    |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
|      | -1.534483 | 0.401679 | 0.208378 |       |      | 0.659022 | 0.121692 | -0.990705 | -1.383529 | 1.594564 | 0.602684 |       | 1.533988 | -0.265571 | 1.740525 |       | 2.078162 | 0.549497 | 2.265874 |       | 0.440947 | -0.032453 | 1.731017 |       |
|      | -0.623237 | -0.364855 | -0.540269 |       |      | 0.996499 | -0.398641 | -1.927495 | -1.383529 | 1.594564 | 0.602684 |       | 1.533988 | -0.265571 | 1.740525 |       | 2.078162 | 0.549497 | 2.265874 |       | 0.440947 | -0.032453 | 1.731017 |       |
|      | 0.659022 | 0.121692 | -0.990705 | -1.383529 | 1.594564 | 0.602684 |       |       | 1.533988 | -0.265571 | 1.740525 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|      | 0.996499 | -0.398641 | -1.927495 |       |      | -1.383529 | 1.594564 | 0.602684 |       | 1.533988 | -0.265571 | 1.740525 |       |       |       |       |       |       |       |       |       |       |       |       |       |
|      |       |       |       |       |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

**3-methyl-3-pentene-2-one_1_am1_reopt**

| Datum                                      | Value               |
|-------------------------------------------|---------------------|
| AM1 Energy                                | -0.062835           |
| AM1 Free Energy (Quasiharmonic)           | 0.054279            |
### 3-methyl-3-pentene-2-one_2_am1_reopt

| Datum                        | Value         |
|------------------------------|---------------|
| AM1 Energy                   | -0.063721     |
| AM1 Free Energy (Quasiharmonic) | 0.053586     |
| Number of Imaginary Frequencies | 0             |

**Frequencies (Top 3 out of 45)**

1. 18.5974 cm\(^{-1}\)
2. 61.6858 cm\(^{-1}\)
3. 88.6111 cm\(^{-1}\)
AM1 Molecular Geometry in Cartesian Coordinates

|      |       |       |      |
|------|-------|-------|------|
| C    | -2.699981 | -0.245194 | 0.021283 |
| H    | -2.930863  | 0.377503  | -0.880064 |
| H    | -2.928793  | 0.365078  | 0.931854 |
| C    | -1.286969  | -0.664194 | 0.018511 |
| H    | -3.378526  | -1.133370 | 0.016087 |
| C    | -0.230119  | 0.170720  | -0.006619 |
| C    | 1.138563   | -0.395364 | -0.005668 |
| C    | 2.278465   | 0.572054  | 0.049068 |
| O    | 1.340704   | -1.617736 | -0.044671 |
| H    | 3.252923   | 0.029641  | -0.020727 |
| H    | 2.206242   | 1.299649  | -0.795262 |
| H    | 2.248062   | 1.136405  | 1.012999 |
| H    | -1.105723  | -1.755861 | 0.039220 |
| C    | -0.355618  | 1.645466  | -0.041497 |
| H    | 0.213241   | 2.108626  | 0.803393 |
| H    | 0.055190   | 2.047180  | -1.002041 |
| H    | -1.423431  | 1.966109  | 0.041443 |

4_4-methyl-3-pentene-2-one_1_am1

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.066135 |
| AM1 Free Energy (Quasiharmonic)            | 0.051166  |
| Number of Imaginary Frequencies            | 0         |

Frequencies (Top 3 out of 45)

1. 44.2906 cm⁻¹
2. 94.5686 cm⁻¹
3. 99.8147 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|      |       |       |      |
|------|-------|-------|------|
| C    | -2.413898 | -0.976257 | -0.000012 |
| H    | -2.170965  | -2.066738 | -0.000248 |
| H    | -3.030345  | -0.749510 | -0.906172 |
| C    | -1.191997  | -0.134689 | -0.000003 |
| H    | -3.030126  | -0.749857 | 0.906382 |
| C    | 0.035676   | -0.690014 | -0.000026 |
4_4methyl3pentene2one_1_reopt_am1_HEI

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.115023 |
| AM1 Free Energy (Quasiharmonic)            | 0.035808  |
| Number of Imaginary Frequencies            | 0         |

Frequencies (Top 3 out of 60)

1. 33.1546 cm⁻¹
2. 52.4727 cm⁻¹
3. 74.9287 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| C   | 1.294828 | 0.060350 | -0.000018 |
| C   | 2.531493 | -0.785102| 0.000046  |
| O   | 1.359654 | 1.298533 | -0.000056 |
| H   | 3.446911 | -0.145579| 0.000284  |
| H   | 2.542138 | -1.436590| 0.907425  |
| H   | 2.542411 | -1.436295| -0.907542 |
| C   | -1.415258| 1.329206 | 0.000048  |
| H   | 0.147655 | -1.787008| -0.000057 |
| H   | -0.932783| 1.791618 | 0.899540  |
| H   | -0.933771| 1.791545 | -0.899999 |
| H   | -2.503418| 1.579184 | 0.000629  |

| 4_4methyl3pentene2one_1_reopt_am1_HEI     |          |
|--------------------------------------------|-----------|
### 4_4-methyl-3-pentene-2-one_2_am1

| Datum                          | Value       |
|--------------------------------|-------------|
| AM1 Energy                     | -0.066135   |
| AM1 Free Energy (Quasiharmonic)| 0.051173    |
| Number of Imaginary Frequencies| 0           |

**Frequencies (Top 3 out of 45)**

1. 44.4700 cm⁻¹
2. 94.7425 cm⁻¹
3. 100.0168 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C    | -2.414016 | -0.976139 | -0.000106 |
|------|-----------|-----------|-----------|
| H    | -2.171178 | -2.066646 | -0.000788 |
| H    | -3.030575 | -0.748987 | -0.006093 |
| C    | -1.192023 | -0.134711 | 0.000058  |
| H    | -3.030101 | -0.750034 | 0.906466  |
| C    | 0.035612  | -0.690039 | 0.000010  |
| C    | 1.294781  | 0.060323  | -0.00063  |
| C    | 2.531434  | -0.785144 | 0.000094  |
| O    | 1.359560  | 1.298492  | -0.000209 |
| H    | 2.541978  | -1.437046 | -0.906991 |
| H    | 3.446864  | -0.145624 | -0.000431 |
| H    | 2.542425  | -1.435937 | 0.907968  |
| C    | -1.414948 | 1.329249  | 0.000150  |
| H    | 0.147721  | -1.787068 | 0.000004  |
| H    | -0.932649 | 1.791263  | 0.899955  |
| H    | -0.932987 | 1.791592  | -0.899647 |
| H    | -2.503018 | 1.579622  | 0.000374  |

### 4_4methyl3pentene2one_2_reopt_am1_HEI
### AM1 Molecular Geometry in Cartesian Coordinates

|        | X              | Y              | Z              |
|--------|----------------|----------------|----------------|
| C      | 1.827164       | 0.055554       | -0.040981      |
| C      | 0.656603       | 0.389099       | 0.650488       |
| C      | -0.601933      | 0.764648       | 0.079189       |
| O      | 2.023720       | 0.052631       | -1.289788      |
| C      | -0.896411      | -2.157696      | -0.106122      |
| H      | -1.091046      | -2.620694      | -1.098283      |
| H      | 0.185137       | -1.880144      | -0.035986      |
| H      | -1.140381      | -2.895151      | 0.689549       |
| S      | -1.883286      | -0.726168      | 0.100757       |
| C      | 2.995175       | -0.332319      | 0.846428       |
| H      | 2.730445       | -1.233559      | 1.448127       |
| H      | 3.896127       | -0.560959      | 0.229789       |
| H      | 3.237606       | 0.502569       | 1.545123       |
| C      | -1.405902      | 1.722493       | 0.929611       |
| H      | -0.948168      | 2.741491       | 0.879685       |
| H      | -2.460345      | 1.790642       | 0.564714       |
| H      | -1.417508      | 1.390851       | 1.995121       |
| H      | 0.684974       | 0.320564       | 1.745778       |
| C      | -0.581537      | 1.184666       | -1.366472      |
| H      | -1.610284      | 1.427753       | -1.726701      |
| H      | 0.068187       | 2.086987       | -1.486394      |
| H      | -0.150891      | 0.368615       | -1.997182      

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### 4_4methyl3pentene2one_3_am1_HEI

| Datum                        | Value     |
|------------------------------|-----------|
| AM1 Energy                   | -0.112158 |
| AM1 Free Energy (Quasiharmonic) | 0.039878  |
### AM1 Molecular Geometry in Cartesian Coordinates

|     |     |     |
|-----|-----|-----|
| C   | 1.871231 | 0.079067 | 0.234142 |
| C   | 0.642736 | 0.516813 | 0.762880 |
| C   | -0.582931 | 0.816449 | 0.110199 |
| O   | 2.902212 | -0.098315 | 0.946082 |
| C   | -0.754237 | -2.173892 | 0.315030 |
| H   | -0.754237 | -2.173892 | 0.315030 |
| H   | 0.219472 | -1.797375 | 0.720640 |
| H   | -1.296549 | -2.723986 | 1.114827 |
| S   | -1.719037 | -0.826618 | -0.244321 |
| C   | 1.996322 | -0.223228 | -1.238283 |
| H   | 2.974110 | -0.719127 | -1.450143 |
| H   | 1.168246 | -0.901857 | -1.556593 |
| H   | 1.943941 | 0.722103 | -1.828940 |
| C   | -1.561601 | 1.566443 | 0.986209 |
| H   | -1.218597 | 2.623612 | 1.114440 |
| H   | -2.580484 | 1.576268 | 0.527859 |
| H   | -1.631954 | 1.092061 | 1.993872 |
| H   | 0.629491 | 0.600182 | 1.861312 |
| C   | -0.560827 | 1.384646 | -1.284483 |
| H   | -1.569124 | 1.778173 | -1.566497 |
| H   | 0.174191 | 2.225833 | -1.340850 |
| H   | -0.277563 | 0.609621 | -2.035660 |

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### 4_4methyl3pentene2one_4_am1_HEI

| Datum                              | Value         |
|------------------------------------|---------------|
| AM1 Energy                         | -0.112158     |
| AM1 Free Energy (Quasiharmonic)    | 0.039874      |
| Number of Imaginary Frequencies    | 0             |

**Frequencies (Top 3 out of 60)**

1. 35.4631 cm⁻¹  
2. 53.0691 cm⁻¹  
3. 91.3905 cm⁻¹
1. 35.4895 cm⁻¹
2. 53.1511 cm⁻¹
3. 91.3619 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|    |    |    |    |
|----|----|----|----|
| C  | -1.871308 | 0.078893 | -0.234098 |
| C  | -0.642931 | 0.517051 | -0.762860 |
| C  | 0.582573 | 0.816891 | -0.110144 |
| O  | -2.902360 | -0.098334 | -0.945937 |
| C  | 0.754635 | -2.173742 | -0.315468 |
| H  | 1.296980 | -2.725371 | -1.115448 |
| H  | 0.552877 | -2.871041 | 0.527270 |
| H  | -0.219099 | -1.797199 | -0.720942 |
| S  | 1.719339 | -0.826567 | 0.244245 |
| C  | -1.996062 | -0.223976 | 1.238233 |
| H  | -2.973740 | -0.720076 | 1.450119 |
| H  | -1.167818 | -0.902592 | 1.556139 |
| H  | -1.943681 | 0.721143 | 1.829231 |
| C  | 1.561315 | 1.566825 | -0.986042 |
| H  | 1.218034 | 2.623837 | -1.114822 |
| H  | 2.580030 | 1.577118 | -0.527340 |
| H  | 1.632164 | 1.092082 | -1.993500 |
| H  | -0.629730 | 0.608547 | -1.861282 |
| C  | 0.560461 | 1.384512 | 1.284738 |
| H  | -0.175614 | 2.224734 | 1.341838 |
| H  | 0.278566 | 0.608806 | 2.035737 |
| H  | 1.568391 | 1.779211 | 1.566423 |

**4_4methyl3pentene2one_5_reopt_am1_HEI**

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| AM1 Energy                                 | -0.111043    |
| AM1 Free Energy (Quasiharmonic)            | 0.040029      |
| Number of Imaginary Frequencies            | 0             |

**Frequencies (Top 3 out of 60)**

1. 45.1109 cm⁻¹
2. 57.3391 cm⁻¹
3. 71.7226 cm⁻¹
AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 2.047840 | -0.078629 | -0.133989 |
| C    | 0.889993  | -0.103425 | 0.652192  |
| C    | -0.374880 | 0.502477  | 0.331005  |
| O    | 2.245651  | 0.547694  | -1.214109 |
| C    | -3.023287 | -0.565188 | -0.521918 |
| H    | -3.534350 | -1.448698 | -0.965129 |
| H    | -3.575444 | -0.255251 | 0.393927  |
| H    | -3.061450 | 0.276625  | -1.249136 |
| S    | -1.373987 | -1.028027 | -0.161560 |
| C    | 3.205834  | -0.884695 | 0.423775  |
| H    | 2.922503  | -1.962223 | 0.476995  |
| H    | 4.105776  | -0.778969 | -0.226782 |
| H    | 3.459268  | -0.532536 | 1.451317  |
| C    | -1.087677 | 1.093753  | 1.528524  |
| H    | -0.542895 | 2.005966  | 1.875826  |
| H    | -2.134105 | 1.386084  | 1.266922  |
| H    | -1.120770 | 0.359977  | 2.368583  |
| H    | 0.922159  | -0.677677 | 1.586436  |
| C    | -0.378218 | 1.462666  | -0.829900 |
| H    | -1.408135 | 1.849707  | -1.026781 |
| H    | 0.296067  | 2.325543  | -0.605656 |
| H    | 0.012336  | 0.956579  | -1.746820 |

4_4methyl3pentene2one_6_am1_HEI_reopt

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.112158 |
| AM1 Free Energy (Quasiharmonic)    | 0.039874 |
| Number of Imaginary Frequencies    | 0       |

Frequencies (Top 3 out of 60)

1. 35.4956 cm⁻¹
2. 53.1673 cm⁻¹
3. 91.3641 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 1.871333 | -0.078953 | -0.234007 |
| C    | 0.642984  | -0.517188 | -0.762786 |
4-hexene-3-one_10_am1_HEI

| Datum                          | Value         |
|--------------------------------|---------------|
| AM1 Energy                     | -0.119434     |
| AM1 Free Energy (Quasiharmonic)| 0.032076      |
| Number of Imaginary Frequencies| 0             |

**Frequencies** (Top 3 out of 60)

1. 34.7078 cm\(^{-1}\)
2. 51.5953 cm\(^{-1}\)
3. 67.4812 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

| C    | -3.151346 | -1.326966 | 0.420160 |
| C    | -1.792792 | -0.704095 | 0.595145 |
| C    | -1.617853 | 0.569682  | -0.215298|
| C    | -0.335229 | 1.143235  | -0.241176|
| C    | 0.811691  | 0.639025  | 0.444247 |
| C    | 1.849392  | 1.677505  | 0.781589 |
| O    | -2.624565 | 1.055901  | -0.803116|
| H    | -3.253589 | -2.242080 | 1.052706 |
### 4-hexene-3-one_11_reopt_am1_HEI

| Datum                                    | Value     |
|------------------------------------------|-----------|
| AM1 Energy                               | -0.123899 |
| AM1 Free Energy (Quasiharmonic)          | 0.028109  |
| Number of Imaginary Frequencies          | 0         |

**Frequencies** (Top 3 out of 60)

1. 37.2129 cm⁻¹  
2. 38.3433 cm⁻¹  
3. 75.2718 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C  | 3.150207   | -0.660788 | -0.821076 |
| C  | 1.735585   | -0.148121 | -0.844977 |
| C  | 1.342980   | 0.566322  | 0.437905  |
| C  | 0.003888   | 0.969391  | 0.565543  |
| C  | -1.015389  | 0.783930  | -0.412606 |
| C  | -2.142985  | 1.778731  | -0.357260 |
| O  | 2.231328   | 0.764511  | 1.314928  |
| H  | 3.410308   | -1.154058 | -1.788910 |
| H  | 3.862407   | 0.179921  | -0.638647 |
| H  | 3.279399   | -1.399428 | 0.006261  |
| H  | 1.021495   | -0.999488 | -1.004977 |
| H  | 1.607244   | 0.565289  | -1.700749 |
| H  | -0.634133  | 0.667500  | -1.457136 |
| H  | -2.543724  | 1.866278  | 0.680999  |
### 4-hexene-3-one_12_reopt_am1_HEI

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.123899 |
| AM1 Free Energy (Quasiharmonic)            | 0.02811 |

**Number of Imaginary Frequencies** 0

**Frequencies** (Top 3 out of 60)

1. 37.2735 cm⁻¹
2. 38.3712 cm⁻¹
3. 75.3480 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -3.150230 | -0.660651 | -0.821153 |
|-----|-----------|-----------|-----------|
| C   | -1.735476 | -0.148345 | -0.844875 |
| C   | -1.342980 | 0.566324  | 0.437909  |
| C   | -0.003909 | 0.969499  | 0.565522  |
| C   | 1.015366  | 0.783996  | -0.412607 |
| C   | 2.142996  | 1.778751  | -0.357320 |
| O   | -2.231350 | 0.764538  | 1.314898  |
| H   | -3.410107 | -1.154468 | -1.788769 |
| H   | -3.279888 | -1.398726 | 0.006620  |
| H   | -3.862299 | 0.180343  | -0.639526 |
| H   | -1.606751 | 0.564793  | -1.700818 |
| H   | -1.021549 | -0.999927 | -1.004482 |
| H   | 0.634146  | 0.667429  | -1.457132 |
| H   | 2.977620  | 1.474513  | -1.035526 |
| H   | 1.774804  | 2.785201  | -0.678030 |
| H   | 2.543684  | 1.866410  | 0.680950  |
| C   | 1.101602  | -1.849231 | 0.872923  |
| H   | 0.251012  | -1.252826 | 1.291237  |
| H   | 0.699913  | -2.756156 | 0.370048  |
| H   | 1.773490  | -2.163287 | 1.701077  |
### 4-hexene-3-one_13_am1_HEI

| Datum                                             | Value       |
|---------------------------------------------------|-------------|
| AM1 Energy                                         | -0.124298   |
| AM1 Free Energy (Quasiharmonic)                   | 0.028038    |
| Number of Imaginary Frequencies                   | 0           |

**Frequencies** (Top 3 out of 60)

1. 39.5920 cm\(^{-1}\)
2. 52.9595 cm\(^{-1}\)
3. 65.5670 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |       |       |       |
|---|-------|-------|-------|
| C | -2.804718 | 0.961476 | -0.858173 |
| C | -2.676931 | -0.427138 | -0.289231 |
| C | -1.347487 | -0.602118 | 0.437273 |
| C | -0.222689 | -0.720179 | -0.384671 |
| C | 1.110570  | -0.846885 | 0.124745 |
| C | 2.009987  | -1.778574 | -0.642475 |
| O | -1.377274 | -0.644230 | 1.700651 |
| H | -3.769352 | 1.078455 | -1.409854 |
| H | -2.770655 | 1.721209 | -0.040076 |
| H | -1.961761 | 1.170005 | -1.561611 |
| H | -2.748039 | -1.183044 | -1.112937 |
| H | -3.516117 | -0.622083 | 0.427672 |
| H | 1.123444  | -1.067837 | 1.220863 |
| H | 1.959627  | -1.568129 | -1.737810 |
| H | 3.072285  | -1.676692 | -0.309127 |
| H | 1.686559  | -2.835452 | -0.472524 |
| C | 0.951250  | 2.039177 | 0.223224 |
| H | 1.110957  | 2.808368 | -0.563609 |
| H | 1.061660  | 2.515427 | 1.221910 |
| H | -0.082369 | 1.619065 | 0.129811 |
| S | 2.130400  | 0.758085 | 0.025547 |
| H | -0.354349 | -0.689372 | -1.470824 |
### 4-hexene-3-one_14_am1_HEI

| Datum                                | Value   |
|--------------------------------------|---------|
| AM1 Energy                           | -0.124298 |
| AM1 Free Energy (Quasiharmonic)      | 0.028034 |
| Number of Imaginary Frequencies      | 0       |

