Electronically supplementary information

Computational Elucidation of the Reaction Mechanism for Synthesis of Pyrrolidinedione Derivatives via Nef-type Rearrangement – Cyclization Reaction

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Figure S1. Structures of reaction complexes, transition states and intermediates for Michael addition of nitromethane, CH₃NO₂ (a), and deprotonated nitromethane, CH₂NO₂⁻ (b), to coumarin 1 (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
Figure S2. Structures of reaction complexes, transition states and intermediates for O-atom migration assisted by a water molecule (a) and assisted by a water molecule in acidic solution (b). (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
Figure S3. Structures of reaction complexes, transition states and intermediates for O-atom migration via formation of a three-membered oxaziridine cycle. (only $\sigma$-skeleton is shown; interatomic distances in Å, angles in degrees).
**Figure S4.** Structures of reaction complexes, transition states and intermediates for O-atom migration via formation of a three-membered oxaziridine cycle, assisted by trimethylamine. (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).

**Figure S5.** Structures of reaction complexes, transition states and intermediates for the transformation between different tautomeric forms of the nitrosohydroxymethyl group in intermediate 6. (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
Figure S6. Structures of reaction complexes, transition states and intermediates for formation of pyrrolidine ring from intermediate 6.2. (only σ-skeleton is shown; interatomic distances in Å, angles in degrees).
Figure S7. (a) Energy diagram of the mechanism for O-atom migration assisted by trimethylamine. (b) Schematic representation of the reaction paths.
**Tables**

**Table S1.** Reaction and activation energies, $E_{\text{rea}}$ and $E_{\text{act}}$ (in kJ/mol), for various reaction steps calculated as single point energy at MP2/6-311+G* level accounting the solvent effect by PCM. The corrections for the zero-point vibrational energy, ZPE (in kJ/mol), and entropy corrections, $S_{\text{tot}}$ and $S_{\text{vib}}$, are obtained from frequency calculations at B3LYP/6-311+G* level. $T$ is equal to 298.15 K.

| Structure | $E_{\text{rea}}$ or $E_{\text{act}}$ (kJ/mol) | ZPE (kJ/mol) | $T*S_{\text{tot}}$ (kJ/mol) | $T*S_{\text{vib}}$ (kJ/mol) | ZPE-TAS (kJ/mol) | E+ZPE-TAS (kJ/mol) |
|-----------|---------------------------------|---------------|-------------------------------|-------------------------------|-------------------|---------------------|
| **Michael addition** | | | | | | |
| **Neutral system** | | | | | | |
| TS [RC 1/2] | 69.6 | -5.3 | -25.5 | -24.5 | 20.1 | 89.7 |
| 2.1 | -166.7 | 13.3 | -20.0 | -19.1 | 33.2 | -133.4 |
| TS [2.1/2.2] | 307.6 | -17.1 | -3.4 | -3.4 | -13.7 | 293.9 |
| 2.2E | 97.3 | -3.7 | -0.5 | -0.6 | -3.3 | 94.0 |
| 2.2Z | 90.0 | -4.0 | -0.5 | -0.5 | -3.5 | 86.5 |
| TS [2.1/2.2]w | 197.8 | -14.6 | -13.1 | -13.1 | -1.5 | 196.3 |
| 2.2w | 88.9 | -3.5 | 1.5 | 1.2 | -5.0 | 83.9 |
| **Negatively charged system** | | | | | | |
| TS [RC 1/-2.1-] | 21.7 | 1.8 | -14.7 | -13.9 | 16.4 | 38.2 |
| 2.1- | -46.1 | 6.3 | -14.9 | -14.1 | 21.2 | -24.9 |
| **Oxygen migration** | | | | | | |
| **Neutral system** | | | | | | |
| TS [2.2w/3.1] | 241.9 | -6.9 | -14.5 | -14.1 | 7.6 | 249.5 |
| 3.1 | 16.6 | 11.1 | -13.5 | -13.0 | 24.5 | 41.1 |
| TS [3.1/6.1w] | 73.5 | -26.1 | -12.7 | -12.8 | -13.4 | 60.1 |
| TS [3.1/5+NH(OH)2] | 58.7 | -12.6 | -6.4 | -6.5 | -6.2 | 52.5 |
| 6.1w | -104.2 | -11.6 | 12.3 | 12.1 | -23.9 | -128.2 |
| TS [2.2w/3.2]w | 130.8 | 58.1 | -22.3 | -22.8 | 80.5 | 211.3 |
| 3.2w | -36.6 | 73.9 | 7.0 | 6.3 | 66.8 | 30.3 |
| TS [3.2/6.1w]w | 142.4 | -9.0 | -30.0 | -29.8 | 21.1 | 163.5 |
| **Protonated system** | | | | | | |
| TS [2.2+2w/3.1+] | 149.2 | 7.1 | -10.2 | -9.4 | 17.3 | 166.6 |
| 3.1+ | 1.3 | 15.2 | -19.0 | -18.2 | 34.2 | 35.4 |
| TS [3.1+/3.2+] | 90.1 | -13.7 | -5.6 | -5.5 | -8.2 | 81.9 |
| TS [2.2+w/3.2+] | 101.5 | -1.0 | -20.6 | -20.4 | 19.6 | 121.2 |
| 3.2+ | 27.0 | 9.9 | -7.6 | -7.5 | 17.5 | 44.5 |
| **Nef reaction** | | | | | | |
| TS [2.2/4'] | 164.0 | -6.9 | -6.0 | -6.0 | -0.8 | 163.2 |
| TS [2.2/4''] | 261.8 | -8.4 | -1.3 | -1.0 | -7.1 | 254.8 |
| 4' | 35.5 | -0.2 | -2.7 | -2.5 | 2.5 | 38.0 |
| 4'' | 29.0 | 0.0 | -2.7 | -2.5 | 2.7 | 31.8 |
| TS [4'/5+(NOH)2] | 149.5 | -8.5 | -4.8 | -5.0 | -3.6 | 145.8 |
| TS [4''/6.3] | 151.8 | -8.3 | -2.0 | -1.7 | -6.3 | 145.5 |
|                  | TS [4''/6.1]w | 6.3          | Base assisted Nef reaction                              |          |          |          |          |          |          |          |          |          |          |
|------------------|---------------|--------------|--------------------------------------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
|                  | 99.5          | -10.6        | -3.8                                                   | -3.6     | -6.8     | 92.6     |          |          |          |          |          |          |          |
|                  | -220.8        | 2.1          | 3.0                                                    | 3.1      | -0.9     | -221.7   |          |          |          |          |          |          |          |
| **TS [2.2/4]b'** | 254.3         | -6.6         | -0.4                                                   | 0.1      | -6.2     | 248.1    |          |          |          |          |          |          |          |
| **TS [2.2/4]b''**| 225.8         | -2.0         | -8.9                                                   | -8.3     | 6.9      | 232.7    |          |          |          |          |          |          |          |
| **4b**           | 21.8          | 0.3          | -1.0                                                   | -0.6     | 1.3      | 23.2     |          |          |          |          |          |          |          |
| **TS [4b/4:bH+]**| -1.8          | -9.1         | -5.9                                                   | -5.7     | -3.1     | -4.9     |          |          |          |          |          |          |          |
| **4::bH+**       | -34.4         | 3.7          | -21.9                                                  | -21.7    | 25.7     | -8.7     |          |          |          |          |          |          |          |
| **TS [4::bH+/6.1b]** | -48.1      | -14.2        | 19.5                                                   | 19.8     | -33.7    | -81.8    |          |          |          |          |          |          |          |
| **TS [4::bH+/6.2-::bH+]** | 276.8   | -17.2        | 18.0                                                   | 17.7     | -35.2    | 241.5    |          |          |          |          |          |          |          |
| **6.1b**         | -60.4         | -5.0         | 25.5                                                   | 25.7     | -30.5    | -90.9    |          |          |          |          |          |          |          |
| **Tautomerisation of 6** |          |              |                                                        |          |          |          |          |          |          |          |          |          |          |
| **TS [6.1/6.2]** | 335.9         | -19.6        | -11.2                                                  | -11.3    | -8.5     | 327.4    |          |          |          |          |          |          |          |
| **6.2'**         | -88.4         | 3.8          | 0.9                                                    | 0.8      | 2.9      | -85.5    |          |          |          |          |          |          |          |
| **6.2''**        | -69.2         | 4.3          | -0.9                                                   | -0.8     | 5.3      | -63.9    |          |          |          |          |          |          |          |
| **TS [6.2/6.3]** | 174.5         | -17.3        | -6.3                                                   | -6.3     | -11.0    | 163.4    |          |          |          |          |          |          |          |
| **6.3**          | -39.6         | -0.8         | 3.2                                                    | 3.0      | -4.1     | -43.6    |          |          |          |          |          |          |          |
| **TS [6.1/6.2]w**| 178.4         | -27.1        | -28.2                                                  | -27.7    | 1.1      | 179.5    |          |          |          |          |          |          |          |
| **6.2w**         | -79.9         | 4.8          | -5.5                                                   | -5.4     | 10.3     | -69.7    |          |          |          |          |          |          |          |
| **TS [6.2/6.3]w**| 87.4          | -31.7        | -22.9                                                  | -22.6    | -8.9     | 78.6     |          |          |          |          |          |          |          |
| **6.3w**         | -37.8         | -1.4         | 2.3                                                    | 2.6      | -3.8     | -41.6    |          |          |          |          |          |          |          |
| **Cyclization**  |              |              |                                                        |          |          |          |          |          |          |          |          |          |          |
| **TS [6.2/7]+w** | 11.9          | -1.5         | -16.4                                                  | -16.0    | 15.0     | 26.9     |          |          |          |          |          |          |          |
| **7+w**          | -2.1          | 3.7          | -9.1                                                   | -8.6     | 12.8     | 10.7     |          |          |          |          |          |          |          |
| **TS [7/8]+w**   | 199.4         | -15.5        | -24.1                                                  | -23.8    | 8.5      | 208.0    |          |          |          |          |          |          |          |
| **TS [7/8]+2w**  | 84.8          | -7.9         | -9.8                                                   | -9.6     | 1.9      | 86.8     |          |          |          |          |          |          |          |
| **8+w**          | -36.2         | -2.0         | -8.4                                                   | -8.4     | 6.4      | -29.8    |          |          |          |          |          |          |          |
| **8+2w**         | -18.6         | -4.6         | 10.3                                                   | 10.0     | -14.9    | -33.5    |          |          |          |          |          |          |          |
| **TS [8+2w/8:H3O+]** | -12.6       | -11.4        | -5.9                                                   | -5.8     | -5.5     | -18.1    |          |          |          |          |          |          |          |
| **8**            | -62.9         | -96.8        | -22.6                                                  | -21.3    | -74.2    | -137.2   |          |          |          |          |          |          |          |

a Activation energy, \( E_{\text{act}} \), and reaction energy, \( E_{\text{rea}} \), of the corresponding reaction step.