#### Frequencies (Top 3 out of 60)

1. 39.5357 cm⁻¹  
2. 52.9262 cm⁻¹  
3. 65.5481 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|        |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |         |
|--------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| C      | 2.804738| 0.961269| -0.858509|        |
| C      | 2.676999| -0.427148| -0.289073|        |
| C      | 1.347521| -0.601952| 0.437411 |        |
| C      | 0.222767| -0.720298| -0.384555|        |
| C      | -1.110509| -0.846927| 0.124829 |        |
| C      | -2.009912| -1.778733| -0.642270|        |
| O      | 1.377237| -0.643678| 1.700806 |        |
| H      | 3.769335| 1.078068| -1.410284|        |
| H      | 1.961736| 1.169539| -1.561966|        |
| H      | 2.770710| 1.721292| -0.040686|        |
| H      | 3.516147| -0.621778| 0.427954 |        |
| H      | 2.748218| -1.183345| -1.112498|        |
| H      | -1.123425| -1.067689| 1.220977 |        |
| H      | -1.959551| -1.568434| -1.737629|        |
| H      | -1.686470| -2.835580| -0.472177|        |
| H      | -3.072211| -1.676825| -0.308940|        |
| C      | -0.951471| 2.039238| 0.223284 |        |
| H      | -1.111130| 2.808412| -0.563572|        |
| H      | -1.062152| 2.515457| 1.221950 |        |
| H      | 0.082227| 1.619284| 0.130080 |        |
| S      | -2.130413| 0.758008| 0.025272 |        |
| H      | 0.354483| -0.689788| -1.470708|        |

### 4-hexene-3-one_16_am1_HEI_reopt

| Datum                                | Value   |
|--------------------------------------|---------|
| AM1 Energy                           | -0.124298 |
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Free Energy (Quasiharmonic)            | 0.028035    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 60)

1. 39.5471 cm⁻¹  
2. 53.0407 cm⁻¹  
3. 65.5582 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | 2.804235 | 0.961406 | -0.858928 |
| C | 2.677088 | -0.426819 | -0.288895 |
| C | 1.347615 | -0.601928 | 0.437520  |
| C | 0.222911 | -0.720180 | -0.384532 |
| C | -1.110384| -0.846989 | 0.124745  |
| C | -2.009672| -1.778757 | -0.642528 |
| O | 1.377293 | -0.643954 | 1.700915  |
| H | 2.769862 | 1.721772  | -0.041440 |
| H | 3.768791 | 1.078387  | -1.410736 |
| H | 1.961146 | 1.168995  | -1.562483 |
| H | 2.748688 | -1.183346 | -1.111984 |
| H | 3.516268 | -0.620770 | 0.428277  |
| H | -1.123352| -1.067883 | 1.220865  |
| H | -1.959244| -1.568326 | -1.737859 |
| H | -1.686176| -2.835605 | -0.472537 |
| H | -3.072002| -1.676955 | -0.309264 |
| C | -0.951603 | 2.039187 | 0.223640  |
| H | -1.062371| 2.515183  | 1.222402  |
| H | -1.111301| 2.808515  | -0.563057 |
| S | 0.082140 | 1.619351  | 0.130389  |
| H | -2.130415| 0.757890  | 0.025291  |
| H | 0.354703 | -0.689450 | -1.470670 |

**4-hexene-3-one_17_reopt_am1_HEI_reopt**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.124298   |
| AM1 Free Energy (Quasiharmonic)            | 0.028032    |
| Number of Imaginary Frequencies            | 0           |
**Frequencies (Top 3 out of 60)**

1. 39.4758 cm⁻¹
2. 52.8730 cm⁻¹
3. 65.5259 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C    | 2.804636 | 0.961428 | -0.858411 |
| C    | 2.677042 | -0.427042 | -0.289069 |
| C    | 1.347552 | -0.602020 | 0.437337  |
| C    | 0.222794 | -0.720237 | -0.384619 |
| C    | -1.110465| -0.846944 | 0.124790  |
| C    | -2.009869| -1.778709 | -0.642352 |
| O    | 1.377271 | -0.643959 | 1.700673  |
| H    | 3.769117 | 1.078293 | -1.410376 |
| H    | 1.961489 | 1.169757 | -1.561679 |
| H    | 2.770781 | 1.721365 | -0.040503 |
| H    | 3.516161 | -0.621583 | 0.428017  |
| H    | 2.748442 | -1.183185 | -1.112522 |
| H    | -1.123346| -1.067777 | 1.220923  |
| H    | -3.072164| -1.676832 | -0.309002 |
| H    | -1.959526| -1.568344 | -1.737699 |
| H    | -1.686415| -2.835564 | -0.472328 |
| C    | -0.951529| 2.039246 | 0.223355  |
| H    | 0.082180 | 1.619342 | 0.130053  |
| H    | -1.062158| 2.515409 | 1.222052  |
| H    | -1.111279| 2.808455 | -0.563448 |
| S    | -2.130430| 0.757977 | 0.025357  |
| H    | 0.354467 | -0.689622 | -1.470773 |

**4-hexene-3-one_18_am1_HEI**

| Datum                              | Value    |
|------------------------------------|----------|
| AM1 Energy                         | -0.119728|
| AM1 Free Energy (Quasiharmonic)    | 0.032039 |
| Number of Imaginary Frequencies    | 0        |

**Frequencies (Top 3 out of 60)**

1. 43.1140 cm⁻¹
2. 44.5036 cm⁻¹
3. 55.8289 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     | X        | Y        | Z        |
|-----|----------|----------|----------|
| C   | 3.056573 | -1.283073| -0.612178|
| C   | 2.945288 | 0.161174 | -0.201350|
| C   | 1.592079 | 0.453858 | 0.438073 |
| C   | 0.508145 | 0.511939 | -0.443988|
| C   | -0.841974| 0.728693 | -0.004494|
| C   | -1.642881| 1.680952 | -0.853512|
| O   | 1.571657 | 0.659997 | 1.685163 |
| H   | 2.974895 | -1.948829| 0.280681 |
| H   | 2.234127 | -1.547973| -1.320519|
| H   | 4.037222 | -1.479454| -1.111174|
| H   | 3.076815 | 0.821296 | -1.097178|
| H   | 3.758132 | 0.411231 | 0.528955 |
| H   | -0.899557| 1.012048 | 1.076305 |
| H   | -1.608459| 1.380528 | -1.928129|
| H   | -2.711378| 1.709756 | -0.526404|
| H   | -1.218739| 2.711502 | -0.763609|
| C   | -3.258492| -0.791232| 0.511500 |
| H   | -3.647247| -1.814032| 0.713504 |
| H   | -3.261546| -0.208536| 1.459656 |
| H   | -3.942484| -0.285848| -0.207246|
| S   | -1.637286| -0.948006| -0.129862|
| H   | 0.679115 | 0.352568 | -1.512674|

**4-hexene-3-one_19_am1_HEI**

| Datum                                      | Value   |
|--------------------------------------------|---------|
| AM1 Energy                                 | -0.119728 |
| AM1 Free Energy (Quasiharmonic)            | 0.032041 |
| Number of Imaginary Frequencies            | 0       |

**Frequencies (Top 3 out of 60)**

1. 43.1394 cm⁻¹
2. 44.5840 cm⁻¹
3. 55.8456 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**
4-hexene-3-one_1_am1_HEI

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| AM1 Energy                                 | -0.123899        |
| AM1 Free Energy (Quasiharmonic)            | 0.02811          |
| Number of Imaginary Frequencies            | 0                |

**Frequencies (Top 3 out of 60)**

1. 37.2648 cm⁻¹
2. 38.3638 cm⁻¹
3. 75.3311 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C   | -3.150182 | 0.660649 | 0.821215 |
|-----|-----------|----------|----------|
| C   | -1.735441 | 0.148307 | 0.844878 |
| C   | -1.342970 | -0.566305| -0.437950|
| C   | -0.003896 | -0.969452| -0.565571|
| C   | 1.015349  | -0.783954| 0.412598 |
### 4-hexene-3-one_1_am1

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.064717   |
| AM1 Free Energy (Quasiharmonic)            | 0.052613    |
| Number of Imaginary Frequencies            | 0           |

#### Frequencies (Top 3 out of 45)

1. 31.6560 cm⁻¹
2. 64.4819 cm⁻¹
3. 109.8221 cm⁻¹

#### AM1 Molecular Geometry in Cartesian Coordinates

|           |               |               |               |
|-----------|---------------|---------------|---------------|
| C         | 2.142954      | -1.778742     | 0.357349      |
| O         | -2.231356     | -0.764507     | -1.314926     |
| H         | -3.410081     | 1.154274      | 1.788922      |
| H         | -3.279801     | 1.398901      | -0.006404     |
| H         | -3.862257     | -0.180294     | 0.639379      |
| H         | -1.606709     | -0.564879     | 1.700777      |
| H         | -1.021485     | 0.999872      | 1.004482      |
| H         | 0.634065      | -0.667409     | 1.457102      |
| H         | 2.543732      | -1.866338     | -0.680891     |
| H         | 2.977524      | -1.474581     | 1.035654      |
| H         | 1.774696      | -2.785200     | 0.677952      |
| C         | 1.101595      | 1.849190      | -0.872932     |
| H         | 0.699751      | 2.756035      | -0.370039     |
| H         | 0.251113      | 1.252718      | -1.291373     |
| H         | 1.773533      | 2.163378      | -1.700995     |
| S         | 1.995911      | 0.876541      | 0.275995      |
| H         | 0.277733      | -1.453244     | -1.508595     |
4-hexene-3-one_2_am1_HEI

| Datum                                | Value  |
|--------------------------------------|--------|
| AM1 Energy                           | -0.123899 |
| AM1 Free Energy (Quasiharmonic)      | 0.02811  |
| Number of Imaginary Frequencies      | 0      |

**Frequencies** (Top 3 out of 60)

1. 37.2091 cm⁻¹  
2. 38.3677 cm⁻¹  
3. 75.3292 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C         | 3.150310 | 0.660385 | 0.821400 |
|-----------|----------|----------|----------|
| C         | 1.735505 | 0.148214 | 0.844898 |
| C         | 1.342978 | -0.566025| -0.438121|
| C         | 0.003917 | -0.969197| -0.565759|
| C         | -1.015262| -0.783969| 0.412537 |
| C         | -2.142751| -1.778889| 0.357205 |
| O         | 2.231317 | -0.763933| -1.315211|
| H         | 3.410208 | 1.153848 | 1.789189 |
| H         | 3.862298 | -0.180619| 0.639512 |
| H         | 3.280070 | 1.398730 | -0.006114|
| H         | 1.021653 | 0.999843 | 1.004684 |
| H         | 1.606646 | -0.565161| 1.700616 |
| H         | -0.633870| -0.667615| 1.457028 |
| H         | -2.543568| -1.866391| -0.681027|
| H         | -1.774353| -2.785346| 0.677647 |
| H         | -2.977328| -1.474932| 1.035593 |
| C         | -1.182064| 1.849016 | -0.873029|
| H         | -0.699889| 2.755831 | -0.370346|
| H         | -1.774394| 2.163257 | -1.700753|
| H         | -0.251842| 1.252476 | -1.291889|
| S         | -1.995888| 0.876444 | 0.276352 |
| H         | -0.277758| -1.452786| -1.508873|
4-hexene-3-one_2_am1

| Datum                                           | Value     |
|------------------------------------------------|-----------|
| AM1 Energy                                      | -0.062711 |
| AM1 Free Energy (Quasiharmonic)                 | 0.054608  |
| Number of Imaginary Frequencies                 | 0         |

**Frequencies (Top 3 out of 45)**

1. 27.6098 cm⁻¹
2. 67.8338 cm⁻¹
3. 107.3319 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

```
C          2.707784       -0.778347        0.000001
C          1.202035       -0.819763        0.000000
C          0.582582        0.550568       -0.000001
C         -0.889243        0.628796        0.000000
C         -1.711633       -0.425923        0.000000
C         -3.182988       -0.312566        0.000001
O            1.266036        1.582784       -0.000002
H            3.121812       -1.814846        0.000002
H            3.083174       -0.238496     -0.902896
H            3.083173       -0.238495      0.902898
H           -0.835180       -1.372650        0.905910
H           -0.835181       -1.372651     -0.905909
H           -1.284007       1.660806        0.000000
H           -1.324228       -1.460077     -0.000000
H           -3.603915       -0.817447        0.906196
H           -3.521963        0.752437        0.000001
H           -3.603916       -0.817447     -0.906194
```

4-hexene-3-one_3_am1_HEI

| Datum                                           | Value     |
|------------------------------------------------|-----------|
| AM1 Energy                                      | -0.119434 |
| AM1 Free Energy (Quasiharmonic)                 | 0.03207   |
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 60)**

1. 34.7006 cm⁻¹  
2. 51.4062 cm⁻¹  
3. 67.2224 cm⁻¹  

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -3.150935 | -1.327289 | 0.419939 |
| C          | -1.792646 | -0.703961 | 0.595311 |
| C          | -1.617009 | 0.569813  | -0.215157|
| C          | -0.335212 | 1.143434  | -0.241070|
| C          | 0.811732  | 0.639206  | 0.444224 |
| C          | 1.849541  | 1.677641  | 0.781368 |
| O          | -2.624566 | 1.056003  | -0.802919|
| H          | -3.253276 | -2.242094 | 1.052902 |
| H          | -3.949961 | -0.599633 | 0.701743 |
| H          | -3.310176 | -1.608804 | -0.648752|
| H          | -0.993481 | -1.428189 | 0.283927 |
| H          | -1.626578 | -0.459872 | 1.677447 |
| H          | 0.579623  | 0.017497  | 1.345381 |
| H          | 1.436386  | 2.396439  | 1.531512 |
| H          | 2.764244  | 1.202500  | 1.213575 |
| H          | 2.144036  | 2.252100  | -0.129404|
| C          | 2.934506  | -1.341530 | 0.096381 |
| H          | 2.645461  | -1.649657 | 1.126121 |
| H          | 3.810434  | -0.658547 | 0.173803 |
| H          | 3.236928  | -2.244028 | -0.479830|
| S          | 1.594623  | -0.587489 | -0.739983|
| H          | -0.200944 | 2.030212  | -0.871321|

**4-hexene-3-one_3_am1**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.064537   |
| AM1 Free Energy (Quasiharmonic)            | 0.053255    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies (Top 3 out of 45)**
1. 45.3104 cm⁻¹
2. 71.1392 cm⁻¹
3. 112.8596 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 2.327082| -1.121168| -0.458703|
| C    | 1.892331| -0.081596| 0.542740 |
| C    | 0.605872| 0.582091 | 0.127667 |
| C    | -0.600216| -0.254514| 0.215355 |
| C    | -1.818583| 0.206116 | -0.098978|
| O    | 0.580832| 1.761701 | -0.248690|
| H    | 3.271145| -1.608936| -0.114852|
| H    | 1.544640| -1.909233| -0.579589|
| H    | 2.514116| -0.653559| -1.455664|
| H    | 2.691412| 0.699832 | 0.648970 |
| H    | 1.741705| -0.556063| 1.548531 |
| H    | -0.441578| -1.289298| 0.557942 |
| H    | -1.945647| 1.250349 | -0.441015|
| H    | -3.533802| -0.652822| -1.029989|
| H    | -2.850888| -1.641569| 0.330134 |
| H    | -3.774460| -0.120136| 0.685276 |

4-hexene-3-one_4_am1_HEI

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.119434 |
| AM1 Free Energy (Quasiharmonic)    | 0.032075 |
| Number of Imaginary Frequencies    | 0       |

Frequencies (Top 3 out of 60)

1. 34.7078 cm⁻¹
2. 51.5933 cm⁻¹
3. 67.4713 cm⁻¹
4-hexene-3-one_4_am1

| Datum                                      | Value         |
|--------------------------------------------|---------------|
| AM1 Energy                                 | -0.062134     |
| AM1 Free Energy (Quasiharmonic)            | 0.055589      |
| Number of Imaginary Frequencies            | 0             |

**Frequencies** (Top 3 out of 45)

1. 21.7747 cm⁻¹
2. 85.3458 cm⁻¹
3. 120.8433 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C     | 1.720980 | -1.497425 | -0.454134 |
|-------|----------|-----------|-----------|
| C     | 1.427579 | -0.502929 | 0.641251  |
| C     | 0.756022 | 0.730194  | 0.096272  |
| C     | -0.711053| 0.739901  | -0.031865 |
| C     | -1.499637| -0.333795 | 0.086990  |
4-hexene-3-one_5_am1_HEI

| Datum                               | Value     |
|-------------------------------------|-----------|
| AM1 Energy                          | -0.123442 |
| AM1 Free Energy (Quasiharmonic)     | 0.028927  |
| Number of Imaginary Frequencies     | 0         |

**Frequencies** (Top 3 out of 60)

1. 28.7070 cm⁻¹  
2. 42.3874 cm⁻¹  
3. 83.1903 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | 2.562674 | 0.772825 | -1.311191 |
|---|----------|----------|-----------|
| C | 1.828821 | -0.444515| -0.813440 |
| C | 1.437654 | -0.301186| 0.650252  |
| C | 0.225515 | 0.327588 | 0.969932  |
| C | -0.697648| 0.893625 | 0.042412  |
| C | -1.545399| 2.010414 | 0.589627  |
| O | 2.239235 | -0.774745| 1.506806  |
| H | 2.863912 | 0.642027 | -2.379317 |
| H | 1.916230 | 1.680544 | -1.235224 |
| H | 3.482742 | 0.946383 | -0.702106 |
| H | 2.491134 | -1.344084| -0.918664 |
| H | 0.911036 | -0.625174| -1.430980 |
| H | -0.244721| 1.180476 | -0.938835 |
| H | -2.348570| 2.293439 | -0.134134 |
| H | -2.024953| 1.709369 | 1.551720  |
| H | -0.907880| 2.909435 | 0.781119  |
4-hexene-3-one_5_am1

Datum Value

AM1 Energy -0.064717

AM1 Free Energy (Quasiharmonic) 0.052613

Number of Imaginary Frequencies 0

Frequencies (Top 3 out of 45)

1. 31.6514 cm⁻¹
2. 64.5198 cm⁻¹
3. 109.8337 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   |   |   |   |
|---|---|---|---|
| C | -1.586870 | -1.897251 | -0.020710 |
| H | -1.412594 | -2.578216 | -0.882344 |
| H | -0.646514 | -1.814524 | 0.581911  |
| H | -2.394737 | -2.320132 | 0.615352  |
| S | -2.056868 | -0.313872 | -0.602407 |
| H | -0.037563 | 0.371370  | 2.034286  |

4-hexene-3-one_6_am1_HEI

|   |   |   |   |
|---|---|---|---|
| C | 3.012646 | -0.138433 | -0.000000 |
| C | 1.661649 | -0.802966 | 0.000008  |
| C | 0.524344 | 0.180980  | -0.000004 |
| C | -0.813733 | -0.432110 | -0.000011 |
| C | -1.937853 | 0.296826  | 0.000008  |
| C | -3.294768 | -0.278980 | 0.000001  |
| O | 0.700461 | 1.406547  | -0.000005 |
| H | 3.821287 | -0.907786 | 0.000034  |
| H | 3.129003 | 0.508732  | -0.902920 |
| H | 3.128985 | 0.508792  | 0.902879  |
| H | 1.554737 | -1.459805 | 0.904729  |
| H | 1.554740 | -1.459835 | -0.904691 |
| H | -0.836766 | -1.533248 | -0.000033 |
| H | -1.882309 | 1.401626  | 0.000030  |
| H | -3.854389 | 0.066860  | -0.906026 |
| H | -3.278319 | -1.396433 | -0.000024 |
| H | -3.854382 | 0.066821  | 0.906047  |
| Datum                              | Value      |
|-----------------------------------|------------|
| AM1 Energy                        | -0.123442  |
| AM1 Free Energy (Quasiharmonic)   | 0.028927   |
| Number of Imaginary Frequencies   | 0          |

**Frequencies** (Top 3 out of 60)

1. 28.7066 cm\(^{-1}\)
2. 42.3871 cm\(^{-1}\)
3. 83.1905 cm\(^{-1}\)

**AM1 Molecular Geometry in Cartesian Coordinates**

|   |          |          |          |
|---|----------|----------|----------|
| C | -2.562672| 0.772822 | -1.311195|
| C | -1.828821| -0.444517| -0.813439|
| C | -1.437654| -0.301183| 0.650253 |
| C | -0.225514| 0.327591 | 0.969932 |
| C | 0.697650 | 0.893624 | 0.042410 |
| C | 1.545400 | 2.010415 | 0.589621 |
| O | -2.239236| -0.774738| 1.506809 |
| H | -2.863909| 0.642020 | -2.379321|
| H | -3.482740| 0.946383 | -0.702112|
| H | -1.916227| 1.680541 | -1.235230|
| H | -0.911035| -0.625180| -1.430977|
| H | -2.491134| -1.344086| -0.918659|
| H | 0.244722 | 1.180473 | -0.938837|
| H | 2.024954 | 1.709373 | 1.551716 |
| H | 2.348572 | 2.293437 | -0.134140|
| H | 0.907881 | 2.909436 | 0.781111 |
| C | 1.586865 | -1.897253| -0.020709|
| H | 1.412583 | -2.578215| -0.882343|
| H | 0.646511 | -1.814523| 0.581915 |
| H | 2.394733 | -2.320137| 0.615350 |
| S | 2.056868 | -0.313874| -0.602404|
| H | 0.037564 | 0.371376 | 2.034286 |

**4-hexene-3-one_7_am1_HEI**

| Datum                              | Value      |
|-----------------------------------|------------|
| AM1 Energy                        | -0.119092  |
| AM1 Free Energy (Quasiharmonic)   | 0.032972   |
### AM1 Molecular Geometry in Cartesian Coordinates

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C    | -2.387497| -1.312068| 1.194473 |
| C    | -1.855940| -1.056307| -0.191237|
| C    | -1.715679| 0.432885 | -0.471069|
| C    | -0.519594| 1.077739 | -0.122770|
| C    | 0.599519 | 0.473536 | 0.528734 |
| C    | 1.452708 | 1.428063 | 1.322858 |
| O    | -2.703249| 1.011613 | -1.009212|
| H    | -2.510809| -2.408201| 1.374150 |
| H    | -1.689589| -0.904990| 1.965726 |
| H    | -3.30524 | -0.817823| 1.326070 |
| H    | -2.52217 | -1.494063| -0.945009|
| H    | -0.86138 | -1.555804| -0.327631|
| H    | 0.347913 | -0.424533| 1.147404 |
| H    | 1.772774 | 2.291208 | 0.691353 |
| H    | 0.869942 | 1.824956 | 2.190546 |
| H    | 2.365689 | 0.915981 | 1.714691 |
| C    | 2.990350 | -1.079520| -0.113757|
| H    | 2.642766 | -1.727748| 0.721598 |
| H    | 3.756093 | -0.378767| 0.289091 |
| H    | 3.465677 | -1.716523| -0.892407|
| S    | 1.653340 | -0.225931| -0.853502|
| H    | -0.426728| 2.132333 | -0.409257|

### 4-hexene-3-one_8_am1_HEI

| Datum                          | Value  |
|--------------------------------|--------|
| AM1 Energy                     | -0.119092|
| AM1 Free Energy (Quasiharmonic)| 0.032972|
| Number of Imaginary Frequencies| 0      |

### Frequencies (Top 3 out of 60)

1. 38.9491 cm⁻¹
2. 52.8933 cm⁻¹
3. 71.6777 cm⁻¹
1. 38.9492 cm⁻¹
2. 52.8932 cm⁻¹
3. 71.6780 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|   | C           | C           | C           | C           | C           | C           | O           | H           | H           | H           | H           | H           | H           | H           | H           | C           | H           | S           | H           | H           | H           |
|---|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|   | 2.387497    | -1.312069   | 1.194473    | 1.855938    | -1.056308   | -0.191236   | 1.715679    | 0.432885    | -0.471068   | 0.519594    | 1.077740    | -0.122770   | -0.599519   | 0.473537    | 0.528734    | -1.452709   | 1.428065    | 1.322857    | 2.703249    | 1.011612    | -1.009212   | 2.510809    | -2.408202   | 1.374149    |
|   | 3.80524     | -0.817823   | 1.326069    | 1.689591    | -0.904990   | 1.965727    | 0.861367    | -1.555803   | -0.327629   | 2.562215    | -1.494064   | -0.945010   | -0.347914   | -0.424532   | 1.147405    | -0.869944   | 1.824957    | 2.190546    | 1.772772    | 2.291211    | 0.691351    | -3.65691    | 0.915985    | 1.714687    |
|   | -2.990346   | -1.079524   | -0.113756   | -3.756891   | -0.378774   | 0.289095    | -3.465674   | -1.716528   | -0.892406   | -2.642759   | -1.727753   | 0.721598    | -1.653341   | -0.225930   | -0.853501   | -0.426729   | 2.132333    | -0.409257   |

**4-hexene-3-one_9_am1_HEI**

| Datum                                   | Value       |
|-----------------------------------------|-------------|
| AM1 Energy                              | -0.119434   |
| AM1 Free Energy (Quasiharmonic)         | 0.03207     |
| Number of Imaginary Frequencies         | 0           |

**Frequencies (Top 3 out of 60)**

1. 34.7033 cm⁻¹
2. 51.4319 cm⁻¹
3. 67.2477 cm⁻¹
AM1 Molecular Geometry in Cartesian Coordinates

|   | 1.682115 | 0.341868 | 1.118383 |
|---|----------|----------|-----------|
| C | 0.337659 | 1.065151 | 1.118203 |

5_3methyl2cyclopentene1one_1_am1_HEI

| Datum                          | Value  |
|--------------------------------|--------|
| AM1 Energy                     | -0.104149 |
| AM1 Free Energy (Quasiharmonic)| 0.030617 |

Number of Imaginary Frequencies | 0

Frequencies (Top 3 out of 54)

1. 51.7338 cm⁻¹
2. 81.3257 cm⁻¹
3. 112.9466 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

|   | 1.682115 | 0.341868 | 1.118383 |
|---|----------|----------|-----------|
| C | 0.337659 | 1.065151 | 1.118203 |
### 5_3-methyl-2-cyclopentene-1-one_1_am1

| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| AM1 Energy                                 | -0.049065              |
| AM1 Free Energy (Quasiharmonic)            | 0.051502               |
| Number of Imaginary Frequencies            | 0                      |

#### Frequencies (Top 3 out of 39)

1. 67.7079 cm⁻¹  
2. 126.1479 cm⁻¹  
3. 167.7430 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

|   |                  |                  |               |
|---|------------------|------------------|---------------|
| C | -0.346901        | 0.701063         | -0.209634     |
| C | 0.627092         | -0.037593        | -0.985165     |
| C | 1.805259         | -0.301433        | -0.268387     |
| H | 2.528136         | 1.048583         | 1.291211      |
| H | 1.722398         | -0.446777        | 1.907181      |
| H | 0.486764         | 2.172633         | 1.180629      |
| H | -0.291746        | 0.755836         | 1.987553      |
| O | 2.843227         | -0.924572        | -0.607307     |
| H | 0.455275         | -0.339060        | -2.011986     |
| C | -1.404572        | -1.993717        | 0.081843      |
| H | -1.436659        | -2.493979        | 1.074360      |
| H | -0.363166        | -2.044788        | -0.325674     |
| H | -2.096939        | -2.521306        | -0.609902     |
| S | -1.898965        | -0.319818        | 0.235951      |
| C | -1.008268        | 1.868614         | -0.889439     |
| H | -0.256914        | 2.676735         | -1.071895     |
| H | -1.432331        | 1.554339         | -1.873142     |
| H | -1.831492        | 2.287721         | -0.259913     |
AM1 Energy
-0.104149

AM1 Free Energy (Quasiharmonic)
0.030616

Number of Imaginary Frequencies
0

Frequencies (Top 3 out of 54)

1.  51.7329 cm⁻¹
2.  81.3425 cm⁻¹
3.  112.9533 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

C  -1.682130  0.342000  -1.118343
C  -0.337632  1.065210  -1.118169
C   0.346887  0.701131   0.209680
C  -0.627111  -0.037504   0.985210
C  -1.805258  -0.301390   0.268389
H  -2.528118   1.048785  -1.291069
H  -1.722507  -0.446579  -1.907201
H  -0.486659   2.172698  -1.180631
H   0.291774   0.755802  -1.987490
O  -2.843195  -0.924596   0.607268
H  -0.455308  -0.338987   2.012028
C   1.404398  -1.993774  -0.818400
H   2.096761  -2.521474   0.609826
H   0.363026  -2.044679   0.325788
H   1.436294  -2.494019  -1.074372
S   1.898956  -0.319935  -0.236005
C   1.008445  1.868584   0.889434
H   0.257062   2.676546   1.072494
H   1.433084   1.554124   1.872830
H   1.831270   2.287971   0.259576
5_3methyl2cyclopentene1one_3_am1_HEI

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.099761 |
| AM1 Free Energy (Quasiharmonic)    | 0.034794 |
| Number of Imaginary Frequencies    | 0       |

**Frequencies** (Top 3 out of 54)

1. 64.7178 cm⁻¹
2. 81.7464 cm⁻¹
3. 85.3463 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |        |        |        |
|-----|--------|--------|--------|
| C   | -1.680197 | 0.228123 | -1.250399 |
| C   | -0.267864 | 0.797580 | -1.145837 |
| C   | 0.221231  | 0.473822 | 0.275654  |
| C   | -0.916538 | -0.080804 | 0.988082 |
| C   | -2.031977 | -0.271565 | 0.157107 |
| H   | -2.411009 | 1.004159 | -1.580092 |
| H   | -1.724458 | -0.621821 | -1.972430 |
| H   | -0.276782 | 1.905098 | -1.307569 |
| H   | 0.480866  | 0.347393 | -1.912080 |
| O   | -3.174710 | -0.726752 | 0.415972 |
| H   | -0.882287 | -0.336411 | 2.040364 |
| C   | 2.888995  | -0.436764 | -0.539094 |
| H   | 3.460229  | 0.274220 | 0.099381 |
| H   | 2.692467  | 0.059067 | -1.516181 |
| H   | 3.512672  | -1.341907 | -0.712485 |
| S   | 1.404851  | -0.956167 | 0.230449 |
| C   | 0.925318  | 1.628384 | 0.934932 |
| H   | 0.229422  | 2.499201 | 1.020898 |
| H   | 1.259806  | 1.343445 | 1.961193 |
| H   | 1.817237  | 1.947590 | 0.341364 |

6_3pentene2zone_1_am1_HEI

| Datum                              | Value   |
|------------------------------------|---------|
| AM1 Energy                         | -0.114108 |
| AM1 Free Energy (Quasiharmonic)    | 0.010621 |
Number of Imaginary Frequencies | 0
---|---
Frequencies (Top 3 out of 51)

1. 35.7916 cm⁻¹
2. 61.1649 cm⁻¹
3. 77.7044 cm⁻¹

AM1 Molecular Geometry in Cartesian Coordinates

| C | 2.941365 | -0.083746 | -0.770233 |
| C | 1.754826 | 0.058388  | 0.161067  |
| C | 0.605982 | 0.609324  | -0.415621 |
| C | -0.615114 | 0.815119 | 0.304057 |
| O | 1.902087 | -0.311220 | 1.362376 |
| C | -1.372614 | 2.065486 | -0.054689 |
| H | 3.817300 | -0.511632 | -0.227996 |
| H | 2.678059 | -0.757000 | -1.619902 |
| H | 3.223729 | 0.913445  | -1.182746 |
| H | 0.626325 | 0.879913  | -1.475979 |
| H | -0.473961 | 0.717060 | 1.408935 |
| H | -2.392915 | 2.062415 | 0.402438 |
| H | -0.818965 | 2.960232 | 0.323812 |
| H | -1.479570 | 2.161794 | -1.161925 |
| S | -1.957313 | -0.491558 | -0.045274 |
| C | -1.060917 | -1.988663 | -0.208659 |
| H | 0.034788 | -1.766465 | -0.241011 |
| H | -1.272803 | -2.659601 | 0.652352 |
| H | -1.362818 | -2.500922 | -1.148128 |

6_3pentene2one_2_reopt2_am1_HEI

| Datum | Value |
|---|---|
| AM1 Energy | -0.114108 |
| AM1 Free Energy (Quasiharmonic) | 0.010618 |
| Number of Imaginary Frequencies | 0 |

Frequencies (Top 3 out of 51)
### 6_3pentene2one_3_am1_HEI

| Datum                                      | Value     |
|--------------------------------------------|-----------|
| AM1 Energy                                 | -0.114344 |
| AM1 Free Energy (Quasiharmonic)            | 0.01104   |
| Number of Imaginary Frequencies            | 0         |

#### Frequencies (Top 3 out of 51)

1. 38.5784 cm⁻¹
2. 57.3498 cm⁻¹
3. 96.4266 cm⁻¹
### 6_3pentene2zone_4_am1_HEI

| Datum                                      | Value    |
|--------------------------------------------|----------|
| AM1 Energy                                 | -0.109674|
| AM1 Free Energy (Quasiharmonic)            | 0.014792 |
| Number of Imaginary Frequencies            | 0        |

**Frequencies (Top 3 out of 51)**

1. 44.2824 cm⁻¹  
2. 58.7359 cm⁻¹  
3. 69.7666 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

|          |          |          |
|----------|----------|----------|
| C        | 3.206808 | -0.221637 | -0.697569 |
| C        | 1.981979 | -0.142166 | 0.190533  |
| C        | 0.865720 | 0.473550  | -0.387031 |
| C        | -0.399913| 0.578757  | 0.281806  |
| O        | 2.075957 | -0.600349 | 1.365578  |
| C        | -1.093386| 1.907428  | 0.131532  |
| H        | 3.489699 | 0.796666  | -1.054350 |
| H        | 4.067765 | -0.662102 | -0.141584 |
### 6_3pentene2zone_5_reopt_am1_HEI

| Datum                                | Value     |
|--------------------------------------|-----------|
| AM1 Energy                           | -0.111805 |
| AM1 Free Energy (Quasiharmonic)      | 0.013072  |
| Number of Imaginary Frequencies      | 0         |

#### Frequencies (Top 3 out of 51)

1. 32.5276 cm\(^{-1}\)
2. 52.3406 cm\(^{-1}\)
3. 72.8465 cm\(^{-1}\)

#### AM1 Molecular Geometry in Cartesian Coordinates

| C         | -2.835950 | -0.882046 | -0.413971 |
|-----------|-----------|-----------|-----------|
| C         | -1.686750 | 0.000993  | 0.035997  |
| C         | -0.614855 | 0.065187  | -0.860135 |
| C         | 0.602398  | 0.799322  | -0.694725 |
| O         | -1.811440 | 0.589104  | 1.148709  |
| C         | 0.589968  | 1.923274  | 0.300744  |
| H         | -3.659011 | -0.867459 | 0.338744  |
| H         | -3.233864 | -0.521847 | -1.391682 |
| H         | -2.480367 | -1.931765 | -0.540487 |
| H         | -0.687386 | -0.537346 | -1.774705 |
| H         | 1.026668  | 1.142296  | -1.675586 |
| H         | 1.597633  | 2.398687  | 0.378874  |
| H         | -0.151052 | 2.698544  | -0.016787 |
| H         | 0.279415  | 1.548884  | 1.307267  |
| S         | 2.086735  | -0.302174 | -0.207011 |
| C         | 1.392752  | -1.600992 | 0.742773  |
| H         | 1.714907  | -1.517452 | 1.803701  |
6_3pentene2one_6_am1_HEI

| Datum                              | Value         |
|------------------------------------|---------------|
| AM1 Energy                         | -0.114344     |
| AM1 Free Energy (Quasiharmonic)    | 0.011039      |
| Number of Imaginary Frequencies    | 0             |

**Frequencies** (Top 3 out of 51)

1. 38.5423 cm⁻¹
2. 57.3249 cm⁻¹
3. 96.4231 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

| C          | -1.894029 | -0.383239 | -1.294027 |
| C          | -1.805269 | 0.138563  | 0.121881  |
| C          | -0.595138 | 0.717409  | 0.535301  |
| C          | 0.563848  | 0.870703  | -0.278888 |
| O          | -2.830865 | 0.025479  | 0.853708  |
| C          | 1.468268  | 2.011682  | 0.100002  |
| H          | -2.868773 | -0.900049 | -1.460631 |
| H          | -1.808773 | 0.461573  | -2.018109 |
| H          | -1.061432 | -1.102851 | -1.483963 |
| H          | -0.537888 | 1.061087  | 1.574871  |
| H          | 0.354925  | 0.869091  | -1.377091 |
| H          | 0.967413  | 2.984191  | -0.133998 |
| H          | 2.430656  | 1.964103  | -0.466371 |
| H          | 1.697970  | 1.989385  | 1.192250  |
| S          | 1.814497  | -0.604772 | -0.217256 |
| C          | 0.952798  | -1.905319 | 0.577559  |
| H          | 0.806817  | -2.751822 | -0.128770 |
| H          | 1.538090  | -2.262354 | 1.452686  |
| H          | -0.046909 | -1.538612 | 0.924581  |

6_3pentene2one_7_am1_HEI
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.109425   |
| AM1 Free Energy (Quasiharmonic)            | 0.016477    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 51)

1. 30.0031 cm⁻¹  
2. 48.7938 cm⁻¹  
3. 92.8518 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|     |     |     |     |
|-----|-----|-----|-----|
| C   | -1.720138 | 0.304379 | 1.276996 |
| C   | -1.731501 | -0.200440 | -0.145528 |
| C   | 0.547190  | 0.810502  | -0.737677 |
| O   | -2.747671 | -0.862027 | -0.511621 |
| C   | 0.492550  | 2.036124  | 0.130184  |
| H   | -1.823492 | 1.415583  | 1.287402  |
| H   | -2.569880 | -0.136151 | 1.851836  |
| H   | -0.760876 | 0.022730  | 1.773684  |
| H   | -0.692364 | -0.415327 | -1.975305 |
| H   | 1.070485  | 1.053399  | -1.699438 |
| H   | -0.383263 | 2.669463  | -0.156763 |
| H   | 1.423475  | 2.643229  | 0.004735  |
| H   | 0.401302  | 1.771953  | 1.210897  |
| S   | 1.988510  | -0.184748 | 0.090952  |
| C   | 1.356813  | -1.800765 | 0.327898  |
| H   | 1.430449  | -2.076246 | 1.402683  |
| H   | 0.283885  | -1.838081 | 0.009083  |
| H   | 1.944060  | -2.529608 | -0.272178 |