b In entropy \( S_{\text{tot}} \) all degrees of freedom are included, while in \( S_{\text{vib}} \) only vibrational degrees of freedom are taken into account.
Table S2. Reaction and activation energies, $E_{\text{rea}}$ and $E_{\text{act}}$ (in kJ/mol), for various reaction steps in the case of the *ethyl ester of 3-coumarin-carboxylic acid* calculated as single point energy at MP2/6-311+G* level accounting the solvent effect by PCM.

| Structure | Erel $^a$ | $E_{\text{rea}}$$^b$ | $E_{\text{act}}$$^b$ |
|-----------|-----------|------------------|------------------|
| **I. Michael addition** | | | |
| 2.1 | -88.7 | - | |
| TS [2.1/2.2] | 218.0 | 306.7 | |
| 2.2E | 5.8 | 94.5 | |
| 2.2Z | -1.4 | 87.3 | |
| 2.1w | -107.4 | - | |
| TS [2.1/2.2]w | 87.4 | 194.8 | |
| 2.2w | - | - | |
| **II. Oxygen migration** | | | |
| Protonated system | | | |
| 2.2'w | 58.5 | | |
| 2.2'2w | 50.1 | | |
| TS [2.2'2w/3.1'] | 208.4 | 158.4 | |
| 3.1' | 62.0 | 11.9 | |
| TS [3.1'/3.2'] | 164.1 | 102.1 | |
| TS [2.2'w/3.2'] | 144.7 | 86.2 | |
| 3.2' | 90.1 | 31.6 | |
| *Nef reaction* | | | |
| TS [2.2/4'] | 277.1 | 271.4 | |
| TS [2.2/4''] | 264.9 | 266.3 | |
| 4' | 43.8 | 38.1 | |
| 4'' | 31.2 | 32.6 | |
| **Tautomerisation of 6** | | | |
| 6.1 | -80.7 | | |
| TS [6.1/6.2] | 252.5 | 333.2 | |
| 6.2' | -171.1 | -90.3 | |
| 6.2'' | -146.4 | -65.7 | |
| TS [6.2/6.3] | 24.9 | 171.3 | |
| 6.3 | -190.7 | -44.2 | |
| 6.1w | -104.2 | | |
| TS [6.1/6.2]w | 69.9 | 174.1 | |
| 6.2w | -182.5 | -78.2 | |
| TS [6.2/6.3]w | -94.9 | 87.5 | |
| 6.3w | -223.5 | -41.0 | |
| **III. Cyclization** | | | |
| 6.2'w | -108.0 | | |
| TS [6.2/7]'w | -116.1 | - | |
| 7''w | -116.8 | -8.8 | |
| TS [7/8]'w | 85.1 | 201.9 | |
| Species                  | $E_{rel}$ | $E_{act}$ | $E_{rea}$ |
|-------------------------|----------|-----------|-----------|
| TS [7/8]*2w             | -49.9    |           | 67.0      |
| 8*2w                    | -        | -         |           |
| 8*2w                    | -123.9   | -         | -7.1      |
| TS [8*2w/8:H2O*]        | -134.4   |           |           |
| 8                       | -199.4   | -         | -75.5     |

\(^a\) Relative energy of the species, $E_{rel}$, with respect to the energy of 1 and nitromethane at the corresponding level.

\(^b\) Activation energy, $E_{act}$, and reaction energy, $E_{rea}$, of the corresponding reaction step.
Description of the results obtained for the mechanism of the Nef rearrangement assisted by triethylamine

In recent experimental studies, we showed that the final product of the new rearrangement, pyrrolidinedion derivative, could be synthesized also in basic media in presence of triethylamine. By this reason, we modeled O-migration, in which such a base (with trimethylamine as a model) can influence the process of oxygen migration in the three-membered transition state $\text{TS} [2.2/4]b$ (Fig. S4, S7):

- forming hydrogen bonds between the NOH group and the base in the transition state $\text{TS} [2.2/4]b'$;
- coordination of the nitrogen atom from the amine to the migrating oxygen atom from $\text{CH}_2\text{NO}_2\text{H}$ in the transition state $\text{TS} [2.2/4]b''$.

The former approach is based on the basic properties of trialkylamine, while the latter one is connected with the possible formation of trialkylamino N-oxide. The formation of hydrogen bond stabilizes the starting compound $2.2b$ by 57.1 kJ mol$^{-1}$ with respect to $2.2Z$, while the stabilization of the transition state $\text{TS} [2.2/4]b'$ is weaker and the energy barrier of the reaction step, 254.3 kJ mol$^{-1}$, increases compared to the reaction without amine, 167.5 (164.1) kJ mol$^{-1}$. The transfer of O atom coordinated to N atom from $\text{Me}_3\text{N}$ through $\text{TS} [2.2/4]b''$ has a slightly lower energy barrier, 225.8 kJ mol$^{-1}$, which is still by ~ 60 kJ mol$^{-1}$ higher than the barrier of the reaction without amine.

The reaction step via the presumed transition state $\text{pseudoTS} [4b/4\cdot\text{bH}^+]$ (which has lower energy than the preceding intermediate) instead of the neutral complex $4b$ spontaneously leads to formation of the ionic couple $4\cdot\text{bH}^+$, in which the NOH group of $4$ is deprotonated and the amine is protonated. The formation of the ionic couple leads to the opening of the three-centered ring and complete migration of the oxygen atom to the carbon atom, which was not possible to achieve in absence of the base (see above). The intermediate $6.1$ can be easily obtained from $[4\cdot\text{bH}^+]$ by reverse protonation of $4\cdot$ from the protonated base. This process is spontaneous via the structure denoted as $\text{TS} [4\cdot\text{bH}^+/6.1b]$ (Figs. S4, S7).

| Intermediate | Transition state | $E_{\text{rel}}$ | $E_{\text{act}}$ or $E_{\text{rea}}$ |
|--------------|-----------------|-----------------|-----------------|
|              | $\text{TS} [2.2/4]b'$ | $-9.4$ | 234.6 |
|              | $\text{TS} [2.2/4]b''$ | $36.3$ | 232.9 |
| $2.2b$       | $\text{L1}$     | 243.9 | 225.8 |
|              | $\text{L2}$     | 254.3 | 211.9 |
|              | $\text{L2}\text{PCM}$ | 243.9 | 225.8 |
| Reaction Step       | Relative Energy, $E_{rel}$ | Activation Energy, $E_{act}$ | Reaction Energy, $E_{rea}$ |
|---------------------|----------------------------|------------------------------|-----------------------------|
| $4\text{b}\cdot\text{bH}^+$ | 49.2                      | -22.3                        | 12.9                        | -1.8                        |
| $6.1\text{b}$       | 37.5                      | -54.9                        | 1.2                         | -34.4                       |
| $4\text{b}\cdot\text{bH}^+/6.1\text{b}$ | -24.6                    | -103.0                       | -62.1                       | -48.1                       |
| $6.1\text{b}$       | 323.3                     | 221.8                        | 285.8                       | 276.8                       |

*a* Relative energy of the species, $E_{rel}$, with respect to the energy of 1 and nitromethane at the corresponding level.

*b* Activation energy, $E_{act}$, and reaction energy, $E_{rea}$, of the corresponding reaction step.
### TS structures (Energies at L1)

|        | TS [RC 1/2] | ImgFreq/IR Inten: -851.5222/12.3334 |
|--------|-------------|-------------------------------------|
| O      | -0.91305    | 1.77920 -0.37935                   |
| C      | 0.29198     | 2.09008 0.26751                    |
| O      | 0.62625     | 3.24331 0.28722                    |
| C      | 1.03737     | 0.96203 0.81543                    |
| C      | 0.49231     | -0.35913 0.81706                  |
| C      | -0.91502    | -0.50894 0.41735                  |
| C      | -1.64923    | -1.68757 0.61692                  |
| H      | -1.17036    | -2.53408 1.10083                  |
| C      | -2.97341    | -1.77691 0.21294                  |
| H      | -3.53217    | -2.69128 0.37821                  |
| C      | -3.58424    | -0.67988 -0.40529                 |
| H      | -4.61850    | -0.74483 -0.72586                 |
| C      | -2.88090    | 0.50124 -0.60122                  |
| H      | -3.33971    | 1.36916 -1.06033                  |
| C      | -1.55200    | 0.58382 -0.18457                  |
| C      | 1.38266     | -1.44969 -0.60819                 |
| H      | 0.90799     | -1.05713 -1.49523                 |
| N      | 2.68510     | -1.06404 -0.45595                 |
| O      | 2.90174     | 0.19732 -0.84144                  |
| O      | 3.52146     | -1.65182 0.22209                  |
| H      | 1.76679     | 1.23321 1.57142                   |
| H      | 0.83484     | -1.01504 1.61442                  |
| H      | 1.19675     | -2.48151 -0.34092                 |
| H      | 2.17026     | 0.77539 -0.24679                  |

|        | TS [2.1/2.2] | ImgFreq/IR inten: -2172.6740/541.3399 |
|--------|-------------|-------------------------------------|
| O      | -0.93507    | 1.76505 -0.38671                   |
| C      | 0.26798     | 2.03500 0.22386                    |
| O      | 0.81958     | 3.06676 -0.02672                  |
| C      | 0.76377     | 0.98993 1.20026                   |
| H      | 1.81734     | 1.19002 1.39487                   |
| H      | 0.22714     | 1.13886 2.14496                   |
| C      | 0.51107     | -0.44375 0.69795                  |
| H      | 0.73051     | -1.13868 1.51859                  |
| C      | -0.95024    | -0.56222 0.32723                  |
| C      | -1.68598    | -1.74050 0.47044                  |
| H      | -1.19747    | -2.62198 0.87642                  |
| C      | -3.02946    | -1.79540 0.10852                  |
| H      | -3.58639    | -2.71823 0.22826                  |
| C      | -3.65518    | -0.65702 -0.40127                 |
| H      | -4.70202    | -0.68998 -0.68358                 |
| C      | -2.94243    | 0.52875 -0.54609                  |
|   |   |   |   |
|---|---|---|---|
| H | -3.40495 | 1.42712 | -0.93846 |
| C | -1.59919 | 0.56355 | -0.18255 |
| C | 1.38161 | -0.78999 | -0.49738 |
| O | 3.38314 | -1.17242 | 0.76573 |
| N | 2.77604 | -0.96737 | -0.24740 |
| O | 3.36489 | -0.73586 | -1.41052 |
| H | 1.04620 | -1.64942 | -1.08034 |
| H | 2.20515 | -0.32454 | -1.66911 |

**TS [2.1/2.2]w**

|   |   |   |   |
|---|---|---|---|
| O | 1.14768 | 1.75540 | 0.29575 |
| C | 0.03690 | 2.05236 | -0.46764 |
| O | -0.50648 | 3.10406 | -0.29021 |
| C | -0.37106 | 1.00513 | -1.47838 |
| H | -1.38849 | 1.22155 | -1.79920 |
| H | 0.27915 | 1.12046 | -2.35426 |
| C | -0.22315 | -0.42561 | -0.92521 |
| H | -0.37086 | -1.12202 | -1.75860 |
| C | 1.18395 | -0.57685 | -0.39264 |
| C | 1.89989 | -1.77497 | -0.44065 |
| H | 1.43425 | -2.64880 | -0.88758 |
| C | 3.19439 | -1.85896 | 0.06656 |
| H | 3.73643 | -2.79712 | 0.01763 |
| C | 3.79179 | -0.73031 | 0.62921 |
| H | 4.80139 | -0.78550 | 1.02226 |
| C | 3.09859 | 0.47503 | 0.68333 |
| H | 3.54039 | 1.36748 | 1.11180 |
| C | 1.80437 | 0.53731 | 0.17447 |
| C | -1.22917 | -0.74303 | 0.16940 |
| O | -2.90162 | -0.90904 | -1.40709 |
| N | -2.53355 | -1.01985 | -0.24705 |
| O | -3.40185 | -1.31705 | 0.68610 |
| H | -0.91988 | -1.47335 | 0.91370 |
| H | -1.72260 | 0.25790 | 1.37339 |
| H | -3.10688 | -0.41850 | 1.69101 |
| O | -2.52133 | 0.41952 | 2.12461 |
| H | -2.19818 | 0.23309 | 3.01520 |

**TS [RC 1/2.1]**

|   |   |   |   |
|---|---|---|---|
| O | 2.30114 | -0.60008 | 0.39959 |
| C | 1.86759 | -1.89151 | -0.03477 |
| O | 2.67164 | -2.79038 | 0.14735 |
| C | 0.58470 | -1.94884 | -0.62933 |
| C | 0.29418 | -0.85764 | -0.68196 |
| C | -0.28475 | 0.46315 | -0.41935 |
| C | 0.38019 | 1.67012 | -0.68385 |

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*ESI*
| Element | TS [2.2w/3.1] | ImgFreq/IR inten: -811.7078/529.1724 |
|---------|---------------|----------------------------------------|
| H       | 1.38970       | 1.63524                                |
| C       | -0.22082      | 2.89416                                |
| H       | 0.31508       | 3.81607                                |
| C       | -1.50695      | 2.93111                                |
| H       | -1.98143      | 3.88438                                |
| C       | -2.18730      | 1.74911                                |
| H       | -3.18895      | 1.75005                                |
| C       | -1.57981      | 0.52119                                |
| C       | 1.78323       | -1.07227                               |
| H       | 1.35299       | -0.64073                               |
| N       | 2.89423       | -0.39996                               |
| O       | 3.57808       | -0.94457                               |
| O       | 3.11813       | 0.78186                                |
| H       | -0.26915      | -2.92858                               |
| H       | 1.11813       | -0.89708                               |
| H       | 1.86258       | -2.14574                               |

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### TS [3.1/6.1]w

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### TS [3.1/5+NH(OH)₂]

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|       |       |       |       |
|-------|-------|-------|-------|
| C     | -3.23210 | 0.31488 | -0.52319 |
| H     | -3.80448 | 1.13784 | -0.93546 |
| C     | -1.90244 | 0.52534 | -0.17245 |
| C     | 1.25197  | -0.57052 | -0.43784 |
| N     | 2.94728  | -0.38843 | 0.21179  |
| O     | 3.66053  | 0.48563  | -0.66475 |
| O     | 3.40616  | -1.63819 | 0.18479  |
| H     | 1.31960  | 0.18398  | -1.23338 |
| H     | 4.49569  | 0.01432  | -0.82750 |
| O     | 1.30268  | -1.81604 | -0.78827 |
| H     | 2.45192  | -2.09338 | -0.38127 |
| H     | 3.04947  | 0.00680  | 1.14707  |

**TS [2.2w/3.2]w**

|       |       |       |       |
|-------|-------|-------|-------|
| O     | -1.83800 | 1.63691 | -0.45776 |
| C     | -0.84715 | 2.30122 | 0.23886 |
| O     | -0.70208 | 3.47054 | 0.04190 |
| C     | -0.05150 | 1.47029 | 1.22423 |
| H     | -0.62514 | 1.45038 | 2.15826 |
| H     | 0.88241  | 1.99263 | 1.41599 |
| C     | 0.15977  | 0.01549 | 0.76338 |
| H     | 0.56903  | -0.55063 | 1.60653 |
| C     | -1.18226 | -0.55699 | 0.36283 |
| C     | -1.54612 | -1.89059 | 0.56307 |
| H     | -0.83675 | -2.57003 | 1.02598 |
| C     | -2.80007 | -2.35815 | 0.18114 |
| H     | -3.06404 | -3.39730 | 0.34427 |
| C     | -3.71400 | -1.48448 | -0.40928 |
| H     | -4.69348 | -1.84065 | -0.71003 |
| C     | -3.37825 | -0.14924 | -0.60677 |
| H     | -4.07190 | 0.55314  | -1.05439 |
| C     | -2.11983 | 0.29989  | -0.21650 |
| C     | 1.18725  | -0.07822 | -0.36449 |
| N     | 2.56259  | 0.32998  | 0.05459 |
| O     | 2.62278  | 1.74601  | -0.17236 |
| O     | 3.44785  | -0.28516 | -0.83293 |
| H     | 0.88094  | 0.44140  | -1.27924 |
| H     | 3.02925  | 1.81289  | -1.05662 |
| O     | 1.35272  | -1.48937 | -0.76321 |
| H     | 2.08864  | -1.35379 | -1.43341 |
| H     | 2.01352  | -2.02178 | 0.00889 |
| H     | 3.65624  | -1.55583 | 0.05575 |
| O     | 3.19966  | -2.37470 | 0.51533 |
| H     | 3.32267  | -2.31942 | 1.46920 |
| TS [3.2/6.1w] | ImgFreq/IR inten: -1326.5756/194.2267 |
|---------------|----------------------------------------|
| TS [2.2*2w/3.1+] | ImgFreq/IR inten: -1487.8898/1295.6481 |