---

**6_cis_3pentene2one_1_am1**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| AM1 Energy                                 | -0.053035   |
| AM1 Free Energy (Quasiharmonic)            | 0.037881    |
| Number of Imaginary Frequencies            | 0           |

**Frequencies** (Top 3 out of 36)

1. 30.0031 cm⁻¹  
2. 48.7938 cm⁻¹  
3. 92.8518 cm⁻¹
1. 32.5662 cm⁻¹  
2. 81.6430 cm⁻¹  
3. 96.2466 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

```
C    -2.292372    -0.249725     0.000011
C    -0.850720    0.154604     0.000000
C     0.105898    -0.959401    -0.000006
C     1.440118    -0.822285    -0.000006
O    -0.511504    1.346630     -0.000013
C     2.154847    0.466124     0.000009
H    -2.955035    0.649150     0.000241
H    -2.511234   -0.863231    -0.907615
H    -2.511128   -0.863624     0.907395
H    -0.349053   -1.963776    -0.000017
H     2.076733   -1.725275    -0.000018
H     3.261311    0.318237    -0.000139
H     1.866792    1.069878    -0.899455
H     1.867015    1.069703     0.899660
```

### 6_cis_3pentene2one_2_am1

| Datum                               | Value       |
|-------------------------------------|-------------|
| AM1 Energy                          | -0.050569   |
| AM1 Free Energy (Quasiharmonic)     | 0.039896    |
| Number of Imaginary Frequencies     | 0           |

**Frequencies** (Top 3 out of 36)

1. 27.9741 cm⁻¹  
2. 76.1613 cm⁻¹  
3. 96.0563 cm⁻¹

### AM1 Molecular Geometry in Cartesian Coordinates

```
C    -1.401905     1.167645     0.373562
C    -0.937914    -0.204114    -0.004796
C     0.246449    -0.694267    0.728355
C     1.511936    -0.371950    0.453848
```
|     |   X   |   Y   |   Z   |
|-----|-------|-------|-------|
| O   | -1.531| -0.890| -0.843|
| C   |  1.952|  0.518| -0.637|
| H   | -1.654|  1.190|  1.461|
| H   | -0.585|  1.905|  0.181|
| H   | -2.304|  1.458| -0.216|
| H   | -0.000| -1.388|  1.549|
| H   |  2.329| -0.793|  1.066|
| H   |  2.560|  1.361| -0.223|
| H   |  2.592| -0.052| -1.357|
| H   |  1.087|  0.948| -1.201|
**methane_thiolate_am1**

| Datum                                    | Value       |
|------------------------------------------|-------------|
| AM1 Energy                               | -0.027104   |
| AM1 Free Energy (Quasiharmonic)          | -0.011189   |
| Number of Imaginary Frequencies          | 0           |

**Frequencies** (Top 3 out of 9)

1. 818.8846 cm⁻¹  
2. 947.8763 cm⁻¹  
3. 947.9178 cm⁻¹

**AM1 Molecular Geometry in Cartesian Coordinates**

|          |           |           |           |
|----------|-----------|-----------|-----------|
| C        | 0.000006  | -1.059692 | -0.000000 |
| H        | -1.039520 | -1.466710 | 0.000000  |
| H        | 0.519698  | -1.466703 | 0.900290  |
| H        | 0.519698  | -1.466703 | -0.900290 |
| S        | 0.000006  | 0.672392  | -0.000000 |

**methane_thiolate_DFT**

| Datum                                    | Value       |
|------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy    | -438.210295 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -438.193051 |
| Number of Imaginary Frequencies          | 0           |

**Frequencies** (Top 3 out of 9)

1. 715.6670 cm⁻¹  
2. 943.2388 cm⁻¹  
3. 947.1466 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 0.000000| -0.000000| -1.124868|
| H       | 0.000000| 1.015083| -1.523719|
| H       | -0.879088| -0.507542| -1.523719|
| H       | 0.879088| -0.507542| -1.523719|
| S       | -0.000000| 0.000000| 0.707523 |
1-pentene-3-one_protonation_TS_10_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.136987 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.999495 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 60)

1. -944.2083 cm⁻¹
2. 29.0860 cm⁻¹
3. 38.4127 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|  |  |  |
|---|---|---|
| C | 0.192136 | 1.583794 | -0.330020 |
| C | 0.036459 | 0.197623 | -0.508830 |
| C | 0.566970 | -0.836216 | 0.425294 |
| O | -0.071000 | 2.434107 | -1.214840 |
| H | -0.123245 | -0.124806 | -1.534874 |
| H | 0.670620 | -0.452860 | 1.440419 |
| H | -0.095860 | -1.703684 | 0.483703 |
| C | 3.231965 | -0.131533 | -0.015906 |
| H | 2.785943 | 0.662698 | -0.613627 |
| H | 4.191877 | -0.407151 | -0.446417 |
| H | 3.385296 | 0.216455 | 1.004170 |
| S | 2.176333 | -1.589213 | -0.052071 |
| C | 0.552747 | 2.098462 | 1.057612 |
| H | -0.201017 | 1.785757 | 1.785185 |
### 1-pentene-3-one_protonation_TS_11_reopt

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1108.136984     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.999708 |
| Number of Imaginary Frequencies            | 1                |

#### Frequencies (Top 3 out of 60)

1. -1018.9924 cm⁻¹  
2. 40.3976 cm⁻¹  
3. 47.7463 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 0.524569 | 1.449650 | -0.126588 |
|-----|----------|----------|-----------|
| C   | -0.004097| 0.323727 | -0.790195 |
| C   | -1.049117| -0.550619| -0.177316 |
| O   | 1.179713 | 2.357211 | -0.689948 |
| H   | 0.006646 | 0.371012 | -1.875639 |
| H   | -1.085944| -1.524240| -0.671884 |
| H   | -0.855568| -0.730670| 0.881621  |
| C   | -3.698580| -1.134646| 0.451967  |
| H   | -4.742696| -0.830556| 0.435909  |
| H   | -3.389555| -1.291473| 1.484052  |
| H   | -3.590381| -2.063445| -0.105821 |
| S   | -2.722979| 0.179000 | -0.310253 |
| C   | 0.375139 | 1.505621 | 1.387555  |
| H   | -0.676571| 1.535075 | 1.678631  |
| H   | 0.813150 | 0.613878 | 1.844465  |
| H   | 0.880821 | 2.389350 | 1.769028  |
| H   | 1.188509 | -0.692634| -0.462688 |
| S   | 2.275838 | -1.672246| -0.044577 |
| C   | 3.501480 | -0.345641| 0.177024  |
### 1-pentene-3-one_protonation_TS_12_reopt

| Datum                                           | Value         |
|------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -1108.139805  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1108.003151  |
| Number of Imaginary Frequencies                 | 1             |

#### Frequencies (Top 3 out of 60)

1. -999.8773 cm\(^{-1}\)
2. 17.4858 cm\(^{-1}\)
3. 32.8648 cm\(^{-1}\)

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | 0.074315 | 1.694339 | 0.046949 |
|-------|----------|----------|----------|
| C     | -0.085462 | 0.333682 | 0.367873 |
| C     | -0.744466 | -0.591117 | -0.597515 |
| O     | -0.100858 | 2.176299 | -1.095819 |
| H     | -0.091206 | 0.060265 | 1.416662 |
| H     | -0.472306 | -0.319650 | -1.617831 |
| H     | -0.440195 | -1.626941 | -0.433926 |
| C     | -2.881585 | -1.135349 | 1.079163 |
| H     | -2.479127 | -0.422661 | 1.796244 |
| H     | -2.432573 | -2.113995 | 1.243955 |
| H     | -3.957864 | -1.209588 | 1.216448 |
| S     | -2.579956 | -0.577580 | -0.607276 |
| C     | 0.631714  | 2.610300  | 1.120292 |
| H     | 0.723011  | 2.120834  | 2.088096 |
| H     | 1.617401  | 2.961401  | 0.806793 |
| H     | -0.010127 | 3.486601  | 1.218641 |
| H     | 1.405665  | 0.027183  | -0.031110 |
| S     | 2.766423  | -0.565343 | -0.429299 |
| C     | 2.466014  | -2.070931 | 0.546802 |
| H     | 1.635854  | -1.893874 | 1.231456 |
| H     | 2.214381  | -2.912326 | -0.095395 |
| H     | 3.347302  | -2.326424 | 1.130329 |
### 1-pentene-3-one_protonation_TS_1

| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -1108.140321  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -1108.002562  |
| Number of Imaginary Frequencies                                       | 1             |

#### Frequencies (Top 3 out of 60)

1. -1068.1219 cm⁻¹
2. 34.3722 cm⁻¹
3. 45.7723 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

```
 C   -0.034372   1.441537   0.121225  
 C    0.112922   0.257499  -0.627875 
 C    0.664816  -0.976073  0.003489  
 O    0.031273   1.522155  1.370481 
 H    0.267474   0.369374  1.576670 
 H    0.540978  -0.925660  1.084914 
 H    0.166346  -1.882889 -0.349538 
 C    3.148146   0.208842  0.355027  
 H    2.969209   0.259333  1.427309 
 H    2.712139   1.082755 -0.126179 
 H    4.218954   0.186550  0.165823 
 S    2.437810  -1.293676 -0.338301 
 C   -0.413434   2.700459 -0.638981 
 H   -0.453620   2.549913 -1.716152 
 H   -1.389928   3.043400 -0.290975 
 H    0.307146   3.487929 -0.413311 
 H   -1.412914  -0.105210 -0.726410 
 S   -2.835920  -0.676871 -0.595620 
 C   -2.540075  -1.138555  1.141254 
 H   -1.768990  -0.489578  1.553850 
 H   -3.453656  -1.013696  1.718265 
 H   -2.211571  -2.172956  1.222941 
```

### 1-pentene-3-one_protonation_TS_2_reopt
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1108.13699 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.999273 |

Number of Imaginary Frequencies

**Frequencies** (Top 3 out of 60)

1. -1004.4300 cm⁻¹
2. 27.0457 cm⁻¹
3. 44.1047 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          | x         | y         | z         |
|----------|-----------|-----------|-----------|
| C        | 0.161010  | 1.283707  | -0.273744 |
| C        | -0.150573 | -0.032645 | -0.667526 |
| C        | -0.915569 | -0.994107 | 0.179832  |
| O        | 0.517594  | 2.187577  | -1.068094 |
| H        | -0.231705 | -0.185694 | -1.740936 |
| H        | -0.583866 | -2.024380 | 0.018893  |
| H        | -0.791829 | -0.786442 | 1.242757  |
| C        | -3.204041 | 0.593501  | 0.254553  |
| H        | -4.244828 | 0.718413  | -0.035142 |
| H        | -2.589880 | 1.302374  | -0.299482 |
| H        | -3.106570 | 0.777689  | 1.323159  |
| S        | -2.719509 | -1.090781 | -0.156165 |
| C        | 0.167708  | 1.608771  | 1.215583  |
| H        | 0.688439  | 0.838301  | 1.787957  |
| H        | 0.662860  | 2.565463  | 1.365592  |
| H        | -0.848559 | 1.675430  | 1.608321  |
| H        | 1.261141  | -0.696877 | -0.342495 |
| S        | 2.563542  | -1.366549 | 0.076313  |
| C        | 3.469339  | 0.211514  | 0.069202  |
| H        | 3.762249  | 0.493248  | -0.939858 |
| H        | 2.845804  | 1.000205  | 0.486630  |
| H        | 4.364217  | 0.114480  | 0.679581  |

---

1-pentene-3-one_protonation_TS_3_reopt

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1108.13646 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1108.000059 |
| Datum                                      | Value                      |
|--------------------------------------------|----------------------------|
| Number of Imaginary Frequencies            | 1                          |

**Frequencies** (Top 3 out of 60)

1.  -990.0203 cm\(^{-1}\)
2.   3.6263 cm\(^{-1}\)
3.   35.7754 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|          |    |     |     |
|----------|----|-----|-----|
| C        |    |     |     |
| 0.193836 | 1.352855 | -0.397617 |
| C        | -0.141741 | -0.002648 | -0.581041 |
| C        | -0.847871 | -0.841253 | 0.431836 |
| O        | 0.641340 | 2.083206 | -1.314973 |
| H        | -0.285661 | -0.290730 | -1.619369 |
| H        | -0.805728 | -1.892684 | 0.142926 |
| H        | -0.396817 | -0.771352 | 1.422430 |
| C        | -3.256412 | -0.661778 | 0.934976 |
| H        | -3.091070 | -1.678481 | -1.288813 |
| H        | -2.772527 | 0.042710 | -1.608613 |
| H        | -4.324856 | -0.460667 | -0.912460 |
| S        | -2.625287 | -0.461030 | 0.739764 |
| C        | 0.050070 | 1.994256 | 0.974394 |
| H        | -0.064561 | 1.283844 | 1.790258 |
| H        | 0.911980 | 2.633198 | 1.165040 |
| H        | -0.837244 | 2.631142 | 0.959696 |
| H        | 1.316197 | -0.665351 | -0.580799 |
| S        | 2.697909 | -1.264987 | -0.448582 |
| C        | 3.095858 | -0.179689 | 0.952103 |
| H        | 3.914579 | 0.492508 | 0.705741 |
| H        | 2.213592 | 0.417352 | 1.186707 |
| H        | 3.367003 | -0.761334 | 1.829942 |

**1-pentene-3-one_protonation_TS_4_reopt**

| Datum                                      | Value                      |
|--------------------------------------------|----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1108.139826               |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1108.002525               |
| Number of Imaginary Frequencies            | 1                          |
**Frequencies (Top 3 out of 60)**

1. -1008.3677 cm\(^{-1}\)
2. 21.7681 cm\(^{-1}\)
3. 29.8230 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 0.275518 | 1.304277 | -0.214150 |
| C | -0.170308 | 0.130591 | 0.425843 |
| C | -1.005414 | -0.849434 | -0.327806 |
| O | 0.273159 | 1.471841 | 0.425843 |
| H | -0.283526 | 0.162205 | 1.503363 |
| H | -0.632227 | -0.953637 | -1.347337 |
| H | -0.983247 | -1.836424 | 0.139231 |
| C | -3.281067 | -0.352440 | 1.176692 |
| H | -2.736142 | 0.423971 | 1.709909 |
| H | -3.112364 | -1.314722 | 1.658250 |
| H | -4.343908 | -0.123171 | 1.201210 |
| S | -2.772924 | -0.410341 | -0.550638 |
| C | 0.851099 | 2.418441 | 0.642726 |
| H | 0.957965 | 2.135023 | 1.688610 |
| H | 1.820667 | 2.722837 | 0.247228 |
| H | 0.187246 | 3.283419 | 0.580355 |
| H | 1.140396 | -0.719416 | 0.229979 |
| S | 2.399135 | -1.546816 | -0.038081 |
| C | 3.457420 | -0.115313 | 0.330703 |
| H | 3.674544 | 0.457808 | -0.568607 |
| H | 2.948565 | 0.533751 | 1.042917 |
| H | 4.393898 | -0.448609 | 0.771566 |

**1-pentene-3-one_protonation_TS_5_reopt**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.140587 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1108.003371 |
| Number of Imaginary Frequencies | 1 |

**Frequencies (Top 3 out of 60)**
1. -1002.6925 cm⁻¹
2. 29.2582 cm⁻¹
3. 38.3473 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| At   | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -0.227127 | 1.536592  | 0.005008  |
| C    | -0.060425 | 0.212857  | 0.451832  |
| C    | -0.575726 | -0.929890 | -0.356194 |
| O    | -0.562512 | 1.862542  | -1.158167 |
| H    | 0.054275  | 0.053942  | 1.518769  |
| H    | -0.629620 | -0.642027 | -1.405853 |
| H    | 0.066179  | -1.810851 | -0.283160 |
| C    | -3.194886 | -0.049376 | -0.052057 |
| H    | -3.181202 | 0.286198  | -1.086865 |
| H    | -2.796201 | 0.736975  | 0.586375  |
| H    | -4.216092 | -0.276629 | 0.245504  |
| S    | -2.225372 | -1.554677 | 0.140547  |
| C    | 0.161855  | 2.650317  | 0.960350  |
| H    | 0.435680  | 2.284801  | 1.948274  |
| H    | 1.005722  | 3.200086  | 0.537956  |
| H    | -0.668590 | 3.351434  | 1.054216  |
| H    | 1.427712  | 0.186910  | -0.051338 |
| S    | 2.851258  | -0.162950 | -0.511497 |
| C    | 2.925799  | -1.603518 | 0.597128  |
| H    | 2.779260  | -2.531077 | 0.047420  |
| H    | 3.888531  | -1.642940 | 1.101176  |
| H    | 2.143339  | -1.516999 | 1.351663  |

1-pentene-3-one_protonation_TS_7_reopt

| Datum                                           | Value                  |
|------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -1108.137601           |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.998458           |
| Number of Imaginary Frequencies                 | 1                      |

Frequencies (Top 3 out of 60)

1. -1153.5855 cm⁻¹
2. 52.2678 cm⁻¹
3. 63.0314 cm⁻¹
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| C   | -0.812307 | 1.577666 | 0.056336 |
| C   | 0.054042  | 0.955759 | -0.872641 |
| C   | 1.534929  | 1.106739 | -0.702448 |
| O   | -0.471349 | 2.021690 | 1.175479 |
| H   | -0.307675 | 0.923088 | -1.896226 |
| H   | 2.013305  | 1.453415 | -1.618726 |
| H   | 1.751836  | 1.828379 | 0.086139 |
| C   | 1.782289  | -0.710492| 1.357479 |
| H   | 2.095176  | 0.063457 | 2.056030 |
| H   | 2.139564  | -1.678215| 1.703400 |
| H   | 0.695844  | -0.730792| 1.288772 |
| S   | 2.476646  | -0.410536| -0.276384|
| C   | -2.277264 | 1.674016 | -0.338526|
| H   | -2.553112 | 0.903826 | -1.059422|
| H   | -2.906127 | 1.587871 | 0.546574 |
| H   | -2.463480 | 2.650159 | -0.791900|
| H   | -0.463365 | -0.526162| -0.724302|
| S   | -1.128464 | -1.924327| -0.628128|
| C   | -2.101135 | -1.467947| 0.839100 |
| H   | -3.131285 | -1.235496| 0.575884 |
| H   | -2.096096 | -2.281902| 1.560782 |
| H   | -1.658025 | -0.587799| 1.305566 |

1-pentene-3-one_protonation_TS_8

| Datum                                                                 | Value         |
|----------------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -1108.140072  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -1108.002551  |
| Number of Imaginary Frequencies                                       | 1             |

Frequencies (Top 3 out of 60)

1. -995.8042 cm⁻¹
2. 27.4723 cm⁻¹
3. 49.9270 cm⁻¹
1-pentene-3-one_protonation_TS_9_reopt

| Datum                                      | Value             |
|--------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1108.133934      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.996042 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 60)