| Element | x1 | y1 | z1 | x2 | y2 | z2 | x3 | y3 | z3 |
|---------|----|----|----|----|----|----|----|----|----|
| O       | -1.48825 | 1.78215 | -0.57039 |
| C       | -0.31750 | 2.11766 | 0.06492 |
| O       | 0.28456 | 3.08227 | -0.31896 |
| C       | 0.09435 | 1.20919 | 1.20043 |
| H       | -0.56392 | 1.42516 | 2.05020 |
| H       | 1.11430 | 1.45374 | 1.47898 |
| C       | -0.08867 | -0.27162 | 0.82358 |
| H       | 0.11606 | -0.89007 | 1.70152 |
| C       | -1.53610 | -0.44677 | 0.40838 |
| C       | -2.28467 | -1.59609 | 0.69444 |
| H       | -1.80269 | -2.43350 | 1.16200 |
| C       | -3.62265 | -1.68059 | 0.29480 |
| H       | -4.18707 | -2.58274 | 0.50497 |
| C       | -4.23391 | -0.60488 | -0.35052 |
| H       | -5.27672 | -0.66395 | -0.64391 |
| C       | -3.50904 | 0.55193 | -0.61821 |
| H       | -3.95680 | 1.40341 | -1.11802 |
| C       | -2.17304 | 0.61561 | -0.23583 |
| C       | 0.86782 | -0.77131 | -0.27462 |
| N       | 2.29988 | -0.85002 | 0.22790 |
| O       | 2.84120 | 0.88298 | 0.21210 |
| O       | 3.00879 | -1.42818 | -0.69996 |
| H       | 0.85589 | -0.14045 | -1.17620 |
| H       | 2.57601 | 1.28489 | -0.63179 |
| O       | 0.49683 | -2.08587 | -0.58100 |
| H       | 1.14618 | -2.43834 | -1.20610 |
| H       | 4.21485 | -1.08506 | -0.32812 |
| O       | 4.94743 | -0.30107 | 0.09120 |
| H       | 4.14204 | 0.45416 | 0.19975 |
| H       | 5.61862 | -0.03409 | -0.54661 |
| O       | -1.11566 | 1.83089 | -0.47678 |
| C       | 0.04886 | 2.18125 | 0.15878 |
| O       | 0.59509 | 3.20183 | -0.12798 |
| C       | 0.56187 | 1.19052 | 1.19283 |
| H       | 0.00035 | 1.34044 | 2.12032 |
| H       | 1.59752 | 1.46111 | 1.40391 |
| C       | 0.35415 | -0.27268 | 0.75347 |
| H       | 0.62309 | -0.95370 | 1.56382 |
| C       | -1.10603 | -0.44790 | 0.38187 |
| C       | -1.82230 | -1.62554 | 0.62004 |
| H       | -1.32576 | -2.46890 | 1.08998 |

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|-----|-------|-------|-------|
| C   | -3.16875 | -1.71265 | 0.27948 |
| H   | -3.71814 | -2.62599 | 0.47591 |
| C   | -3.81183 | -0.61630 | -0.29855 |
| H   | -4.86240 | -0.67848 | -0.55874 |
| C   | -3.11841 | 0.56721  | -0.53262 |
| H   | -3.60015 | 1.43378  | -0.96996 |
| C   | -1.77326 | 0.63938  | -0.18946 |
| C   | 1.21741  | -0.60487 | -0.45022 |
| N   | 2.70824  | -0.85723 | -0.26222 |
| O   | 3.14975  | -0.99463 | 1.04385 |
| O   | 3.42057  | 0.12860  | -0.94396 |
| H   | 1.10531  | 0.06219  | -1.30313 |
| H   | 3.26225  | -0.09887 | 1.41615 |
| O   | 1.03074  | -2.01634 | -0.89329 |
| H   | 0.52177  | -2.15688 | -1.70936 |
| H   | 2.21889  | -2.04646 | -0.83979 |
| H   | 4.28554  | -0.26088 | -1.16196 |

TS [3.1+/3.2+]  
-818.9847008  
ImgFreq/IR inten: -790.2056/1952.7991

|     |       |       |       |
|-----|-------|-------|-------|
| O   | -0.88616 | 1.83313  | -0.36178 |
| C   | 0.27450  | 1.75721  | 0.21731 |
| O   | 1.28439  | 2.21150  | -0.38698 |
| C   | 0.41588  | 0.88812  | 1.41642 |
| H   | -0.37291 | 1.09468  | 2.14204 |
| H   | 1.38492  | 1.00944  | 1.88939 |
| C   | 0.18713  | -0.51735 | 0.80402 |
| H   | 0.33997  | -1.27948 | 1.56857 |
| C   | -1.25950 | -0.48516 | 0.32770 |
| C   | -2.13958 | -1.56318 | 0.40072 |
| H   | -1.78042 | -2.51918 | 0.76726 |
| C   | -3.47772 | -1.41404 | 0.02973 |
| H   | -4.14893 | -2.26226 | 0.09742 |
| C   | -3.95677 | -0.18233 | -0.41011 |
| H   | -4.99760 | -0.06908 | -0.68964 |
| C   | -3.10033 | 0.91646  | -0.49809 |
| H   | -3.44091 | 1.88186  | -0.85311 |
| C   | -1.78322 | 0.73458  | -0.12876 |
| C   | 1.18455  | -0.81044 | -0.35991 |
| N   | 2.47555  | -0.01764 | -0.19098 |
| O   | 3.33413  | -0.29883 | -1.24724 |
| O   | 3.06353  | -0.45020 | 1.02359 |
| H   | 0.80166  | -0.41951 | -1.30653 |
| H   | 3.49187  | -1.26396 | -1.21847 |
| O   | 1.47596  | -2.16603 | -0.45459 |
| H   | 1.21921  | -2.52498 | -1.31264 |
| H   | 2.06745  | 1.40283  | -0.25442 |
|         | TS [2.2*4'] | ImgFreq/IR inten: |
|---------|-------------|-------------------|
|         |             |                   |
| O       | 1.63521     | 1.67808           | -0.23923 |
| C       | 0.48239     | 2.35135           | 0.05631 |
| O       | 0.43611     | 3.53451           | -0.11618 |
| C       | -0.65024    | 1.52364           | 0.62899 |
| H       | -1.57025    | 2.09403           | 0.51745 |
| H       | -0.45003    | 1.40975           | 1.70220 |
| C       | -0.75716    | 0.12878           | -0.04307 |
| H       | -1.11317    | 0.25933           | -1.06771 |
| C       | 0.60883     | -0.52709          | -0.03366 |
| C       | 0.80697     | -1.90988          | 0.01753 |
| H       | -0.05697    | -2.56481          | 0.04224 |
| C       | 2.09190     | -2.44706          | 0.01218 |

| O       | 3.86240     | 0.09337           | 1.12889 |
| C       | -1.40383    | 1.81772           | -0.30938 |
| O       | -0.22882    | 2.05621           | 0.21438 |
| C       | 0.58681     | 2.76695           | -0.40433 |
| H       | 0.19405     | 1.23805           | 1.39307 |
| H       | -0.58407    | 1.21746           | 2.15753 |
| C       | 1.11336     | 1.62393           | 1.82670 |
| C       | 0.32699     | -0.17677          | 0.78394 |
| H       | 0.64066     | -0.86778          | 1.56517 |
| C       | -1.07151    | -0.53019          | 0.29225 |
| C       | -1.59882    | -1.82074          | 0.32963 |
| H       | -0.97016    | -2.64309          | 0.65525 |
| C       | -2.92665    | -2.05561          | -0.02792 |
| H       | -3.32096    | -3.06438          | 0.00893 |
| C       | -3.74906    | -0.99898          | 0.41574 |
| H       | -4.78288    | -1.18336          | -0.68408 |
| C       | -3.24973    | 0.30184           | -0.46528 |
| H       | -3.86218    | 1.13851           | -0.77981 |
| C       | -1.92895    | 0.50270           | -0.11402 |
| C       | 1.40460     | -0.21815          | -0.33980 |
| N       | 2.24356     | -1.36803          | -0.24042 |
| O       | 2.87272     | -1.47424          | 1.00485 |
| O       | 3.22626     | -1.21078          | -1.24854 |
| H       | 0.97946     | -0.21240          | -1.34147 |
| H       | 3.52669     | -0.75330          | 1.08057 |
| H       | 3.44291     | -2.10641          | -1.54853 |
| O       | 2.28222     | 1.04891           | -0.27308 |
| H       | 2.94264     | 0.99603           | -0.98604 |
| H       | 1.62353     | 2.05728           | -0.33038 |
H  2.22573  -3.52256  0.04958
C  3.19987  -1.60257  -0.04818
H  4.20306  -2.01508  -0.05300
C  3.02388  -0.22403  -0.11178
H  3.86513   0.45665  -0.17357
C  1.73459   0.29653  -0.10691
C  -1.78458  -0.63916   0.70611
N  -3.15396  -0.72851   0.32624
O  -3.40095   0.25041  -0.68479
O  -2.62327  -1.94979  -0.29455
H  -4.36318   0.23477  -0.77085
H  -1.57817  -1.06110   1.68295

TS [2.2/4'']  
-742.1249367  ImgFreq/IR inten: -914.2135/43.8485
O   0.49836   1.65963   0.58338
C  -0.63987   1.89507  -0.17301
O  -1.31415   2.83917   0.10627
C  -0.88889   0.94736  -1.32687
H  -0.33674   1.34084  -2.18776
H  -1.95145   0.97078  -1.55856
C  -0.41206  -0.48333  -1.05771
H  -0.42184  -1.05413  -1.99385
C  1.00522  -0.45683  -0.50415
C  1.94641  -1.46274  -0.74056
H  1.67345  -2.31012  -1.36325
C  3.22443  -1.38371  -0.19750
H  3.94666  -2.16853  -0.39269
C  3.57244  -0.28610   0.59289
H  4.56745  -0.21657   1.01912
C  2.65223   0.72771   0.83354
H  2.90141   1.59199   1.43822
C  1.37379   0.63387   0.28742
C  -1.23512  -1.25756  -0.07698
N  -2.30925  -0.76228   0.51158
O  -2.73606  -1.55987   1.59977
O  -3.15332  -0.79610  -0.63028
H  -3.28990  -0.96359   2.12412
H  -0.87442  -2.23961   0.23810

TS [4'/5+(NOH)2]  
-742.1536390  ImgFreq/IR inten: -170.4202/2.0477
O   1.08385   1.81242   0.34357
C  -0.17588   2.15954  -0.08158
O  -0.59639   3.24504   0.19834
C  -0.90942   1.12950  -0.91333
H  -0.55001   1.24445  -1.94294
H  -1.96677   1.38901  -0.90416

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| Atom | C   | H   | C   |
|------|-----|-----|-----|
|      | -0.66429 | -0.31765 | -0.46616 |
|      | -1.04241 | -1.01040 | -1.22145 |
|      | 0.82533  | -0.53069  | -0.28391 |
|      | 1.44458  | -1.77027  | -0.46670 |
|      | 0.83615  | -2.62441  | -0.74655 |
|      | 2.81670  | -1.91752  | -0.28867 |
|      | 3.28078  | -2.88659  | -0.43603 |
|      | 3.59062  | -0.81571  | 0.07911  |
|      | 4.66115  | -0.92224  | 0.21827  |
|      | 2.99401  | 0.42603   | 0.27017  |
|      | 3.57031  | 1.29720   | 0.55978  |
|      | 1.61966  | 0.55426   | 0.09234  |
|      | -1.36548 | -0.66617  | 0.84794  |
|      | -3.48198 | -0.48570  | 0.45796  |
|      | -3.73104 | -0.88929  | -0.71862 |
|      | -1.71667 | -1.81003  | 1.13080  |
|      | -4.43835 | -1.58056  | -0.72399 |
|      | -1.34998 | 0.12041   | 1.62329  |

**TS [4''/6.3]**

-742.1545510

| Atom | C   | H   | C   |
|------|-----|-----|-----|
|      | 0.30364 | 1.75450 | 0.50909 |
|      | -0.89761 | 1.91598 | -0.15770 |
|      | -1.61976 | 2.80030 | 0.19533  |
|      | -1.15424 | 0.99566 | -1.33055 |
|      | -0.74045 | 1.50099 | -2.21137 |
|      | -2.23288 | 0.92727 | -1.47034 |
|      | -0.53632 | -0.39966 | -1.20136 |
|      | -0.51161 | -0.86480 | -2.19020 |
|      | 0.84523  | -0.33445 | -0.62288 |
|      | 1.81640  | -1.31855 | -0.85527 |
|      | 1.57349  | -2.15160 | -1.50872 |
|      | 3.07812  | -1.23541 | -0.28053 |
|      | 3.81709  | -2.00447 | -0.47702 |
|      | 3.39218  | -0.15146 | 0.54576  |
|      | 4.37596  | -0.07809 | 0.99697  |
|      | 2.45069  | 0.83963  | 0.78950  |
|      | 2.67024  | 1.69142  | 1.42272  |
|      | 1.18657  | 0.74147  | 0.20868  |
|      | -1.43227 | -1.36793 | -0.34640 |
|      | -1.31381 | -0.87066 | 1.07574  |
|      | -2.05089 | -1.51019 | 1.89173  |
|      | -2.72942 | -1.35119 | -0.55024 |
|      | -2.55297 | -2.21966 | 1.39935  |
|      | -0.92324 | -2.36543 | -0.35427 |
| TS [4''/6.1]w       | ImgFreq/IR inten: -1006.4768/581.8438 |
|---------------------|----------------------------------------|
| O                   | -1.35245 1.57632 -0.65636              |
| C                   | -0.37710 2.26192 0.03711               |
| O                   | -0.06970 3.35149 -0.34798              |
| C                   | 0.16608 1.59510 1.28193                |
| H                   | -0.49665 1.89725 2.10175               |
| H                   | 1.14882 2.01739 1.48599                |
| C                   | 0.22069 0.06232 1.22472                |
| H                   | 0.32745 -0.31266 2.24833               |
| C                   | -1.04999 -0.48236 0.61801              |
| C                   | -1.54687 -1.75654 0.91249              |
| H                   | -1.01235 -2.37765 1.62626              |
| C                   | -2.71235 -2.23230 0.31977              |
| H                   | -3.08141 -3.22245 0.56412              |
| C                   | -3.40602 -1.42419 -0.58271             |
| H                   | -4.31757 -1.78331 -1.04858             |
| C                   | -2.93674 -0.15101 -0.88460             |
| H                   | -3.45848 0.49851 -1.57807              |
| C                   | -1.76486 0.30796 -0.28601              |
| C                   | 1.46845 -0.46756 0.49673               |
| N                   | 1.53765 0.05668 -0.88240               |
| O                   | 2.22571 -0.62631 -1.68639              |
| O                   | 2.65138 0.11441 0.86665                |
| H                   | 2.97476 -1.34641 -1.16342              |
| H                   | 1.46552 -1.57184 0.50266               |
| O                   | 3.90433 -1.66855 -0.31508              |
| H                   | 4.80486 -1.54244 -0.63560              |
| H                   | 3.63958 -0.91207 0.36201               |

| TS [2.2/4]b'        | ImgFreq/IR inten: -894.6979/67.2922   |
|---------------------|----------------------------------------|
| O                   | -1.39132 1.65929 0.22523               |
| C                   | -0.58332 1.33600 1.30198               |
| O                   | 0.26157 2.11850 1.62393                |
| C                   | -0.89149 0.03203 2.00234               |
| H                   | -1.70060 0.23197 2.71431               |
| H                   | -0.00539 -0.27282 2.55367              |
| C                   | -1.34823 -1.06949 1.04066              |
| H                   | -1.73051 -1.92162 1.61397              |
| C                   | -2.45500 -0.52816 0.14841              |
| C                   | -3.50394 -1.30897 -0.34383             |
| H                   | -3.55482 -2.35974 -0.07277             |
| C                   | -4.48104 -0.75506 -1.16500             |
| H                   | -5.29134 -1.37221 -1.53704             |
| C                   | -4.41485 0.59842 -1.50126              |
| H                   | -5.17341 1.03823 -2.13989              |
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|----|----|----|----|----|----|
| C  | -3.38209 | 1.39371 | -1.01675 |
| H  | -3.31220 | 2.44748 | -1.26071 |
| C  | -2.40823 | 0.82430 | -0.19976 |
| C  | -0.27782 | -1.59275 | 0.12976 |
| N  | 0.95670 | -1.12822 | 0.13236 |
| O  | 1.70625 | -1.48920 | -0.97925 |
| O  | 1.31590 | -1.75978 | 1.37704 |
| H  | 2.49672 | -0.85581 | -0.95518 |
| H  | -0.56711 | -2.29749 | -0.65443 |
| N  | 3.81118 | 0.22047 | -0.71349 |
| C  | 4.37740 | -0.19610 | 0.57612 |
| C  | 4.79005 | 0.08750 | -1.79402 |
| C  | 3.28229 | 1.58784 | -0.64123 |
| H  | 2.81066 | 1.85052 | -1.59063 |
| H  | 4.07609 | 2.32237 | -0.43250 |
| H  | 2.53089 | 1.65759 | 0.14590 |
| H  | 4.32992 | 0.35948 | -2.74649 |
| H  | 5.12983 | -0.94809 | -1.86080 |
| H  | 5.66967 | 0.73224 | -1.63792 |
| H  | 3.59887 | -0.18525 | 1.34005 |
| H  | 5.20434 | 0.45962 | 0.89061 |
| H  | 4.75170 | -1.21841 | 0.49771 |

**TS [2.2/4]b″**

-916.6623065  

|    |    |    |    |    |    |
|----|----|----|----|----|----|
| O  | 3.04867 | -0.12165 | 0.84069 |
| C  | 2.85927 | -1.44705 | 0.50974 |
| O  | 3.57226 | -2.26553 | 1.01503 |
| C  | 1.74981 | -1.73007 | -0.47627 |
| H  | 1.49152 | -2.78241 | -0.39193 |
| H  | 2.14337 | -1.55795 | -1.48607 |
| C  | 0.52870 | -0.81799 | -0.22394 |
| H  | 0.15738 | -1.02962 | 0.78474 |
| C  | 1.02147 | 0.61393 | -0.28419 |
| C  | 0.32992 | 1.68271 | -0.85998 |
| H  | -0.64539 | 1.50020 | -1.29446 |
| C  | 0.87070 | 2.96793 | -0.88056 |
| H  | 0.31562 | 3.78085 | -1.33728 |
| C  | 2.12515 | 3.20437 | -0.32071 |
| H  | 2.55234 | 4.20157 | -0.33171 |
| C  | 2.84135 | 2.15326 | 0.24421 |
| H  | 3.82476 | 2.30058 | 0.67601 |
| C  | 2.28776 | 0.87731 | 0.24854 |
| C  | -0.61126 | -1.11825 | -1.17882 |
| N  | -1.16692 | -2.31671 | -1.32756 |
| O  | -0.90302 | -3.12603 | -0.21193 |
| O  | -2.09936 | -0.60157 | -0.46276 |

*ImgFreq/IR inten: -623.7936/365.4912*
|       |       |       |       |
|-------|-------|-------|-------|
| H     | -1.46457 | -3.89596 | -0.35935 |
| H     | -0.60052 | -0.58036 | -2.12286 |
| N     | -3.10331 | 0.55232  | 0.54768  |
| C     | -3.53325 | 1.65652  | -0.30560 |
| C     | -4.19966 | -0.34201 | 0.91284  |
| C     | -2.30456 | 0.97107  | 1.69661  |
| H     | -3.79019 | -1.20840 | 1.42905  |
| H     | -4.69667 | -0.68256 | 0.00649  |
| H     | -4.92422 | 0.16902  | 1.56295  |
| H     | -2.67232 | 2.26555  | -0.57624 |
| H     | -4.26740 | 2.29259  | 0.20937  |
| H     | -3.97868 | 1.24970  | -1.21215 |
| H     | -1.94442 | 0.08456  | 2.21703  |
| H     | -2.90052 | 1.57949  | 2.39126  |
| H     | -1.44933 | 1.55180  | 1.35488  |