1. -1094.7929 cm⁻¹
2. 25.9374 cm⁻¹
3. 39.2682 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | C   | O   | H   | H   | H   | C   | H   | H   | S   | C   | H   | H   | H   | S   | C   | H   | H   | H   | H   |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| -0.525852 | 1.384653 | 0.170331 |
| -0.001606 | 0.356638 | -0.640138 |
| 1.079894 | -0.525720 | -0.107719 |
| -0.381137 | 1.448457 | 1.412663 |
| -0.039038 | 0.500576 | -1.714306 |
| 0.928531 | -0.692300 | 0.959191 |
| 1.097090 | -1.496197 | -0.610028 |
| 3.758092 | -1.084187 | 0.370429 |
| 3.508533 | -1.252970 | 1.416573 |
| 4.796818 | -0.769718 | 0.298770 |
| 3.627277 | -2.009204 | -0.188836 |
| 2.730004 | 0.226512 | -0.323688 |
| -1.371311 | 2.457956 | -0.494507 |
| -1.610242 | 2.225185 | -1.531039 |
| -2.293074 | 2.603224 | 0.069225 |
| -0.820208 | 3.400496 | -0.467494 |
| -1.113616 | -0.721672 | -0.385480 |
| -2.155282 | -1.788503 | -0.048771 |
| -3.451749 | -0.523528 | 0.105855 |
| -3.539546 | -0.170366 | 1.131411 |
| -3.204753 | 0.322764 | -0.534460 |
| -4.409036 | -0.930510 | -0.210994 |
3-methyl-2-butenal_protonation_TS_10_reopt

| Datum                                      | Value            |
|--------------------------------------------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1147.436455     |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1147.26978     |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 69)

1.  -1175.9246 cm⁻¹
2.   52.6194 cm⁻¹
3.   69.6868 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 0.631021 | 1.879727 | -0.936571 |
| C   | 0.251488 | 0.524988 | -1.028848 |
| C   | 1.061690 | -0.638488|-0.486732 |
| O   | 1.445552 | 2.426495 | -0.173372 |
| H   | -0.270800| 0.298995 | -1.956939 |
| C   | 0.783854 | -1.878892|-1.338412 |
| C   | 2.567984 | -0.370466|-0.483054 |
| C   | 0.645088 | 0.383897 | 2.131422 |
| H   | -0.035305| 1.113496 | 1.698497 |
### 3-methyl-2-butenal_protonation_TS_1_reopt

| Datum                                                                 | Value              |
|----------------------------------------------------------------------|--------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -1147.441623       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -1147.27582        |

#### Number of Imaginary Frequencies
1

#### Frequencies (Top 3 out of 69)

1. -1093.8698 cm⁻¹  
2. 39.6484 cm⁻¹  
3. 59.0033 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 0.137943| 1.834641| 0.130609|
| C      | -0.010766| 0.522834| -0.346179|
| C      | 0.721243| -0.660137| 0.226618|
| O      | -0.271253| 2.876863| -0.421246|
| H      | -0.258055| 0.440248| -1.404183|
| C      | 0.017318| -1.956686| -0.177835|
| C      | 0.842830| -0.613783| 1.748944|
| C      | 3.161747| 0.757901| -0.194060|
| H      | 2.602207| 1.542896| -0.698793|
| H      | 4.173464| 0.727950| -0.593430|
| H      | 3.213507| 0.971530| 0.872042|
3-methyl-2-butenal_protonation_TS_2_reopt

| Datum                                                                 | Value                  |
|----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -1147.438764           |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -1147.272518           |
| Number of Imaginary Frequencies                                      | 1                      |

**Frequencies (Top 3 out of 69)**

1.  -1078.3241 cm⁻¹
2.   48.2433 cm⁻¹
3.   63.7634 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C       | 0.226682 | 1.661898 | -0.749050 |
|---------|----------|----------|-----------|
| C       | 0.221069 | 1.021339 | 0.411730  |
| C       | 1.450980 | 0.136991 | 0.500770  |
| O       | -1.019884| 2.630967 | -0.806920 |
| H       | 0.055238 | 1.584159 | 1.331930  |
| C       | 1.340491 | -0.780109| 1.719980  |
| C       | 2.724969 | 0.982383 | 0.632250  |
| C       | 0.208873 | -1.765001| -1.226700 |
| H       | -0.069376| -2.312671| -0.329080 |
| H       | 0.372044 | -2.470321| -2.039270 |
| H       | -0.593378| -1.083132| -1.495800 |
| S       | 1.758181 | -0.876449| -1.003460 |
| H       | 0.106578 | 1.207279 | -1.701640 |
3-methyl-2-butenal_protonation_TS_3_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1147.437211 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1147.270935 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 69)

1. -1121.9394 cm⁻¹
2. 30.2048 cm⁻¹
3. 54.1747 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.247427  | 1.743800  | -0.768360 |
|-------|-----------|-----------|-----------|
| C     | 0.014032  | 0.933240  | 0.349750  |
| C     | 1.360381  | 0.282278  | 0.591930  |
| O     | -1.236726 | 2.483791  | -0.935580 |
| H     | -0.520648 | 1.222210  | 1.253710  |
| C     | 1.520621  | 0.010478  | 2.087400  |
| C     | 2.544742  | 1.122357  | 0.107910  |
| C     | 1.023290  | -1.110521 | -1.876570 |
| H     | -0.008570 | -0.765660 | -1.922440 |
| H     | 1.103269  | -2.062011 | -2.398830 |
| H     | 1.680351  | -0.390122 | -2.361250 |
| S     | 1.512809  | -1.413642 | -0.172150 |
| H     | 0.466953  | 1.652039  | -1.609220 |
| H     | -1.011759 | -0.159289 | 0.063280  |
| S     | -2.196010 | -1.181068 | -0.007040 |
### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | -0.291049| 1.589295 | -0.365816|
| C       | -0.025977| 0.247715 | -0.697514|
| C       | 0.846128 | -0.700445| 0.088689 |
| O       | -0.197974| 2.166915 | 0.735629 |
| H       | -0.037847| 0.052570 | -1.767421|
| C       | 0.694128 | -0.564502| 1.602126 |
| C       | 0.546899 | -2.144890| -0.319629|
| C       | 2.880424 | 1.282180 | -0.158759|
| H       | 2.604329 | 1.604689 | 0.842733 |
| H       | 2.289958 | 1.833096 | -0.888103|
| H       | 3.937312 | 1.480369 | -0.325238|
| S       | 2.642952 | -0.489708| -0.360599|
| H       | -0.711331| 2.167668 | -1.214857|
| H       | -1.435107| -0.305371| -0.293817|
| S       | -2.838197| -0.819074| 0.104507 |
| C       | -3.633725| 0.740207 | -0.376552|
| H       | -4.478299| 0.553409 | -1.035677|
**3-methyl-2-butenal_protonation_TS_6**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1147.439336 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1147.273047 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 69)

1. -1097.5178 cm⁻¹
2. 35.3099 cm⁻¹
3. 65.1184 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 1.776022 | -0.786328 |
|-------|----------|------------|
| C     | 0.607338 | -0.792468 |
| C     | 0.452112 | 0.158456   |
| O     | 2.638444 | 0.111896   |
| H     | 0.157922 | -1.774345 |
| C     | 1.613593 | 0.000403   |
| C     | 0.360713 | 1.621525   |
| C     | -2.352875 | -0.257120 |
| H     | -2.201762 | -1.021010 |
| H     | -2.427366 | 0.718585   |
| H     | -3.278817 | -0.459938 |
| S     | -1.032510 | -0.290981 |
| H     | 1.888821 | -1.686515 |
| H     | -0.365211 | -0.270660 |
| S     | -1.283224 | 0.206814   |
| C     | -0.014211 | -0.040984 |
| H     | 0.512897 | 0.884264   |
| H     | 0.709302 | -0.778131 |
| H     | -0.471564 | -0.415121 |
3-methyl-2-butenal_protonation_TS_7_reopt

| Datum                                      | Value                  |
|--------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy       | -1147.440189           |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1147.275746           |
| Number of Imaginary Frequencies            | 1                      |

**Frequencies** (Top 3 out of 69)

1.  -1059.8766 cm⁻¹
2.       22.1064 cm⁻¹
3.       44.1965 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Datum | Value                  |
|-------|------------------------|
| C     | 0.515550               |
| C     | 0.244806               |
| C     | -0.898999              |
| O     | 1.298895               |
| H     | 0.515701               |
| C     | -0.906315              |
| C     | -0.819376              |
| C     | -3.780232              |
| H     | -4.713740              |
| H     | -3.771871              |
| H     | -3.726847              |
| S     | -2.448079              |
| H     | 0.038291               |
| H     | 1.490747               |
| S     | 2.788388               |
| C     | 3.639830               |
| H     | 2.901138               |
| H     | 4.274652               |
| H     | 4.253560               |
| H     | 0.024965               |
| H     | -0.997392              |
### 3-methyl-2-butenal_protonation_TS_8_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1147.441318 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1147.277115 |

Number of Imaginary Frequencies

**Frequencies** (Top 3 out of 69)

1. -1054.1596 cm\(^{-1}\)
2. 5.3900 cm\(^{-1}\)
3. 46.4428 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | -0.244041 | 1.718214 | 0.076830 |
|-----|-----------|----------|----------|
| C   | -0.060428 | 0.421258 | -0.432575|
| C   | 0.826787  | -0.625051| 0.189517 |
| O   | 0.002966  | 2.153342 | 1.218264 |
| H   | -0.150120 | 0.361449 | -1.514687|
| C   | 0.486467  | -0.915995| 1.651991 |
| C   | 0.730849  | -1.917611| -0.619227|
| C   | 2.861834  | 0.542873 | -1.425693|
| H   | 2.666742  | -0.218477| -2.179063|
| H   | 3.903102  | 0.849871 | -1.498863|
| H   | 2.219692  | 1.403922 | -1.601059|
| S   | 2.619096  | -0.095587| 0.238985 |
| H   | -0.731375 | 2.408707 | -0.642738|
| H   | -1.475967 | -0.173507| -0.069267|
| S   | -2.890196 | -0.721365| 0.170437 |
| C   | -3.619614 | 0.530716 | -0.924762|
| H   | -4.449033 | 1.033567 | -0.433308|
| H   | -2.856558 | 1.274356 | -1.163292|
| H   | -3.976449 | 0.086837 | -1.851339|
| H   | 0.502828  | -0.002361| 2.240436 |
| H   | -0.513036 | -1.351127| 1.711352 |
| H   | 1.192870  | -1.634542| 2.073494 |
| H   | -0.309828 | -2.250393| -0.647170|
3-methyl-2-butenal_protonation_TS_9

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -1147.439548
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1147.273434

Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 69)

1. -1027.5393 cm⁻¹
2. 48.4677 cm⁻¹
3. 57.2637 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C   | 0.745222 | 1.708499 | -0.735187 |
| C   | 0.220939 | 1.146326 | 0.435186  |
| C   | 1.722336 | 2.487070 | -0.817035 |
| O   | 0.496105 | 1.653444 | 1.359598  |
| H   | -2.80891 | 1.425948 | 0.174898  |
| C   | -1.332626| -0.119068| 1.893205  |
| C   | -2.81763 | -1.466268| -0.785851 |
| H   | -3.182914| -1.699252| 0.210307  |
| H   | -2.823223| -2.377526| -1.380436 |
| H   | -3.459596| -0.731457| -1.257652 |
| S   | -1.094515| -0.911460| -0.740191 |
| O   | 0.278866 | 1.362855 | -1.678434 |
| C   | 1.334887 | 0.048380 | 0.702521  |
| S   | 2.459691 | 0.967734 | 0.869283  |
| C   | 2.565500 | -1.241649| -0.920868 |
| H   | 3.564741 | -1.019500| -1.288657 |
| H   | 2.318699 | -2.268423| -1.175188 |
| H   | 1.852873 | -0.578522| -1.416410 |
| H   | -3.258253| 0.956426 | 0.302078  |
| H   | -2.226824| 2.276056 | 0.858240  |
| H   | -2.200361| 1.801014 | -0.845622 |
| H   | -1.362985| 0.694007 | 2.623073  |
| H   | -2.70306 | -0.670152| 1.976499  |
| H   | -0.509314| -0.784537| 2.151369  |
4-methyl-3-pentene-2-one_protonation_TS_10

| Datum                                                                 | Value               |
|----------------------------------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -1186.755256        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -1186.562928        |
| Number of Imaginary Frequencies                                      | 1                   |

**Frequencies (Top 3 out of 78)**

1.  -1007.9453 cm⁻¹
2.   40.3662 cm⁻¹
3.   58.0755 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  C    | 0.676669  | 1.751809  | -0.282253  |
|-------|-----------|-----------|------------|
|  C    | -0.083019 | 0.593433  | -0.521588  |
|  C    | -1.420954 | 0.360898  | 0.162037   |
|  O    | 0.510334  | 2.558061  | 0.665056   |
|  H    | 0.035409  | 0.145844  | -1.502637  |
|  C    | -1.271655 | 0.132065  | 1.667235   |
|  C    | -2.387650 | 1.526020  | -0.080285  |
|  C    | -1.058524 | -2.401759 | -0.426873  |
|  H    | -1.488119 | -3.282211 | -0.900851  |
|  H    | -0.856885 | -2.622105 | 0.618778   |
|  H    | -0.125288 | -2.141937 | -0.922524  |
|  S    | -2.270663 | -1.081104 | -0.604062  |
|  C    | 1.900669  | 1.954721  | -1.160530  |
|  H    | 1.890455  | 1.336401  | -2.056564  |
|  H    | 1.979787  | 3.085252  | -1.440534  |
|  H    | 2.787821  | 1.697107  | -0.575018  |
|  H    | 1.000345  | -0.258283 | 0.313165   |
|  S    | 2.105141  | -1.092117 | 0.973237   |
|  C    | 2.918608  | -1.399501 | -0.622843  |
|  H    | 2.221543  | -1.165131 | -1.428881  |
|  H    | 3.803857  | -0.777877 | -0.742734  |
|  H    | 3.207015  | -2.444801 | -0.706705  |
|  H    | -2.249305 | 0.039397  | 2.142480   |
|  H    | -0.694136 | -0.768132 | 1.877459   |
|  H    | -0.741896 | 0.982392  | 2.098337   |
|  H    | -3.358124 | 1.339494  | 0.385730   |
4-methyl-3-pentene-2-one_protonation_TS_11_reopt

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -1186.756016
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1186.564588

Number of Imaginary Frequencies | 1

**Frequencies** (Top 3 out of 78)

1. -1082.7908 cm⁻¹
2. 26.8571 cm⁻¹
3. 47.7604 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |
|---|---|---|
| C | 0.648202 | 1.603335 | -0.062976 |
| C | 0.150390 | 0.445777 | -0.700631 |
| C | -0.939621 | -0.433921 | -0.138744 |
| O | 0.397620 | 1.984550 | 1.103399 |
| H | 0.192655 | 0.469002 | -1.786353 |
| C | -1.149131 | -1.628458 | -1.066866 |
| C | -0.620531 | -0.935061 | 1.269189 |
| C | -3.795771 | -0.583406 | 0.294529 |
| H | -3.964500 | -1.293918 | -0.511488 |
| H | -4.703639 | -0.001561 | 0.442712 |
| H | -3.575622 | -1.118901 | 1.216092 |
| S | -2.487875 | 0.595859 | -0.112205 |
| C | 1.672053 | 2.412061 | -0.845977 |
| H | 1.784986 | 2.079349 | -1.875985 |
| H | 1.390233 | 3.465481 | -0.832293 |
| H | 2.638394 | 2.324602 | -0.343127 |
| H | 1.461128 | -0.463169 | -0.649744 |
| S | 2.714006 | -1.331026 | -0.490347 |
| C | 3.019712 | -0.696541 | 1.188378 |
| H | 2.295355 | 0.088803 | 1.401232 |
| H | 4.022765 | -0.282566 | 1.265068 |
| H | 2.906876 | -1.485745 | 1.928972 |
| H | -0.213330 | -2.187056 | -1.141082 |
| H | -1.914614 | -2.303918 | -0.683780 |
| H | -1.439708 | -1.301785 | -2.066049 |
4-methyl-3-pentene-2-one_protonation_TS_13

| Datum                                           | Value   |
|-------------------------------------------------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy           | -1186.752871 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1186.561331 |

Number of Imaginary Frequencies

Frequencies (Top 3 out of 78)

1. -1098.5444 cm⁻¹
2. 41.3053 cm⁻¹
3. 47.2732 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |  C          |  C          |      |     |
|---|-------------|-------------|------|-----|
| H | -1.353209   | -1.629216   | -0.189830 |
| C | -0.381777   | -0.678955   | -0.558493 |
| C | 0.953020    | -0.586731   | 0.166702  |
| O | -1.373970   | -2.281376   | 0.880175  |
| H | -0.365465   | -0.414926   | -1.611688 |
| C | 0.793894    | -0.150330   | 1.623765  |
| C | 1.711331    | -1.914659   | 0.105632  |
| C | 3.542665    | 0.598962    | -0.075185 |
| H | 4.104206    | 1.431544    | -0.493940 |
| H | 4.033569    | -0.330509   | -0.353596 |
| H | 3.531457    | 0.700187    | 1.008240  |
| S | 1.880110    | 0.708331    | -0.764866 |
| C | -2.558713   | -1.759358   | -1.105847 |
| H | -2.435266   | -1.236403   | -2.052177 |
| H | -2.759610   | -2.813969   | -1.295756 |
| H | -3.429033   | -1.345271   | -0.590104 |
| H | -1.348020   | 0.487016    | -0.061049 |
| S | -2.248234   | 1.675395    | 0.372186  |
| C | -1.038012   | 2.940598    | -0.115447 |
| H | -0.211372   | 2.986399    | 0.591141  |
| H | -0.632690   | 2.717529    | -1.101020 |
| H | -1.528947   | 3.910756    | -0.148895 |
| H | 1.763964    | -0.058142   | 2.115302  |
| H | 0.273025    | 0.804501    | 1.685742  |
4-methyl-3-pentene-2-one_protonation_TS_1_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1186.755951 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1186.564489 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 78)

1. -1076.6895 cm⁻¹
2. 16.3528 cm⁻¹
3. 58.4288 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.322113 | 1.401187 | 0.013155 |
| C     | -0.032735 | 0.161489 | -0.561277 |
| C     | -0.982502 | -0.845667 | 0.031572 |
| O     | 0.168823 | 1.748906 | 1.206635 |
| H     | -0.003225 | 0.140226 | -1.647860 |
| C     | -0.768029 | -2.209286 | -0.630917 |
| C     | -0.860390 | -1.004695 | 1.545397 |
| C     | -2.876657 | 1.284232 | 0.109662 |
| C     | -2.220899 | 1.902287 | -0.500443 |
| H     | -2.611970 | 1.409912 | 1.156937 |
| H     | -3.909620 | 1.589376 | -0.045087 |
| S     | -2.757876 | -0.440999 | -0.388386 |
| C     | 1.015032 | 2.393194 | -0.914262 |
| H     | 1.408370 | 1.926111 | -1.816129 |
| H     | 0.291608 | 3.157001 | -1.218013 |
| H     | 1.822497 | 2.892525 | -0.379894 |
| H     | 1.364762 | -0.554424 | -0.332436 |
| S     | 2.726083 | -1.237333 | -0.098772 |
| C     | 3.572945 | 0.349772 | 0.184606 |
| H     | 4.534202 | 0.165674 | 0.659188 |
| H     | 3.741545 | 0.874423 | -0.753591 |
| H     | 2.974423 | 0.981768 | 0.837378 |
| H     | -1.531154 | -2.923458 | -0.315249 |
4-methyl-3-pentene-2-one_protonation_TS_2