**TS [4b/4::bH+]**

-916.7322648  
ImgFreq/IR inten: -860.8006/6016.3728

|       |       |       |       |
|-------|-------|-------|-------|
| O     | 1.18397 | -1.31140 | 1.06682 |
| C     | 0.48519 | -0.46830 | 1.90035 |
| O     | -0.38370 | -0.94334 | 2.57896 |
| C     | 0.92689 | 0.97629  | 1.91939 |
| H     | 1.76840 | 1.04148  | 2.61989 |
| H     | 0.10841 | 1.57028  | 2.32217 |
| C     | 1.36394 | 1.49871  | 0.54272 |
| H     | 1.86747 | 2.46192  | 0.68166 |
| C     | 2.31601 | 0.51387  | -0.08774 |
| C     | 3.32760 | 0.88299  | -0.97867 |
| H     | 3.45423 | 1.93407  | -1.22262 |
| C     | 4.17105 | -0.06726 | -1.54867 |
| H     | 4.94994 | 0.24188  | -2.23750 |
| C     | 4.01350 | -1.41482 | -1.22394 |
| H     | 4.66856 | -2.16256 | -1.65861 |
| C     | 3.01691 | -1.80651 | -0.33541 |
| H     | 2.87400 | -2.84625 | -0.06343 |
| C     | 2.17926 | -0.84229 | 0.21775 |
| C     | 0.15395 | 1.79229  | -0.36791 |
| N     | -0.86590 | 0.77344  | -0.33508 |
| O     | -1.48392 | 0.61103  | -1.46171 |
| O     | -0.87687 | 2.49441  | 0.19068 |
| H     | -2.50880 | 0.03355  | -1.10169 |
| H     | 0.45349 | 2.09137  | -1.38114 |
| N     | -3.54199 | -0.51826 | -0.59118 |
| C     | -3.09648 | -1.72614 | 0.14128 |
| C     | -4.14013 | 0.47872  | 0.32619 |
| C     | -4.45959 | -0.85845 | -1.69557 |
| H     | -4.71686 | 0.04746  | -2.24546 |
|        |            |            |            |
|--------|------------|------------|------------|
|        | -5.37709   | -1.32072   | -1.31610   |
|        | -3.96593   | -1.55284   | -2.37636   |
|        | -4.38601   | 1.38013    | -0.23529   |
|        | -3.41229   | 0.73873    | 1.09224    |
|        | -5.04718   | 0.07921    | 0.79227    |
|        | -2.59300   | -2.40031   | -0.55248   |
|        | -3.95287   | -2.24348   | 0.58735    |
|        | -2.39374   | -1.44051   | 0.92242    |

**TS [4·bH*/6.1]b**

|        | ImgFreq/IR inten: -820.5050/5432.8938 |
|--------|----------------------------------------|
|        | -916.7603690                           |
| O      | 1.18397                                |
| C      | 0.48519                                |
| O      | -0.38370                               |
| C      | 0.92689                                |
| H      | 1.76840                                |
| H      | 0.10841                                |
| C      | 1.36394                                |
| H      | 1.86747                                |
| C      | 2.31601                                |
| C      | 3.32760                                |
| H      | 3.45423                                |
| C      | 4.17105                                |
| H      | 4.94994                                |
| C      | 4.01350                                |
| H      | 4.66856                                |
| C      | 3.01691                                |
| H      | 2.87400                                |
| C      | 2.17926                                |
| C      | 0.15395                                |
| N      | -0.86590                               |
| O      | -1.48392                               |
| O      | -0.87687                               |
| H      | -2.50880                               |
| H      | 0.45349                                |
| N      | -3.54199                               |
| C      | -3.09648                               |
| C      | -4.14013                               |
| C      | -4.45959                               |
| H      | -4.71686                               |
| H      | -5.37709                               |
| H      | -3.96593                               |
| H      | -4.38601                               |
| H      | -3.41229                               |
| H      | -5.04718                               |
| H      | -2.59300                               |
| H      | -3.95287                               |
|        |      |        |        |
|--------|------|--------|--------|
|        | H    | TS [4·bH*6.2]·bH* | ImgFreq/IR inten: |
|        | -916.6279092 | - | -1485.9711/2006.5186 |
| H      | -2.39374 | -1.44051 | 0.92242 |
| C      | -2.06978 | 1.48418 | -0.89267 |
| O      | -1.23231 | 2.16121 | -0.03979 |
| O      | -0.70629 | 3.16397 | -0.43594 |
| C      | -1.11213 | 1.60333 | 1.35923 |
| H      | -1.97168 | 1.99022 | 1.92203 |
| H      | -0.21063 | 2.02012 | 1.80398 |
| C      | -1.11754 | 0.06377 | 1.42054 |
| H      | -1.28352 | -0.23042 | 2.46290 |
| C      | -2.26313 | -0.45205 | 0.58093 |
| C      | -2.91958 | -1.65727 | 0.84237 |
| H      | -2.59673 | -2.25157 | 1.69187 |
| C      | -3.96236 | -2.10272 | 0.03465 |
| H      | -4.45815 | -3.04199 | 0.25659 |
| C      | -4.36593 | -1.33545 | 1.05885 |
| H      | -5.17916 | -1.67198 | 1.69370 |
| C      | -3.72652 | -0.13256 | -1.33981 |
| H      | -4.01647 | 0.48262 | -2.18420 |
| C      | -2.68204 | 0.29329 | -0.52274 |
| C      | 0.18024 | -0.62093 | 0.99140 |
| N      | 0.88129 | -0.06545 | -0.14484 |
| O      | 1.54764 | -1.27662 | -0.56881 |
| O      | 1.38821 | 0.17782 | 1.25110 |
| H      | 3.00039 | -0.84830 | -0.45486 |
| H      | 0.93403 | -1.77729 | 0.29112 |
| N      | 4.00473 | -0.42730 | -0.36907 |
| C      | 3.87091 | 1.04087 | -0.59720 |
| C      | 4.48007 | -0.72618 | 1.00928 |
| C      | 4.84054 | -1.07735 | -1.40995 |
| H      | 4.85349 | -2.15279 | -1.23694 |
| H      | 5.85839 | -0.68554 | -1.37204 |
| H      | 4.40447 | -0.87914 | -2.38789 |
| H      | 4.53574 | -1.80675 | 1.13692 |
| H      | 3.75274 | -0.32050 | 1.70897 |
| H      | 5.46553 | -0.28348 | 1.16547 |
| H      | 3.44333 | 1.20591 | -1.58449 |
| H      | 4.85345 | 1.51157 | -0.52834 |
| H      | 3.19319 | 1.44592 | 0.15012 |

|        |      | TS [6.1/6.2] | ImgFreq/IR inten: -2359.5993/442.3123 |
|--------|------|-------------|-------------------------------|
| H      | -742.1181135 | ImgFreq/IR inten: -2359.5993/442.3123 |
| O      | 0.42755 | 1.76403 | 0.60656 |
| C      | -0.77569 | 2.01984 | -0.00956 |
| O      | -1.45177 | 2.91531 | 0.40569 |

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*ESI*
| Element | X1    | Y1    | Z1    |
|---------|-------|-------|-------|
| C       | -1.10618 | 1.16702 | -1.21536 |
| H       | -0.60007 | 1.62863 | -2.07209 |
| H       | -2.17804 | 1.23782 | -1.39116 |
| C       | -0.64165 | -0.29912 | -1.09019 |
| H       | -0.68648 | -0.74526 | -2.08917 |
| C       | 0.78676 | -0.32640 | -0.59663 |
| C       | 1.68196 | -1.35222 | -0.91545 |
| H       | 1.34213 | -2.16759 | -1.54767 |
| C       | 2.98797 | -1.34213 | -0.43818 |
| H       | 3.66759 | -2.14678 | -0.69691 |
| C       | 3.41908 | -0.28950 | 0.37254 |
| H       | 4.43608 | -0.27239 | 0.74970 |
| C       | 2.54907 | 0.74359 | 0.69840 |
| H       | 2.85746 | 1.57206 | 1.32557 |
| C       | 1.24276 | 0.71587 | 0.21341 |
| C       | -1.55008 | -1.15656 | -0.21619 |
| O       | -2.92581 | -0.97337 | -0.54957 |
| N       | -1.38468 | -0.99295 | 1.18149 |
| O       | -1.75613 | -2.09627 | 1.67493 |
| H       | -3.28654 | -1.77623 | -0.93747 |
| H       | -1.77404 | -2.53961 | 0.47121 |

**TS [6.2/6.3]**

| Element | X1    | Y1    | Z1    |
|---------|-------|-------|-------|
| O       | -0.12819 | -1.83583 | 0.25735 |
| C       | 1.05676 | -1.79696 | -0.43943 |
| O       | 1.81981 | -2.70914 | -0.32106 |
| C       | 1.25744 | -0.63030 | -1.38393 |
| H       | 0.86249 | -0.95891 | -2.35248 |
| H       | 2.33145 | -0.49941 | -1.51264 |
| C       | 0.54203 | 0.68189 | -1.00741 |
| H       | 0.44453 | 1.28860 | -1.91017 |
| C       | -0.84493 | 0.38349 | -0.46810 |
| C       | -1.88549 | 1.31441 | -0.53609 |
| H       | -1.69463 | 2.28342 | -0.98678 |
| C       | -3.14571 | 1.01614 | -0.02870 |
| H       | -3.94169 | 1.75011 | -0.08861 |
| C       | -3.37914 | -0.23100 | 0.55333 |
| H       | -4.35974 | -0.47426 | 0.94830 |
| C       | -2.35802 | -1.17145 | 0.62617 |
| H       | -2.51389 | -2.14879 | 1.06833 |
| C       | -1.09904 | -0.85574 | 0.11969 |
| C       | 1.29765 | 1.55358 | -0.03733 |
| O       | 1.40832 | 2.83195 | -0.17108 |
| N       | 1.92257 | 1.26709 | 1.07929 |
| O       | 2.24011 | -0.05191 | 1.43425 |
| H       | 2.12097 | 2.58602 | 0.95222 |