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1186.754312 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1186.561718 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 78)

1. -1150.2111 cm⁻¹
2. 67.9011 cm⁻¹
3. 69.8893 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | 0.952568 | 1.543033 | -0.452405 |
|--------|----------|----------|-----------|
| C      | -0.082801| 0.605029 | -0.637223 |
| C      | -1.251808| 0.522792 | 0.329955  |
| O      | 1.168465 | 2.212525 | 0.585828  |
| H      | -0.302315| 0.353807 | -1.670183 |
| C      | -0.819968| 0.006610 | 1.703535  |
| C      | -1.952615| 1.876852 | 0.495438  |
| C      | -1.686928| 2.099834 | -0.702764 |
| H      | -1.239173| 2.509676 | 0.199318  |
| H      | -0.911279| 1.950052 | -1.451137 |
| H      | -2.425390| 2.801037 | -1.086660 |
| S      | -2.565780| -0.564687| -0.363316 |
| C      | 1.958417 | 1.677967 | -1.585764 |
| H      | 1.691354 | 1.095080 | -2.465172 |
| H      | 2.048493 | 2.729176 | -1.863274 |
| H      | 2.937186 | 1.348387 | -1.230278 |
| H      | 0.867509 | -0.660678| -0.414344 |
| S      | 1.836866 | -1.841272| -0.154920 |
| C      | 2.758492 | -0.939007| 1.127509  |
| H      | 3.551641 | -1.576585| 1.512487  |
| H      | 3.201225 | -0.031483| 0.722796  |
| H      | 2.096717 | -0.667057| 1.947660  |
### 4-methyl-3-pentene-2-one_protonation_TS_3_reopt

| Datum                                                                 | Value                      |
|-----------------------------------------------------------------------|----------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -1186.753875               |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -1186.562041               |
| Number of Imaginary Frequencies                                       | 1                          |

#### Frequencies (Top 3 out of 78)

1.   -1090.9089 cm\(^{-1}\)
2.      29.4148 cm\(^{-1}\)
3.      58.7516 cm\(^{-1}\)

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C          | 0.897985 | 1.588577 | -0.357969 |
| C          | -0.038766 | 0.550947 | -0.515565 |
| C          | -1.087081 | 0.260626 | 0.543288  |
| O          | 1.103709  | 2.253547 | 0.689192  |
| H          | -0.313767 | 0.329565 | -1.541560 |
| C          | -0.444482 | -0.194374 | 1.857763 |
| C          | -1.986570 | 1.469132 | 0.806987  |
| C          | -3.058150 | -0.524946 | -1.363371 |
| H          | -2.401876 | -0.061954 | -2.097895 |
| H          | -3.807001 | 0.192722 | -1.037004 |
| H          | -3.559829 | -1.371315 | -1.827622 |
| S          | -2.115399 | -1.180453 | 0.026901  |
| C          | 1.815147  | 1.863023 | -1.539839 |
| H          | 1.539226  | 1.305408 | -2.433007 |
| H          | 1.811767  | 2.930708 | -1.763204 |
| H          | 2.835522  | 1.589569 | -1.259696 |
| H          | 0.976228  | -0.697005 | -0.538716 |
| S          | 1.993495  | -1.833009 | -0.477921 |
| C          | 2.924953  | -1.008678 | 0.850503  |
| H          | 3.980582  | -0.947427 | 0.594870  |
| H          | 2.531476  | -0.00691 | 0.976702  |
4-methyl-3-pentene-2-one_protonation_TS_4_reopt

| Datum                                               | Value             |
|-----------------------------------------------------|-------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy               | -1186.752635      |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1186.56083       |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 78)

1. -981.7047 cm⁻¹
2.  31.9115 cm⁻¹
3.  46.8750 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C        | 0.101879 | 1.689222 | -0.153751 |
| C        | -0.055399| 0.294950 | -0.346138 |
| C        | 0.792639 | -0.729399|  0.359803 |
| O        | -0.704587|  2.456688| -0.945415 |
| H        | -0.334550|  0.007287| -1.357969 |
| C        | 0.603536 | -0.803141|  1.877502 |
| C        | 0.450118 | -2.102285| -0.224231 |
| C        | 2.743779 | -0.105070| -1.615547 |
| H        | 3.788973 |  0.097312| -1.839795 |
| H        | 2.144649 |  0.769498| -1.861245 |
| H        | 2.414106 | -0.953679| -2.212490 |
| S        | 2.637715 | -0.455579|  0.146689 |
| C        | 0.483040 |  2.316051|  1.100033 |
| H        | 1.468073 |  1.914738|  1.334124 |
| H        | 0.548242 |  3.392606|  0.957840 |
| H        | -0.172497|  2.120206|  1.952294 |
| H        | -1.529721|  0.016236|  0.249859 |
| S        | -2.970522| -0.377071|  0.526467 |
| C        | -3.263615| -0.773876| -1.222671 |
| H        | -3.249340|  0.126818| -1.833292 |
**4-methyl-3-pentene-2-one_protonation_TS_5_reopt**

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1186.752721 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1186.561277 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 78)

1. -1132.6521 cm⁻¹
2. 37.4035 cm⁻¹
3. 49.0152 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.839904 | 1.808139 | -0.285898 |
|-------|----------|----------|-----------|
| C     | 0.059498 | 0.648626 | -0.446887 |
| C     | -1.048802 | 0.291286 | 0.531182 |
| O     | 0.921117 | 2.498918 | 0.758437 |
| H     | -0.072560 | 0.311300 | -1.468791 |
| C     | -0.502278 | -0.096890 | 1.908338 |
| C     | -2.050157 | 1.437172 | 0.691220 |
| C     | -2.790610 | -0.653027 | -1.518820 |
| H     | -3.187599 | -1.538687 | -2.010299 |
| H     | -2.105227 | -0.152230 | -2.200533 |
| H     | -3.614446 | 0.012380 | -1.272148 |
| S     | -1.929208 | -1.222682 | -0.040877 |
| C     | 1.785013 | 2.157863 | -1.423128 |
| H     | 1.615459 | 1.562891 | -2.318503 |
| H     | 1.685348 | 3.216200 | -1.666600 |
| H     | 2.810816 | 1.993176 | -1.083535 |
| H     | 1.341832 | -0.233692 | -0.122802 |
| S     | 2.562030 | -1.159318 | 0.158029 |
| C     | 1.641924 | -2.697912 | -0.141514 |
4-methyl-3-pentene-2-one_protonation_TS_7_reopt

| Datum                                                                 | Value                  |
|-----------------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                 | -1186.750717           |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)            | -1186.559093           |
| Number of Imaginary Frequencies                                       | 1                      |

**Frequencies** (Top 3 out of 78)

1.  -1159.4093 cm⁻¹  
2.   31.3621 cm⁻¹  
3.   39.1516 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  C  | -0.396061  | 1.735589  | 0.316451  |
|  C  | 0.183659  | 0.889009  | -0.696309 |
|  C  | 1.405779  | 0.113699  | -0.614419 |
|  O  | -0.023781 | 1.780859  | 1.511111  |
|  H  | -0.125691 | 1.230249  | -1.702909 |
|  C  | 1.817229  | -0.280231 | -2.036139 |
|  C  | 2.537379  | 0.914229  | 0.030841  |
|  C  | 0.974849  | -1.120561 | 1.962121  |
|  H  | 0.812199  | -2.066821 | 2.476241  |
|  H  | 0.100059  | -0.485471 | 2.056201  |
|  H  | 1.833869  | -0.619641 | 2.403931  |
|  S  | 1.273419  | -1.533951 | 0.234591  |
|  C  | -1.572531 | 2.622149  | -0.068469 |
|  H  | -1.843861 | 2.545909  | -1.119349 |
|  H  | -2.435631 | 2.340299  | 0.538451  |
|  H  | -1.331701 | 3.659789  | 0.167501  |
|  H  | -1.127471 | -0.077491 | -0.835029 |
|  S  | -2.376241 | -0.988781 | -0.950289 |
### 4-methyl-3-pentene-2-one_protonation_TS_8_reopt

| Datum                                                                 | Value              |
|----------------------------------------------------------------------|--------------------|
| M06-2X/def2tzvp-IEFPCM(water) Energy                                 | -1186.747652       |
| M06-2X/def2tzvp-IEFPCM(water) Free Energy (Quasiharmonic)           | -1186.55511        |
| Number of Imaginary Frequencies                                      | 1                  |

**Frequencies** (Top 3 out of 78)

1. -930.4322 cm⁻¹
2. 36.6042 cm⁻¹
3. 57.9506 cm⁻¹

**M06-2X/def2tzvp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C          | -2.383731  | -1.304361  | 0.838801 |
|------------|------------|------------|----------|
| H          | -1.625051  | -2.038691  | 1.103841 |
| H          | -2.175261  | -0.379451  | 1.376441 |
| H          | -3.361131  | -1.673221  | 1.142371 |
| H          | 1.973299   | 0.623809   | -2.627379|
| H          | 2.742689   | -0.857221  | -2.035439|
| H          | 1.035939   | -0.870781  | -2.518299|
| H          | 3.463819   | 0.337049   | 0.041341 |
| H          | 2.701379   | 1.826439   | -0.548619|
| H          | 2.278539   | 1.204949   | 1.045721 |

| C          | -0.747668  | 1.800857   | -0.701103 |
|------------|------------|------------|-----------|
| C          | -0.021201  | 0.609841   | -0.538436 |
| C          | 1.226671   | 0.389591   | 0.296029  |
| O          | -1.618168  | 1.943256   | -1.601263 |
| H          | -0.097346  | -0.032131  | -1.41206  |
| C          | 2.452968   | 1.106821   | -0.276137 |
| C          | 1.078722   | 0.743431   | 1.781602  |
| C          | 1.643847   | -1.939507  | -1.357057 |
| H          | 0.651641   | -1.961502  | -1.802804 |
| H          | 2.050751   | -2.948988  | -1.361232 |
| H          | 2.299771   | -1.299438  | -1.943521 |
| S          | 1.591711   | -1.427372  | 0.369129  |
| C          | -0.622499  | 2.938494   | 0.301958  |
| H          | -1.022090  | 2.633420   | 1.271826  |
| H          | 0.410227   | 3.249518   | 0.455863  |
| H          | -1.198701  | 3.786380   | -0.06954  |
| H          | -1.229566  | -0.102460  | 0.297169  |
4-methyl-3-pentene-2-one_protonation_TS_9_reopt

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1186.753897|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1186.563242|
| Number of Imaginary Frequencies            | 1           |

**Frequencies (Top 3 out of 78)**

1. -1089.6460 cm⁻¹
2. 12.8769 cm⁻¹
3. 33.7368 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | 1.207621 | 1.530293 | -0.241002 |
| C   | 0.198520 | 0.634326 | -0.643652 |
| C   | -1.072231 | 0.456292 | 0.170408  |
| O   | 1.279252 | 2.124830 | 0.862798  |
| H   | 0.093548 | 0.513393 | -1.718479 |
| C   | -0.774093 | -0.181852 | 1.563096  |
| C   | -1.857601 | 1.763531 | 0.292843  |
| C   | -3.615781 | -0.851487 | 0.079977  |
| H   | -4.197007 | -1.638342 | -0.396373 |
| H   | -4.164368 | 0.084228 | 0.002345  |
| H   | -3.474506 | -1.111404 | 1.126952  |
| S   | -2.444273 | -0.775758 | -0.800521 |
| C   | 2.369771 | 1.717363 | -1.204276 |
| H   | 2.199285 | 1.252958 | -2.173803 |
| H   | 2.565256 | 2.781725 | -1.339102 |
| H   | 3.263052 | 1.272091 | -0.758667 |
methylacrolein_protonation_TS_1_reopt

| Datum | Value          |
|-------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.136422 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.998439 |

Number of Imaginary Frequencies

1

Frequencies (Top 3 out of 60)

1. -930.2421 cm⁻¹
2. 24.0723 cm⁻¹
3. 38.8007 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | 0.120017 | 1.460805 | 0.217421 |
|-------|----------|----------|----------|
| C     | -0.078499 | 0.085202 | 0.417730 |
| C     | -0.824682 | -0.684596 | -0.626272 |
| O     | -0.018282 | 2.107941 | -0.843206 |
| C     | -0.056996 | -0.471197 | 1.815479 |
| H     | -0.741167 | -0.176565 | -1.586201 |
| H     | -0.429565 | -1.699353 | -0.739027 |
| C     | -3.102021 | 0.743278 | 0.075542 |
| H     | -2.885814 | 1.389003 | -0.773103 |
| H     | -2.578425 | 1.117720 | 0.954022 |
| H     | -4.172643 | 0.735462 | 0.267325 |
| S     | -2.603473 | -0.951146 | -0.274883 |
| H     | 0.510906 | 1.996083 | 1.107536 |
| H     | 1.297310 | -0.363856 | -0.120332 |
| S     | 2.655332 | -0.891162 | -0.587454 |
**methylacrolein_protonation_TS_2_reopt_reopt**

| Datum | Value          |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.137199 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.999759 |

**Number of Imaginary Frequencies**

1

**Frequencies (Top 3 out of 60)**

1. -922.9743 cm⁻¹
2. 14.9769 cm⁻¹
3. 38.7436 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.107166 | 1.415810 | -0.463421 |
|-------|-----------|----------|-----------|
| C     | 0.117002  | 0.272627 | 0.321045  |
| C     | 0.752084  | -0.914999| -0.323892 |
| O     | -0.481712 | 2.542063 | -0.073947 |
| C     | 0.254239  | 0.415914 | 1.813086  |
| H     | 0.335875  | -1.851676| 0.058149  |
| H     | 0.591877  | -0.896946| -1.404126 |
| C     | 3.114379  | 0.586213 | -0.620799 |
| H     | 2.690416  | 1.300983 | -0.009040 |
| H     | 2.827097  | 0.657017 | -1.660508 |
| H     | 4.198901  | 0.528326 | -0.541824 |
| S     | 2.558151  | -1.103251| -0.036505 |
| H     | 0.002658  | 1.250677 | -1.555554 |
| H     | -1.346737 | -0.192606| 0.382836  |
| S     | -2.777587 | -0.732841| 0.476178  |
| C     | -3.049274 | -0.398066| -1.286579 |
| H     | -3.868151 | 0.312132 | -1.425102 |
| H     | -2.139856 | 0.051329 | -1.701144 |
| H     | -3.271507 | -1.303654| -1.833058 |
| H     | -0.370553 | 1.234283 | 2.170126  |
methylacrolein_protonation_TS_3_reopt

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.133857 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.996697 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 60)

1.  -926.3897 cm⁻¹
2.   3.7999 cm⁻¹
3.  47.5535 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|     | X      | Y      | Z      |
|-----|--------|--------|--------|
| C   | -0.606630 | 1.673269 | -0.444912 |
| C   | 0.841129 | -0.332855 | -0.713729 |
| C   | -1.196259 | 2.614497 | 0.127012 |
| C   | 0.370185 | 0.628567 | 1.620725 |
| H   | 0.723727 | -1.381641 | -0.422613 |
| H   | 0.519464 | -0.247072 | -1.753104 |
| C   | 3.200786 | -1.128842 | 0.587739 |
| H   | 2.807695 | -0.803251 | 1.547645 |
| H   | 4.287615 | -1.090528 | 0.615766 |
| H   | 2.888236 | -2.152903 | 0.391537 |
| S   | 2.658778 | -0.043391 | -0.749255 |
| H   | -0.639371 | 1.633881 | -1.553671 |
| H   | -1.229979 | -0.270795 | 0.358879 |
| S   | -2.431389 | -1.193912 | 0.584127 |
| C   | -3.053262 | -0.832477 | -1.083526 |
| H   | -3.094412 | -1.734127 | -1.690169 |
| H   | -2.376305 | -0.120803 | -1.562228 |
| H   | -4.045847 | -0.389979 | -1.041289 |
| H   | 0.345874 | -0.373329 | 2.063356 |
| H   | 1.366626 | 1.043580 | 1.803094 |
| H   | -0.353937 | 1.250000 | 2.146949 |
methylacrolein_protonation_TS_4_reopt

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1108.131732 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.993454 |

Number of Imaginary Frequencies 1

Frequencies (Top 3 out of 60)

1.  -1041.7608 cm⁻¹
2.   37.3803 cm⁻¹
3.   48.8750 cm⁻¹

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |       |       |       |
|---|-------|-------|-------|
| C | 0.51386 | 1.888465 | 0.464100 |
| C | -0.006162 | 0.589246 | 0.594844 |
| C | -0.640309 | -0.043146 | -0.602799 |
| O | 0.687265 | 2.548642 | -0.581494 |
| C | -0.438342 | 0.107954 | 1.955353 |
| H | -0.273493 | 0.442351 | -1.505862 |
| H | -0.405342 | -1.109857 | -0.673863 |
| C | -2.941310 | -1.481675 | 0.101026 |
| H | -2.604121 | -1.510535 | 1.134376 |
| H | -2.526090 | -2.328150 | -0.442913 |
| H | -4.027159 | -1.544300 | 0.078068 |
| S | -2.472142 | 0.066750 | -0.700212 |
| H | 0.864061 | 2.329402 | 1.420122 |
| H | 1.337229 | -0.158579 | 0.591819 |
| S | 2.540185 | -1.115132 | 0.410269 |
| C | 2.633600 | -0.701022 | -1.361000 |
| H | 2.211410 | 0.290195 | -1.520900 |
| H | 3.670826 | -0.698339 | -1.688295 |
| H | 2.077602 | -1.418221 | -1.961956 |
| H | -0.236121 | -0.962817 | 2.076795 |
| H | 0.105755 | 0.635886 | 2.741336 |
| H | -1.507741 | 0.259005 | 2.133188 |

methylacrolein_protonation_TS_5

| Datum                                      | Value        |
|--------------------------------------------|--------------|
| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.135022 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.997976 |

Number of Imaginary Frequencies 1

**Frequencies** (Top 3 out of 60)

1. -946.9167 cm⁻¹
2. 19.8091 cm⁻¹
3. 44.4485 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | -0.549770 | 1.408555 | -0.881528 |
|-------|-----------|----------|-----------|
| C     | -0.047499 | 0.652678 | 0.189303  |
| C     | 0.935866  | -0.432455| -0.109925 |
| O     | -1.251957 | 2.439229 | -0.819135 |
| C     | -0.047941 | 1.236379 | 1.578819  |
| H     | 0.846219  | -1.254904| 0.605990  |
| H     | 0.775224  | -0.836898| -1.111639 |
| C     | 3.524246  | -1.413745| -0.274716 |
| H     | 3.263344  | -1.841329| -1.241326 |
| H     | 3.270048  | -2.117695| 0.515905  |
| H     | 4.594132  | -1.220648| -0.248318 |
| S     | 2.669716  | 0.154626 | -0.022523 |
| H     | -0.339611 | 0.977982 | -1.882925 |
| H     | -1.314533 | -0.183582| 0.426415  |
| S     | -2.538232 | -1.055338| 0.723956  |
| C     | -2.859202 | -1.264701| -1.051599 |
| H     | -2.805007 | -2.312497| -1.337803 |
| H     | -3.839433 | -0.876176| -1.318089 |
| H     | -2.102524 | -0.710903| -1.612023 |
| H     | -0.906822 | 1.895845 | 1.703127  |
| H     | -0.117672 | 0.443680 | 2.330947  |
| H     | 0.854340  | 1.814407 | 1.797763  |

**methylacrolein_protonation_TS_6**

| Datum | Value         |
|-------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.130865 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.991997 |
**Number of Imaginary Frequencies**

1

**Frequencies** (Top 3 out of 60)

1. -942.8719 cm\(^{-1}\)
2. 38.3853 cm\(^{-1}\)
3. 62.9647 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |   |   |   |
|---|---|---|---|
| C | -1.000302 | -1.813533 | 0.025984 |
| C | 0.082808  | -1.009233 | 0.395765 |
| C | 1.146458  | -0.841372 | -0.670801 |
| O | -1.305411 | -2.177780 | -1.134652 |
| C | 0.449702  | -0.897705 | 1.852061 |
| H | 1.558456  | -1.810342 | -0.971562 |
| H | 0.714673  | -0.400524 | -1.572976 |
| C | 1.892210  | 1.778756  | -0.095519 |
| H | 1.193155  | 1.837479  | 0.736190  |
| H | 1.376687  | 2.042943  | -1.017995 |
| H | 2.711084  | 2.475359  | 0.071414  |
| S | 2.608446  | 0.131116  | -0.230282 |
| H | -1.676217 | -2.095225 | 0.858625  |
| H | -0.734940 | 0.321313  | 0.126427  |
| S | -1.524169 | 1.599374  | -0.169067 |
| C | -3.123299 | 0.797989  | 0.137974  |
| H | -3.633649 | 0.562220  | -0.793501 |
| H | -2.955745 | -0.130197 | 0.686059  |
| H | -3.759458 | 1.444096  | 0.738247  |
| H | 0.732982  | 0.120736  | 2.133401  |
| H | -0.405736 | -1.178460 | 2.470153  |
| H | 1.288102  | -1.544400 | 2.129533  |

**methy lacrolein_protonation_TS_7**

**Datum** | **Value**
---|---
M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.130916
M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.991613
Number of Imaginary Frequencies | 1
**Frequencies** (Top 3 out of 60)

1. -948.0305 cm⁻¹
2. 49.9439 cm⁻¹
3. 67.8978 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  |  |  |
|---|---|---|
| C  | -0.018582 | 1.222970 | 1.169594 |
| C  | -0.173211 | 1.175408 | -0.219399 |
| C  | -1.380755 | 0.582251 | -0.905635 |
| O  | 0.837390  | 1.881524 | 1.810611  |
| C  | 0.531968  | 2.198670 | -1.073506 |
| H  | -2.054250 | 1.372386 | -1.255093 |
| H  | -1.060742 | 0.037657 | -1.802348 |
| C  | -1.364371 | -1.917536| 0.322918  |
| H  | -0.609674 | -1.664120| 1.062942  |
| H  | -0.873779 | -2.215062| -0.602504 |
| H  | -1.972551 | -2.739759| 0.693531  |
| S  | -2.471321 | -0.527695| 0.020690  |
| H  | -0.688821 | 0.553971 | 1.738662  |
| H  | 0.897097  | 0.084564 | -0.463439 |
| S  | 2.035962  | -0.861830| -0.874399 |
| C  | 2.096380  | -1.638886| 0.766894  |
| H  | 3.128119  | -1.734574| 1.097615  |
| H  | 1.560637  | -1.011701| 1.480588  |
| H  | 1.636966  | -2.625504| 0.754834  |
| H  | 1.413541  | 2.576705 | -0.557836 |
| H  | 0.857227  | 1.760105 | -2.023521 |
| H  | -0.115722 | 3.048272 | -1.314182 |

**methylacrolein_protonation_TS_8**

| Datum | Value             |
|-------|------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1108.130689 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1107.992128 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 60)
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | 0.407338 | 1.810054 | 0.715651 |
| C    | -0.273551 | 1.192797 | -0.354575 |
| C    | -1.677688 | 0.721618 | -0.093465 |
| O    | 0.123905 | 1.770489 | 1.928422 |
| C    | 0.003948 | 1.661808 | -1.763102 |
| H    | -1.965769 | 0.944225 | 0.934078 |
| H    | -2.380701 | 1.229045 | -0.758742 |
| C    | -1.237835 | -1.704547 | 1.127162 |
| H    | -1.751137 | -1.346271 | 2.017982 |
| H    | -0.192546 | -1.401607 | 1.147016 |
| H    | -1.294021 | -2.790464 | 1.089773 |
| S    | -2.028741 | -1.054150 | -0.354668 |
| H    | 1.335254 | 2.338328 | 0.412378 |
| H    | 0.692092 | 0.017517 | -0.472138 |
| S    | 1.786401 | -1.076936 | -0.811672 |
| C    | 2.697585 | -0.744228 | 0.725739 |
| H    | 3.737038 | -1.043328 | 0.608970 |
| H    | 2.671092 | 0.321250 | 0.952565 |
| H    | 2.271789 | -1.289326 | 1.567361 |
| H    | -0.706127 | 2.427176 | -2.091977 |
| H    | 1.011553 | 2.073300 | -1.846490 |
| H    | -0.061094 | 0.828595 | -2.471182 |

methylacrylate_protonation_TS_10

| Datum                                          | Value       |
|------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy          | -1183.375966|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.233336|

Number of Imaginary Frequencies

Frequencies (Top 3 out of 63)

| Frequency | Unit  |
|-----------|-------|
| -965.9366 | cm⁻¹  |
| 18.0541   | cm⁻¹  |
| 46.1626   | cm⁻¹  |
M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |   |   |
|---|---|---|
| C | -0.048542 | 0.983074 | 0.509377 |
| C | 0.207931  | -0.060711 | -0.404834 |
| C | 1.095219  | -1.177656 | 0.030203  |
| O | 0.171735  | 0.969952  | 1.725991  |
| H | 0.201697  | 0.158453  | -1.463485 |
| H | 0.799112  | -2.129512 | -0.419438 |
| H | 1.049471  | -1.292721 | 1.112542  |
| C | 3.261206  | 0.535787  | 0.365162  |
| H | 4.297338  | 0.769621  | 0.130980  |
| H | 3.139586  | 0.453214  | 1.443098  |
| H | 2.617484  | 1.328844  | -0.011203 |
| S | 2.861169  | -1.023306 | -0.441868 |
| O | -0.681474 | 2.126278  | 0.062699  |
| C | -1.080102 | 2.222045  | -1.290804 |
| H | -1.158869 | -0.896182 | -0.295455 |
| S | -2.417116 | -1.709141 | -0.106827 |
| C | -3.380899 | -0.239796 | 0.368806  |
| H | -4.069246 | -0.493586 | 1.171390  |
| H | -2.703275 | 0.536114  | 0.722712  |
| H | -3.951172 | 0.147774  | -0.472661 |
| H | -1.733153 | 1.392286  | -1.569395 |
| H | -1.625488 | 3.157620  | -1.385356 |
| H | -0.219308 | 2.240927  | -1.961598 |

methylacrylate_protonation_TS_11_reopt

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1183.375213   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.231854  |

Number of Imaginary Frequencies

| Frequencies (Top 3 out of 63) |
|--------------------------------|
| 1. -1139.4638 cm⁻¹            |
| 2. 48.2610 cm⁻¹               |
| 3. 55.9449 cm⁻¹               |

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates
### methylacrylate_protonation_TS_12_reopt

| Datum | Value               |
|-------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1183.376546       |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.234796       |

#### Number of Imaginary Frequencies

1

#### Frequencies (Top 3 out of 63)

| Frequency | Value (cm⁻¹) |
|-----------|--------------|
| 1.        | -862.5931    |
| 2.        | 32.5350      |
| 3.        | 43.0538      |

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C      | -0.536903 | 1.029010 | 0.701114 |
| C      | -0.144751 | -0.171089| 0.987178 |
| C      | -1.193936 | -0.724097| 0.086896 |
### methylacrylate_protonation_TS_13

| Datum                                      | Value          |
|--------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1183.375235   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.233378  |
| Number of Imaginary Frequencies            | 1              |

**Frequencies (Top 3 out of 63)**

1.  -1047.0807 cm⁻¹
2.     33.2710 cm⁻¹
3.     42.1065 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|         |          |          |          |
|---------|----------|----------|----------|
| C       | 0.882790 | -1.231648| -0.185473|
| C       | -0.056263| -0.531671| -0.971850|
| C       | -1.444448| -1.075025| -1.076604|
| O       | 0.665796 | -2.064732| 0.699482 |
| H       | 0.346183 | -0.032404| -1.845743|
| H       | -1.511922| -2.051590| -0.595968|
| H       | -1.762643| -1.189776| -2.113308|
### methylacrylate_protonation_TS_14

| Datum                                                   | Value                  |
|---------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -1183.377904           |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.236272           |

Number of Imaginary Frequencies: 1

**Frequencies** (Top 3 out of 63)

1. -915.0001 cm⁻¹
2. 44.4193 cm⁻¹
3. 48.6996 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     |       |       |       |     |     |     |
|-----|-------|-------|-------|-----|-----|-----|
| C   | -2.331470 | -0.218761 | 1.398098 |
| H   | -2.465730 | -1.244200 | 1.738440 |
| H   | -2.971502 | 0.441608  | 1.979216 |
| H   | -1.291448 | 0.072991  | 1.533204 |
| S   | -2.791524 | -0.060599 | -0.336263 |
| O   | 2.178109  | -0.830665 | -0.427326 |
| C   | 3.160291  | -1.342580 | 0.455549 |
| H   | 0.032284  | 0.814420  | -0.060190 |
| S   | 0.354994  | 2.136679  | 0.618381 |
| C   | 1.510672  | 2.625334  | -0.697608 |
| H   | 0.975704  | 2.981079  | -1.576017 |
| H   | 2.154265  | 3.423724  | -0.335457 |
| H   | 2.125163  | 1.771339  | -0.975454 |
| H   | 4.107424  | -0.914893 | 0.136978 |
| H   | 2.953691  | -1.050632 | 1.485438 |
| H   | 3.212592  | -2.429670 | 0.405069 |
methylacrylate_protonation_TS_15

| Datum                                                   | Value       |
|---------------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                   | -1183.37358 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.230813 |
| Number of Imaginary Frequencies                        | 1           |

Frequencies (Top 3 out of 63)

1. -1033.2368 cm\(^{-1}\)
2. 38.2393 cm\(^{-1}\)
3. 49.6542 cm\(^{-1}\)

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C   | -1.470792 | -0.736636 | -0.551259 |
| C   | -0.272684 | -0.215115 | -1.086370 |
| C   | -0.075147 | 1.252717  | -1.301032 |
| O   | -1.824660 | -1.921001 | -0.543300 |
| H   | 0.193466  | -0.872873 | -1.811146 |
| H   | -1.006637 | 1.807201  | -1.193378 |
| H   | 0.317547  | 1.457385  | -2.297475 |
| C   | 0.273402  | 1.903484  | 1.368936  |
| H   | 0.074052  | 0.848433  | 1.546502  |
| H   | -0.662937 | 2.458695  | 1.365388  |
| H   | 0.920680  | 2.286067  | 2.155425  |
| S   | 1.135043  | 2.009846  | -0.199387 |
| O   | -2.252434 | 0.197514  | 0.884088  |
| C   | -3.418282 | -0.297751 | 0.721966  |
| H   | 0.665802  | -0.830327 | 0.079340  |
### methylacrylate_protonation_TS_1_reopt

| Datum                                      | Value               |
|--------------------------------------------|---------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1183.376885        |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.234779 |
| Number of Imaginary Frequencies            | 1                   |

**Frequencies** (Top 3 out of 63)

1. -878.4689 cm⁻¹
2. 29.0385 cm⁻¹
3. 41.8408 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|    | 0.126431 | 0.840243 | 0.678655 |
|----|----------|----------|----------|
| C  | -0.194605| -0.530739| 0.700669 |
| C  | -0.961880| -1.196652| -0.384775|
| O  | 0.619328 | 1.504719 | 1.599395 |
| H  | -0.283108| -0.948313| 1.697665 |
| H  | -0.697474| -2.252926| -0.474408|
| H  | -0.765166| -0.726617| -1.347141|
| C  | -3.157159| 0.499864 | -0.049937|
| H  | -2.589163| 0.942496 | 0.766693 |
| H  | -4.220805| 0.602492 | 0.153165 |
| H  | -2.911794| 1.011425 | -0.978243|
| S  | -2.793978| -1.259583| -0.170656|
| O  | -0.076021| 1.446407 | -0.544845|
| C  | 0.419396 | 2.766121 | -0.669361|
| H  | 1.322887 | -1.128462| 0.437610 |
| S  | 2.698962 | -1.590943| 0.086219 |
| C  | 3.116624 | -0.006507| -0.703805|
| H  | 3.527955 | 0.697201 | 0.016784 |
| H  | 3.848004 | -0.174062| -1.490703|
**SI_protonation_extension.md**

**methylacrylate_protonation_TS_2**

| Datum | Value         |
|-------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1183.378412 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.23601 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 63)

1. -778.6910 cm⁻¹
2. 37.6889 cm⁻¹
3. 50.6403 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|  | x   | y   | z   |
|---|-----|-----|-----|
| H | 2.218606 | 0.423782 | -1.144412 |
| H | 1.500127 | 2.795488 | -0.521616 |
| H | 0.179615 | 3.086596 | -1.680084 |
| H | -0.048719 | 3.436337 | 0.050592 |

|  | x   | y   | z   |
|---|-----|-----|-----|
| C | -0.159654 | 0.894876 | 0.041148 |
| C | 0.289642 | -0.262466 | -0.620446 |
| C | 1.204716 | -1.196264 | 0.087991 |
| O | -0.175835 | 1.116782 | 1.257638 |
| H | 0.352616 | -0.212523 | -1.700720 |
| H | 1.045089 | -2.237186 | -0.206385 |
| H | 1.043426 | -1.129998 | 1.164131 |
| C | 3.181410 | 0.746956 | 0.349582 |
| H | 2.508545 | 1.396910 | -0.207275 |
| H | 4.209764 | 1.050115 | 0.166373 |
| H | 2.964057 | 0.825397 | 1.413000 |
| S | 3.003752 | -0.953360 | -0.215626 |
| O | -0.703745 | 1.831784 | -0.818210 |
| C | -1.368813 | 2.918204 | -0.201166 |
| H | -1.052091 | -1.192403 | -0.340076 |
| S | -2.263188 | -1.979340 | 0.012354 |
| C | -3.279001 | -0.479226 | 0.175541 |
| H | -2.843123 | 0.314894 | -0.427427 |
| H | -4.287634 | -0.676164 | -0.17391 |
| H | -3.325763 | -0.147326 | 1.212399 |
| H | -0.691621 | 3.493599 | 0.429055 |
| H | -1.741922 | 3.544685 | -1.007374 |
| H | -2.203526 | 2.572183 | 0.410711 |
methylacrylate_protonation_TS_3_reopt

| Datum                                           | Value       |
|-------------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy            | -1183.376267|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.234537|
| Number of Imaginary Frequencies                 | 1           |

**Frequencies (Top 3 out of 63)**

1. -857.6460 cm\(^{-1}\)
2. 28.9630 cm\(^{-1}\)
3. 38.3391 cm\(^{-1}\)

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|       |       |       |       |
|-------|-------|-------|-------|
| C     | 0.296431 | 0.907042 | 0.695218 |
| C     | -0.312173 | -0.359648 | 0.601763 |
| C     | -1.102310 | -0.774430 | -0.586333 |
| O     | 0.860463  | 1.396111  | 1.681555  |
| H     | -0.561983 | -0.806311 | 1.556694  |
| H     | -1.204127 | -1.860712 | -0.626246 |
| H     | -0.623538 | -0.455257 | -1.511614 |
| C     | -3.526887 | -0.819581 | 0.761137  |
| H     | -3.475599 | -1.907215 | 0.729157  |
| H     | -4.568954 | -0.513586 | 0.817012  |
| H     | -3.000653 | -0.455259 | 1.641404  |
| S     | -2.819787 | -0.107474 | -0.734676 |
| O     | 0.298243  | 1.609783  | -0.491597 |
| C     | 1.083731  | 2.787383  | -0.509311 |
| H     | 1.063580  | -1.261216 | 0.385531  |
| S     | 2.335744  | -1.970772 | 0.062113  |
| C     | 3.100247  | -0.464038 | -0.611403 |
| H     | 2.336398  | 0.145012  | -1.092055 |
| H     | 3.575625  | 0.121075  | 0.173066  |
| H     | 3.848959  | -0.737291 | -1.351022 |
| H     | 2.134261  | 2.560140  | -0.321295 |
| H     | 0.973342  | 3.212210  | -1.503727 |
| H     | 0.743487  | 3.502817  | 0.238018  |
### methylacrylate_protonation_TS_6_reopt

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                      | -1183.374595  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.232044  |
| Number of Imaginary Frequencies                            | 1             |

#### Frequencies (Top 3 out of 63)

1. -999.3999 cm⁻¹
2. 29.1736 cm⁻¹
3. 52.6002 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.410618  | -0.906462 | 0.086721  |
| C | 0.121516  | -0.990884 | -0.480275|
| C | -0.967389 | -1.620133 | 0.325770 |
| O | 1.729731  | -0.976450 | 1.277750 |
| H | 0.097779  | -1.147343 | -1.552460|
| H | -0.616368 | -1.817963 | 1.338490 |
| H | -1.305514 | -2.566776 | -0.101953|
| C | -2.941102 | -0.380588 | -1.158223|
| H | -3.870711 | 0.183641  | -1.187014|
| H | -3.089164 | -1.338301 | -1.656041|
| H | -2.162285 | 0.186969  | -1.664859|
| S | -2.494310 | -0.626808 | 0.568363 |
| O | 2.380586  | -0.629859 | -0.851800|
| C | 3.668898  | -0.334543 | -0.342439|
| H | -0.024887 | 0.637001  | -0.575199|
| S | -0.095093 | 2.152406  | -0.577814|
| C | -0.029285 | 2.266318  | 1.235751 |
| H | -0.507317 | 3.188204  | 1.559775 |
| H | -0.568360 | 1.421818  | 1.662177 |
| H | 0.997138  | 2.256712  | 1.596092 |
| H | 4.080431  | -1.178352 | 0.210528 |
| H | 4.294969  | -0.121685 | -1.205068|
| H | 3.642661  | 0.534729  | 0.315318 |

### methylacrylate_protonation_TS_7

| Datum                                                      | Value         |
|------------------------------------------------------------|---------------|
| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1183.376105|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.232545|
| Number of Imaginary Frequencies            | 1           |

**Frequencies** (Top 3 out of 63)

1. -1058.2632 cm⁻¹
2. 50.5981 cm⁻¹
3. 59.1614 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1183.377721|

**methylacrylate_protonation_TS_9_reopt**

| Datum                                      | Value       |
|--------------------------------------------|-------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy      | -1183.377721|
### M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)

| Datum | Value   |
|-------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1183.236608 |