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*ESI*
|       | TS [6.1/6.2]w       | ImgFreq/IR inten:  |       |
|-------|---------------------|--------------------|-------|
|       | -818.6277658        |                    |       |
| O     | -0.17672            | -1.92095           | 0.65956|
| C     | 1.00489             | -2.10932           | -0.01706|
| O     | 1.77664             | -2.93073           | 0.38556|
| C     | 1.19975             | -1.25564           | -1.25135|
| H     | 0.63631             | -1.72099           | -2.06874|
| H     | 2.25402             | -1.27360           | -1.51368|
| C     | 0.67100             | 0.18514            | -1.05687|
| H     | 0.70638             | 0.68574            | -2.02832|
| C     | -0.76489            | 0.07350            | -0.60191|
| C     | -1.78192            | 0.92900            | -1.03225|
| H     | -1.53290            | 1.75804            | -1.68687|
| C     | -3.09855            | 0.74325            | -0.62041|
| H     | -3.87316            | 1.42251            | -0.95972|
| C     | -3.41726            | -0.32270           | 0.22193|
| H     | -4.44058            | -0.47390           | 0.54874|
| C     | -2.42632            | -1.20719           | 0.63429|
| H     | -2.64703            | -2.05172           | 1.27676|
| C     | -1.11675            | -1.00596           | 0.21205|
| C     | 1.65049             | 0.95176            | -0.12461|
| O     | 2.93870             | 0.85745            | -0.64084|
| N     | 1.60611             | 1.05087            | 1.21370|
| O     | 0.46352             | 1.28364            | 1.77341|
| H     | 3.55795             | 1.00147            | 0.09110|
| H     | 1.03227             | 2.32781            | -0.18048|
| H     | -0.08834            | 2.40681            | 0.92537|
| O     | 0.13864             | 3.05983            | 0.12535|
| H     | 0.50355             | 3.87696            | 0.49282|
|       | TS [6.2/6.3]w       | ImgFreq/IR inten:  |       |
|       | -818.7069622        |                    |       |
| O     | -1.55031            | 1.58862            | -0.32618|
| C     | -0.51589            | 2.25439            | 0.28275|
| O     | -0.34387            | 3.40888            | 0.02013|
| C     | 0.25164             | 1.49666            | 1.34413|
| H     | -0.30897            | 1.64930            | 2.27439|
| H     | 1.21065             | 1.99747            | 1.47452|
| C     | 0.40406             | -0.02295           | 1.12946|
| H     | 0.54826             | -0.48052           | 2.11007|
| C     | -0.85634            | -0.59849           | 0.51629|
| C     | -1.16147            | -1.96026           | 0.61622|
| H     | -0.46608            | -2.61585           | 1.13214|
| C     | -2.32992            | -2.47907           | 0.06933|
| H     | -2.54662            | -3.53804           | 0.15732|
| C     | -3.22241            | -1.62796           | -0.58512|
|   |   |   |
|---|---|---|
| H | -4.14011 | -2.02014 | -1.01051 |
| C | -2.94129 | -0.27120 | -0.69173 |
| H | -3.61711 | 0.41245 | -1.19287 |
| C | -1.76157 | 0.23248 | -0.14499 |
| C | 1.66267 | -0.43662 | 0.37246 |
| O | 2.50533 | -1.18167 | 1.00490 |
| N | 1.94228 | -0.09643 | -0.86479 |
| O | 1.08016 | 0.84969 | -1.44761 |
| H | 3.47864 | -1.33604 | 0.22825 |
| H | 0.78689 | 0.45506 | -2.28042 |
| H | 3.16646 | -0.51171 | -1.16774 |
| O | 4.08394 | -1.18486 | -0.80379 |
| H | 4.91311 | -0.70410 | -0.70410 |

**TS [6.2/7]^+w**

|   |   |   |
|---|---|---|
| O | -0.54915 | -1.09261 | 0.13240 |
| C | -1.24055 | -0.12272 | 0.77942 |
| O | -2.48773 | -0.42659 | 1.00717 |
| C | -0.47822 | 0.64732 | 1.83680 |
| H | -0.09265 | -0.04521 | 2.58759 |
| H | -1.14299 | 1.36581 | 2.31375 |
| C | 0.65632 | 1.30580 | 1.03219 |
| H | 1.23802 | 2.04202 | 1.58430 |
| C | 1.51139 | 0.18696 | 0.45112 |
| C | 2.89674 | 0.25362 | 0.30298 |
| H | 3.42661 | 1.14291 | 0.62819 |
| C | 3.59618 | -0.81662 | -0.24855 |
| H | 4.67369 | -0.76099 | -0.35004 |
| C | 2.91208 | -1.95868 | -0.66600 |
| H | 3.45651 | -2.79180 | -1.09544 |
| C | 1.52806 | -2.04165 | -0.53388 |
| H | 0.97993 | -2.92094 | -0.85134 |
| C | 0.84932 | -0.96883 | 0.02257 |
| C | -0.05796 | 1.90068 | -0.15266 |
| O | 0.49542 | 2.80552 | -0.91622 |
| N | -1.19049 | 1.30788 | -0.35300 |
| O | -1.76824 | 1.49263 | -1.59681 |
| H | -0.04448 | 2.98320 | -1.70746 |
| H | -2.72628 | 1.53329 | -1.44991 |
| O | -3.66463 | -2.21265 | -0.52750 |
| H | -2.84883 | -1.14925 | 0.41683 |
| H | -3.25017 | -2.94789 | -0.99255 |
| H | -4.58148 | -2.45189 | -0.34904 |
| TS [7/8]⁺w          | ImgFreq/IR inten:         |
|---------------------|--------------------------|
| -819.0097791        | -1840.9797/1056.4662     |
| O                   | -0.52154                 |
| C                   | 0.65838                  |
| O                   | 0.95958                  |
| C                   | 0.09893                  |
| H                   | -0.83302                 |
| H                   | 0.83403                  |
| C                   | -0.07923                 |
| H                   | -0.13298                 |
| C                   | -1.30317                 |
| C                   | -2.24073                 |
| H                   | -2.08869                 |
| C                   | -3.37769                 |
| H                   | -4.10456                 |
| C                   | -3.58543                 |
| H                   | -4.47252                 |
| C                   | -2.65686                 |
| H                   | -2.79600                 |
| C                   | -1.53877                 |
| C                   | 1.17662                  |
| O                   | 1.64525                  |
| N                   | 1.61161                  |
| O                   | 2.54083                  |
| H                   | 2.45033                  |
| H                   | 2.69841                  |
| H                   | -0.18799                 |
| O                   | 3.66270                  |
| H                   | 4.07266                  |
| H                   | 4.07208                  |

| TS [7/8]⁻²w         | ImgFreq/IR inten:         |
|---------------------|--------------------------|
| -819.0457766        | -392.6944/79.8358        |
| O                   | 0.36530                  |
| C                   | 1.56486                  |
| O                   | 2.63578                  |
| C                   | 0.82979                  |
| H                   | 0.38480                  |
| H                   | 1.53924                  |
| C                   | -0.22730                 |
| H                   | -0.61779                 |
| C                   | -1.32993                 |
| C                   | -2.67339                 |
| H                   | -2.96074                 |
| C                   | -3.64112                 |
| H                   | -4.68327                 |
\[
\begin{array}{ccc}
C & -3.26291 & 1.23432 & -0.62582 \\
H & -4.01185 & 1.88910 & -1.05707 \\
C & -1.92664 & 1.62462 & -0.64112 \\
H & -1.63084 & 2.56685 & -1.09045 \\
C & -0.96386 & 0.78695 & -0.08353 \\
C & 0.55259 & -1.83613 & -0.12316 \\
O & 0.22547 & -2.89280 & -0.80726 \\
N & 1.51991 & -1.01459 & -0.38205 \\
O & 2.26922 & -1.07937 & -1.51738 \\
H & 0.77776 & -3.02099 & -1.59910 \\
H & 3.09376 & -0.60279 & -1.29803 \\
H & 0.97212 & 2.41909 & -0.25917 \\
O & 1.84158 & 3.06489 & -0.24887 \\
H & 1.75771 & 3.86004 & 0.29705 \\
\end{array}
\]

| TS [8w2H3O+] | ImgFreq/IR inten: -565.7872/3670.1894 |
|----------------|-----------------------------------|
| -819.0948271 |                                   |

| O  | -0.58889 | -0.26831 | 1.67487 |
| C  | 1.74675  | -1.76937 | -0.06437|
| O  | 2.57743  | -2.50008 | 0.39216 |
| C  | 0.37404  | -1.97313 | -0.64597|
| H  | -0.25903 | -2.44515 | 0.10617 |
| H  | 0.43487  | -2.65413 | -1.49722|
| C  | -0.13575 | -0.55352 | -1.04088|
| H  | -0.16889 | -0.46308 | -2.13145|
| C  | -1.49526 | -0.16365 | -0.49862|
| C  | -2.57603 | 0.06144  | -1.35249|
| H  | -2.43303 | -0.01821 | -2.42587|
| C  | -3.83302 | 0.38226  | -0.84624|
| H  | -4.66327 | 0.55052  | -1.52184|
| C  | -4.01342 | 0.48437  | 0.53098 |
| H  | -4.98776 | 0.73255  | 0.93673 |
| C  | -2.94541 | 0.27031  | 1.39999 |
| H  | -3.08738 | 0.35302  | 2.47408 |
| C  | -1.69463 | -0.05023 | 0.88299 |
| C  | 0.97830  | 0.37561  | -0.59009|
| O  | 0.96132  | 1.62113  | -0.67983|
| N  | 1.98944  | -0.36407 | -0.12788|
| O  | 3.15433  | 0.17124  | 0.36554 |
| H  | 1.94193  | 2.34136  | -0.25947|
| H  | 3.65266  | -0.60919 | 0.68697 |
| H  | -0.81049 | -0.18153 | 2.61029 |
| O  | 2.82185  | 2.99373  | 0.14086 |
| H  | 3.65066  | 2.52692  | 0.30803 |
| H  | 2.96195  | 3.88924  | -0.19189|