### Number of Imaginary Frequencies

1

### Frequencies (Top 3 out of 63)

1.  -770.8678 cm⁻¹
2.   25.0740 cm⁻¹
3.   31.7548 cm⁻¹

### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 0.299820| 1.205280| 0.078228|
| C    | 0.047022| -0.078924| -0.433247|
| C    | 0.510225| -1.273751| 0.318711|
| O    | 0.620336| 1.515520| 1.232234|
| H    | -0.070768| -0.165310| -1.506770|
| H    | -0.167073| -2.123572| 0.203030|
| H    | 0.572552| -1.045061| 1.382727|
| C    | 3.187333| -0.534115| 0.102527|
| H    | 2.816961| 0.317929| -0.464991|
| H    | 4.190767| -0.784034| -0.234648|
| H    | 3.212336| -0.281391| 1.160744|
| S    | 2.139071| -1.968942| -0.188753|
| O    | 0.051841| 2.206211| -0.840086|
| C    | 0.153482| 3.531582| -0.351608|
| H    | -1.523026| -0.089988| 0.118827|
| S    | -2.920815| -0.386733| 0.523374|
| C    | -3.060045| -1.757956| -0.662656|
| H    | -2.296882| -1.641332| -1.431911|
| H    | -2.921217| -2.718612| -0.171560|
| H    | -4.037835| -1.742190| -1.137549|
| H    | -0.079775| 4.182919| -1.189975|
| H    | -0.552008| 3.710324| 0.459669|
| H    | 1.159430| 3.744570| 0.009566|

### methyltiglate_protonation_TS_1_reopt

| Datum | Value   |
|-------|---------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1261.99563 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1261.800001 |
| Datum                                           | Value          |
|------------------------------------------------|----------------|
| Number of Imaginary Frequencies                | 1              |

**Frequencies** (Top 3 out of 81)

1. -693.8495 cm⁻¹  
2. 33.4657 cm⁻¹  
3. 43.7981 cm⁻¹  

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

```
C           0.310638        0.988741       -0.251810  
C          -0.248789       -0.156170        0.351040  
C          -1.272408       -0.890723       -0.452600  
O           0.311498        1.293361       -1.454590  
C          -0.315179       -0.263281        1.852440  
H          -1.118698       -0.652532       -1.503930  
C          -1.277585       -2.406543       -0.277950  
C          -2.833452        1.435144       -0.108510  
H          -2.146123        1.758956        0.671700  
H          -3.814323        1.870402        0.070740  
H          -2.458563        1.765745       -1.074910  
S          -3.022479       -0.355366       -0.076550  
O           0.985307        1.805512        0.635230  
C           1.708265        2.877394        0.061660  
H           1.112303       -1.102888        0.077250  
S           2.367884       -1.872855       -0.090760  
C           3.395661       -0.376353       -0.201280  
C           3.369240       0.182697        0.731440  
H           4.421412       -0.671041       -0.409780  
H           3.041630       0.264256       -1.006380  
H           2.173834       3.407185        0.889200  
H           2.478325       2.515465       -0.620570  
H           1.051003       3.553072       -0.484790  
H          -1.132150       0.322568        2.293630  
H          -0.468737       -1.300241        2.160670  
H           0.613640       0.073401        2.311760  
H          -2.063114       -2.867604       -0.878440  
H          -0.320054       -2.820691       -0.596030  
H          -1.443464       -2.687453        0.762330
```
| Datum                                                                 | Value         |
|----------------------------------------------------------------------|--------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -1261.995398 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)          | -1261.800611 |
| Number of Imaginary Frequencies                                      | 1            |
| **Frequencies** (Top 3 out of 81)                                    |              |
| 1.  -819.7602 cm\(^{-1}\)                                           |              |
| 2.   17.6361 cm\(^{-1}\)                                            |              |
| 3.  38.8570 cm\(^{-1}\)                                            |              |
| **M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian**   |              |
| **Coordinates**                                                      |              |
| C          | 0.283495 | 0.989773 | 0.514684 |
| C          | -0.196050| -0.338950| 0.501949 |
| C          | -1.026111| -0.825645| -0.639927|
| O          | 0.822556 | 1.582585 | 1.459174 |
| C          | -0.391926| -1.013170| 1.834289 |
| H          | -0.751768| -0.292401| -1.546307|
| C          | -0.918758| -2.326814| -0.890915|
| C          | -2.877752| 1.130785 | 0.300456 |
| H          | -3.919753| 1.401552 | 0.458582 |
| H          | -2.410508| 1.854219 | -0.363554|
| H          | -2.357342| 1.129812 | 1.257047 |
| S          | -2.863579| -0.518484| -0.423252|
| O          | 0.194963 | 1.635067 | -0.703644|
| C          | 0.813699 | 2.904888 | -0.775092|
| H          | 1.300303 | -0.967027| 0.218704 |
| S          | 2.695598 | -1.476280| 0.045834 |
| C          | 3.254417 | 0.105409 | -0.659605|
| H          | 3.245476 | 0.886353 | 0.097843 |
| H          | 4.266558 | -0.013453| -1.038918|
| H          | 2.603590 | 0.405656 | -1.478580|
| H          | 0.635137 | 3.273279 | -1.782326|
| H          | 0.387424 | 3.596229 | -0.048757|
| H          | 1.887274 | 2.830438 | -0.596859|
| H          | 0.020932 | -2.028625| 1.847861 |
| H          | 0.108907 | -0.447091| 2.617446 |
| H          | -1.452974| -1.097578| 2.098924 |
| H          | -1.557314| -2.634628| -1.720336|
| H          | 0.112321 | -2.586725| -1.133650|
| H          | -1.216810| -2.892657| -0.007701|
**methyltiglate_protonation_TS_3_reopt**

| Datum                                                        | Value           |
|--------------------------------------------------------------|-----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                        | -1261.991964    |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)  | -1261.795405    |

Number of Imaginary Frequencies

**Frequencies (Top 3 out of 81)**

1. -407.1640 cm⁻¹
2. 40.1474 cm⁻¹
3. 46.2775 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.223820 | 0.946490 | 0.685121 |
| C     | 0.182719 | -0.397790 | 0.618361 |
| C     | 0.952799 | -1.021370 | -0.501849 |
| O     | -0.753180 | 1.506890 | 1.660341 |
| C     | 0.286739 | -1.120620 | 1.936861 |
| H     | 0.776689 | -2.100600 | -0.437169 |
| C     | 0.631189 | -0.599070 | -1.932429 |
| C     | 3.033690 | 0.768269 | 0.128651 |
| H     | 2.687900 | 1.391789 | -0.693139 |
| H     | 4.097640 | 0.931978 | 0.285911 |
| H     | 2.487670 | 1.032349 | 1.033531 |
| S     | 2.805199 | -0.978641 | -0.243519 |
| O     | -0.064930 | 1.677820 | -0.476329 |
| C     | -0.671310 | 2.955100 | -0.488799 |
| H     | -1.355571 | -1.036320 | 0.284561 |
| S     | -2.687941 | -1.553549 | -0.008499 |
| C     | -3.217541 | 0.029351 | -0.731209 |
| H     | -3.684840 | 0.665711 | 0.017051 |
| H     | -2.347151 | 0.543141 | -1.137699 |
| H     | -3.927121 | -0.155299 | -1.533819 |
| H     | -0.262669 | 3.601130 | 0.287501 |
| H     | -0.461770 | 3.380270 | -1.467619 |
| H     | -1.750720 | 2.881380 | -0.345939 |
| H     | -0.482021 | -0.776220 | 2.627371 |
| H     | 0.152759 | -2.198820 | 1.795621 |
| H     | 1.259479 | -0.893831 | 2.425481 |
| H     | 1.080669 | -1.316671 | 2.631409 |
| H     | -0.451241 | -0.573090 | -2.076549 |
| H     | 1.022269 | 0.388319 | -2.161599 |
**methyltiglate_protonation_TS_4_reopt**

| Datum                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                                | -1261.992008   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic)           | -1261.796031   |
| Number of Imaginary Frequencies                                      | 1              |

**Frequencies** (Top 3 out of 81)

1. -478.5907 cm⁻¹
2.  20.9729 cm⁻¹
3.  49.6857 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|     | X     | Y     | Z     |
|-----|-------|-------|-------|
| C   | -0.229769 | 1.025769 | -0.182711 |
| C   | 0.212720  | -0.113752 | 0.514549  |
| C   | 1.124090  | -1.108342 | -0.130911 |
| O   | -0.152608 | 1.291409  | -1.390981 |
| C   | 0.256490  | -0.101992 | 2.022099  |
| H   | 0.994729  | -2.059992 | 0.397029  |
| C   | 0.927059  | -1.370282 | -1.619271 |
| C   | 2.995891  | 0.983476  | -0.177901 |
| H   | 4.035032  | 1.298165  | -0.110041 |
| H   | 2.397002  | 1.548927  | 0.534779  |
| H   | 2.621541  | 1.169306  | -1.182551 |
| S   | 2.932440  | -0.774434 | 0.209959  |
| O   | -0.891228 | 1.931529  | 0.639609  |
| C   | -1.491467 | 3.030010  | -0.015681 |
| H   | -1.194220 | 1.043151  | 0.424779  |
| S   | -2.440961 | -1.812779 | 0.396799  |
| C   | -3.231700 | -0.602019 | -0.705471 |
| H   | -4.306610 | -0.764968 | -0.697381 |
| H   | -3.024439 | 0.406541  | -0.352541 |
| H   | -2.865570 | -0.702879 | -1.724751 |
| H   | -0.753837 | 3.628319  | -0.550831 |
| H   | -2.250497 | 2.702980  | -0.729171 |
| H   | -1.957597 | 3.631120  | 0.760579  |
| H   | 1.146441  | 0.398308  | 2.424509  |
| H   | -0.618409 | 0.386799  | 2.447299  |
| H   | 0.276640  | -1.129602 | 2.400929  |
| H   | 1.479169  | -2.262343 | -1.915511 |
| H   | -0.133921 | -1.524731 | -1.828661 |
| H   | 1.261690  | -0.528093 | -2.218411 |
# methyltiglate_protonation_TS_5

| Datum                                                      | Value                  |
|------------------------------------------------------------|------------------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                       | -1261.99038            |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1261.795169           |
| Number of Imaginary Frequencies                           | 1                      |

**Frequencies** (Top 3 out of 81)

1. -725.4892 cm⁻¹
2. 39.1792 cm⁻¹
3. 43.0756 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|   |        |        |        |
|---|--------|--------|--------|
| C | 1.51532| -0.694738 | -0.319497 |
| C | 0.353065 | -0.643826 | 0.460380 |
| C | -0.927940 | -0.907891 | -0.296733 |
| O | 1.590941 | -0.679845 | -1.560865 |
| C | 0.370546 | -0.932486 | 1.939050 |
| H | -0.893887 | -0.358996 | -1.239822 |
| C | -1.148637 | -2.390666 | -0.594368 |
| C | -3.598498 | -0.218283 | -0.674322 |
| H | -4.488591 | 0.261765 | -0.273590 |
| H | -3.854183 | -1.230717 | -0.978437 |
| H | -3.250232 | 0.346122 | -1.538825 |
| S | -2.349127 | -0.205606 | 0.625721 |
| O | 2.690798 | -0.660213 | 0.411082 |
| C | 3.880300 | -0.528554 | -0.343622 |
| H | 0.481950 | 1.033732 | 0.493567 |
| S | 0.515241 | 2.521351 | 0.490242 |
| C | -0.561105 | 2.685855 | -0.966265 |
| H | -0.788341 | 3.738952 | -1.115609 |
| H | -0.071232 | 2.303565 | -1.859127 |
| H | -1.490006 | 2.141709 | -0.803466 |
| H | 4.016836 | -1.369174 | -1.023667 |
| H | 3.880395 | 0.392465 | -0.927050 |
| H | 4.694969 | -0.504777 | 0.376206 |
| H | 0.022677 | -1.944085 | 2.181724 |
| H | 1.374829 | -0.825714 | 2.342727 |
| H | -0.276052 | -0.239748 | 2.489858 |
| H | -2.084731 | -2.578084 | -1.122389 |
### methyltiglate_protonation_TS_6_reopt

| Datum                                             | Value          |
|--------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy             | -1261.995126   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1261.799784   |
| Number of Imaginary Frequencies                   | 1              |

#### Frequencies (Top 3 out of 81)

1. -741.6843 cm⁻¹
2.  30.0098 cm⁻¹
3.  40.2793 cm⁻¹

#### M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

|      |       |       |       |
|------|-------|-------|-------|
| C    | -0.144500 | 1.277300 | -0.279488 |
| C    | -0.130199 | -0.036990 | 0.227772 |
| C    | -0.871418 | -1.062590 | -0.566018 |
| O    | -0.393300 | 1.647310 | -1.437048 |
| C    |  0.034711 | -0.260080 | 1.710402 |
| H    | -0.976199 | -0.697250 | -1.586438 |
| C    | -0.239548 | -2.450740 | -0.596248 |
| C    | -3.176209 |  0.375269 |  0.171762 |
| H    | -2.588780 |  0.913619 |  0.914022 |
| H    | -4.219079 |  0.355208 |  0.480932 |
| H    | -3.090289 |  0.881639 | -0.787568 |
| S    | -2.615378 | -1.330971 |  0.040972 |
| O    |  0.273200 |  2.219120 |  0.639342 |
| C    |  0.449919 |  3.532970 |  0.141692 |
| H    |  1.464871 | -0.176969 | -0.290028 |
| S    |  2.907561 | -0.376768 | -0.597078 |
| C    |  3.161862 | -1.622628 |  0.702412 |
| H    |  2.366042 | -2.364649 |  0.673702 |
| H    |  4.111402 | -2.123178 |  0.528042 |
| H    |  3.181892 | -1.163028 |  1.687882 |
| H    |  0.782439 |  4.134271 |  0.984152 |
| H    |  1.201479 |  3.559831 | -0.647378 |
| H    | -0.482281 |  3.936380 | -0.252678 |
| H    | -0.833879 |  0.064990 |  2.297472 |
| H    |  0.183982 | -1.319430 |  1.926552 |
methyltiglate_protonation_TS_7_reopt

| Datum                                                | Value          |
|------------------------------------------------------|----------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy                | -1261.994203   |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1261.798487   |
| Number of Imaginary Frequencies                      | 1              |

**Frequencies** (Top 3 out of 81)

1.  -768.7556 cm⁻¹  
2.   34.4900 cm⁻¹  
3.   44.7793 cm⁻¹  

M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates

| C     | -0.631339 | -1.056821 | -0.111015 |
|-------|-----------|-----------|-----------|
| C     | 0.092307  | -0.065563 | 0.578511  |
| C     | 1.307117  | 0.472371  | -0.116941 |
| O     | -0.529914 | -1.360068 | -1.309533 |
| C     | 0.021994  | 0.079082  | 2.077397  |
| H     | 1.110982  | 0.522022  | -1.189236 |
| C     | 1.739003  | 1.842945  | 0.388037  |
| C     | 3.995878  | 0.017431  | -0.927060 |
| H     | 4.432810  | 0.878545  | -0.426621 |
| H     | 3.601450  | 0.320345  | -1.896575 |
| H     | 4.770966  | -0.729999 | -1.082591 |
| S     | 2.689984  | -0.747910 | 0.060557  |
| O     | -1.604822 | -1.677966 | 0.647937  |
| C     | -2.466766 | -2.553248 | -0.052497 |
| H     | -0.954078 | 1.131002  | 0.121458  |
| S     | -1.925418 | 2.189206  | -0.276259 |
| C     | -3.232031 | 0.980285  | -0.653335 |
| H     | -4.103884 | 1.511684  | -1.027476 |
| H     | -2.889759 | 0.279685  | -1.412124 |
| H     | -3.512275 | 0.423751  | 0.238393  |
| H     | -3.158346 | -2.953074 | 0.685120  |
| H     | -3.023520 | -2.024225 | -0.827014 |
| H     | -1.913756 | -3.368355 | -0.518052 |
methyltiglate_protonation_TS_8_reopt

| Datum | Value |
|-------|-------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy | -1261.991981 |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1261.796391 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 81)

1. -854.1472 cm⁻¹
2. 12.8854 cm⁻¹
3. 37.4884 cm⁻¹

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

| C     | 0.396893 | 0.995141 | 0.644963 |
|-------|----------|----------|----------|
| C     | -0.219863| -0.269602| 0.565895 |
| C     | -0.996953| -0.661136| -0.657079|
| O     | 0.944212 | 1.512026 | 1.630295 |
| C     | -0.440747| -1.025360| 1.852881 |
| H     | -0.432276| -0.389626| -1.551000|
| C     | -1.296707| -2.156234| -0.701360|
| C     | -3.352642| 0.223366 | 0.669766 |
| H     | -4.291111| 0.766841 | 0.594056 |
| H     | -2.719602| 0.705582 | 1.412262 |
| H     | -3.562642| -0.800872| 0.973555 |
| S     | -2.572596| 0.290689 | -0.952702|
| O     | 0.444758 | 1.659351 | -0.562964|
| C     | 1.188374 | 2.862111 | -0.577472|
| H     | 1.178645 | -1.003551| 0.177157 |
| S     | 2.471835 | -1.692770| -0.152662|
| C     | 3.284510 | -0.134318| -0.626549 |
| H     | 2.821258 | 0.291450 | -1.514021 |
| H     | 3.217692 | 0.587167 | 0.185233 |
| H     | 4.332646 | -0.334631| -0.836431 |
| H     | 1.111551 | 3.254479 | -1.588558 |
### methyltiglate_protonation_TS_9_reopt

| Datum                                              | Value         |
|----------------------------------------------------|---------------|
| M06-2X/def2tzvpp-IEFPCM(water) Energy              | -1261.989248  |
| M06-2X/def2tzvpp-IEFPCM(water) Free Energy (Quasiharmonic) | -1261.792692  |
| Number of Imaginary Frequencies                    | 1             |

**Frequencies (Top 3 out of 81)**

1. -1009.6959 cm$^{-1}$
2. 38.6576 cm$^{-1}$
3. 45.4220 cm$^{-1}$

**M06-2X/def2tzvpp-IEFPCM(water) Molecular Geometry in Cartesian Coordinates**

|           | X     | Y     | Z     |
|-----------|-------|-------|-------|
| C         | 0.938151 | -1.236577 | 0.277975 |
| C         | -0.138681 | -0.468832 | 0.775850 |
| C         | -1.531645 | -0.710002 | 0.255500 |
| O         | 2.040404 | -1.409486 | 0.812877 |
| C         | -0.024012 | -0.008120 | 2.208526 |
| H         | -1.491118 | -1.380486 | -0.599819 |
| C         | -2.479583 | -1.307370 | 1.297463 |
| C         | -1.598357 | 0.830108 | -2.047313 |
| H         | -0.520590 | 0.730111 | -1.938821 |
| H         | -1.822384 | 1.785202 | -2.517625 |
| H         | -1.987018 | 0.022137 | -2.665034 |
| S         | -2.369219 | 0.804517 | -0.417072 |
| O         | 0.725455 | -1.766974 | -0.979912 |
| C         | 1.828674 | -2.435526 | -1.561601 |
| H         | 0.418315 | 0.931133 | 0.186205 |
| S         | 0.972537 | 2.320574 | -0.103712 |
| C         | 2.708976 | 1.927870 | 0.275044 |
| H         | 2.828260 | 1.664565 | 1.323716 |
| H         | 3.057566 | 1.096740 | -0.333048 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | 3.319889| 2.802691| 0.060915|
| H       | 2.141490| -3.287112| -0.957884|
| H       | 1.494184| -2.780895| -2.536678|
| H       | 2.679390| -1.764271| -1.681738|
| H       | 0.986212| 0.345245 | 2.414548 |
| H       | -0.704184| 0.829321 | 2.390373 |
| H       | -0.260288| -0.786151| 2.943497 |
| H       | -3.436506| -1.568930| 0.848844 |
| H       | -2.034862| -2.200040| 1.733104 |
| H       | -2.669453| -0.600192| 2.109603 |