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**Ethyl ester of 3-coumarin-carboxylic acid**

| TS [2.1/2.2] | ImgFreq/IR inten: -2165.4786/564.3904 |
|--------------|----------------------------------------|
| -1009.3959879 |                                        |
| O            | -0.42107 0.59259 1.76819              |
| C            | -0.15167 -0.72609 1.50586             |
| O            | -0.18152 -1.51689 2.40225             |
| C            | 0.18679 -1.06641 0.06061              |
| H            | 0.68866 -2.03723 0.08643              |
| C            | -1.05275 -1.26946 -0.82409            |
| C            | 1.11172 0.00610 -0.56112              |
| H            | 1.19314 -0.21324 -1.63147             |
| C            | 0.45371 1.35424 -0.36938              |
| C            | 0.55575 2.39653 -1.29308              |
| H            | 1.12367 2.23938 -2.20539              |
| C            | -0.06778 3.61979 -1.06222             |
| H            | 0.01930 4.41859 -1.79051              |
| C            | -0.81033 3.80958 0.10423              |
| H            | -1.30043 4.75932 0.29018              |
| C            | -0.93173 2.78143 1.03337              |
| H            | -1.50358 2.90221 1.94621              |
| C            | -0.29774 1.56726 0.78713              |
| C            | 2.48885 0.00142 0.07696               |
| O            | 3.32780 -1.87752 -1.15614             |
| N            | 3.35353 -1.08627 -0.25725             |
| O            | 4.21098 -1.16000 0.74978              |
| H            | 3.05898 0.92106 -0.06310              |
| H            | 3.37219 -0.36356 1.23960              |
| O            | -0.98673 -1.39563 -2.02068            |
| O            | -2.18164 -1.31384 -0.11122            |
| C            | -3.41651 -1.54908 -0.84518            |
| C            | -4.54999 -1.54834 0.15652             |
| H            | -3.32322 -2.50293 -1.36792            |
| H            | -3.52159 -0.76276 -1.59515            |
| H            | -4.41663 -2.33194 0.90521             |
| H            | -5.49616 -1.72808 -0.36108            |
| H            | -6.62159 -0.58845 0.67244             |

| TS [2.1/2.2]w | ImgFreq/IR inten: -1383.0074/101.7790 |
|---------------|----------------------------------------|
| -1085.8869486 |                                        |
| O             | -0.42203 0.58579 1.70505              |
| C             | -0.23935 -0.73614 1.36795             |
| O             | -0.17390 -1.54862 2.24295             |
| C             | -0.09689 -1.03163 -0.11674            |
| H             | 0.37003 -2.01608 -0.19412             |
| C             | -1.44409 -1.15364 -0.84257            |
| C             | 0.79053 0.03159 -0.80485              |
| H             | 0.74433 -0.16170 -1.88107             |

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*ESI*
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | 0.19344 | 1.38862 | -0.50412 |
| C       | 0.20452 | 2.45348 | -1.40686 |
| H       | 0.65211 | 2.30921 | -2.38565 |
| C       | -0.35879 | 3.68214 | -1.07074 |
| H       | -0.34450 | 4.49817 | -1.78500 |
| C       | -0.95014 | 3.85501 | 0.18148  |
| H       | -1.39467 | 4.80804 | 0.44795  |
| C       | -0.97946 | 2.80446 | 1.09375  |
| H       | -1.43472 | 2.91098 | 2.07180  |
| C       | -0.40702 | 1.58635 | 0.74029  |
| H       | -0.34450 | 4.49817 | -1.78500 |
| C       | -0.95014 | 3.85501 | 0.18148  |
| O       | 2.23181 | -0.01107 | -0.32654 |
| C       | 2.56637 | -1.99594 | -1.44658 |
| N       | 3.01750 | -1.06761 | -0.79276 |
| O       | 4.26854 | -1.08684 | -0.41006 |
| C       | 2.75985 | 0.92174  | -0.40946 |
| H       | 2.75985 | 0.92174  | -0.40946 |
| C       | -1.55177 | -1.13969 | -2.04221 |
| O       | -2.46228 | -1.30882 | 0.01223  |
| C       | -3.78355 | -1.49508 | -0.56648 |
| H       | -4.76244 | -1.66286 | 0.57484  |
| C       | -3.74946 | -2.37109 | -1.21710 |
| H       | -4.01080 | -0.62514 | -1.18588 |
| C       | -5.76961 | -1.81028 | 0.17552  |
| H       | -4.77696 | -0.77963 | 1.21713  |
| C       | -4.50850 | -2.52958 | 1.18858  |
| H       | 4.19916  | -0.73043 | 0.92429  |
| C       | 4.64422  | -0.43116 | 1.83634  |
| H       | 4.01142  | 0.35637  | 2.25743  |

TS [2.2\cdot2w/3.1⁺]

| -1086.2166867 | Imgfreq/IR inten: |
|----------------|-------------------|
| -1423.7935/1170.4711 |

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| O       | -1.02935 | -1.47900 | 1.70118  |
| C       | 0.21885  | -0.95961 | 1.81259  |
| O       | 0.90205  | -1.24335 | 2.74835  |
| C       | 0.70014  | 0.04697  | 0.76247  |
| C       | 1.94231  | -0.39556 | -0.01995 |
| H       | 1.09104  | 0.85976  | 1.38479  |
| C       | -0.36576 | 0.61524  | -0.23255 |
| H       | 0.07365  | 0.69310  | -1.22961 |
| C       | -1.60530 | -0.24874 | -0.32985 |
| C       | -2.49642 | -0.11929 | -1.40615 |
| H       | -2.28795 | 0.60590  | -2.18642 |
| C       | -3.62453 | -0.92500 | -1.50121 |
| H       | -4.29902 | -0.81416 | -2.34235 |
| C       | -3.87062 | -1.89069 | -0.52266 |
| H       | -4.74498 | -2.52765 | -0.59257 |

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*ESI*
| Element | X1 | Y1 | Z1 | X2 | Y2 | Z2 | X3 | Y3 | Z3 | X4 | Y4 | Z4 |
|---------|----|----|----|----|----|----|----|----|----|----|----|----|
| C       | -2.98516 | -2.05524 | 0.53455 |
| H       | -3.13941 | -2.81087 | 1.29575 |
| C       | -1.86137 | -1.23765 | 0.61817 |
| C       | -0.66486 | 2.03199 | 0.21703 |
| N       | 0.39426 | 3.08719 | -0.03732 |
| O       | 1.30890 | 2.81340 | -1.02466 |
| O       | 1.00880 | 3.38051 | 1.19393 |
| H       | -0.98753 | 2.13078 | 1.25158 |
| H       | 1.86542 | 2.01421 | -0.78551 |
| O       | -1.62608 | 2.76447 | -0.66048 |
| H       | -2.52392 | 2.88809 | -0.30867 |
| H       | -0.82157 | 3.61732 | -0.61217 |
| O       | 1.47856 | 4.22095 | 1.05697 |
| O       | 2.56443 | 0.43805 | -0.66246 |
| O       | 2.22417 | -1.66438 | 0.07067 |
| C       | 3.43700 | -2.18262 | -0.59839 |
| H       | 3.74320 | -2.99760 | 0.05396 |
| H       | 4.18761 | -1.39446 | -0.58117 |
| C       | 3.11447 | -2.65235 | -2.00030 |
| H       | 4.00909 | -3.10345 | -2.43736 |
| H       | 2.81210 | -1.82467 | -2.64487 |
| H       | 2.32806 | -3.40965 | -1.99442 |

**TS [2.2e+3.2e]**

-1086.2448778  ImgFreq/IR inten: -820.6690/2136.9112

| Element | X1 | Y1 | Z1 | X2 | Y2 | Z2 | X3 | Y3 | Z3 | X4 | Y4 | Z4 |
|---------|----|----|----|----|----|----|----|----|----|----|----|----|
| O       | -0.42009 | 0.16650 | 1.78406 |
| C       | 0.29870 | -0.78281 | 1.26769 |
| O       | 1.22023 | -1.29170 | 1.96435 |
| C       | 0.23783 | -1.02623 | -0.20531 |
| C       | -1.14990 | -1.37231 | -0.78435 |
| H       | 0.87581 | -1.87135 | -0.45885 |
| C       | 0.80635 | 0.29667 | -0.76530 |
| H       | 0.87067 | 0.22345 | -1.85134 |
| C       | -0.18939 | 1.36460 | -0.33448 |
| C       | -0.55722 | 2.45995 | -1.11339 |
| H       | -0.08661 | 2.60701 | -2.07967 |
| C       | -1.54213 | 3.34529 | -0.67210 |
| H       | -1.81845 | 4.18982 | -1.29266 |
| C       | -2.18166 | 3.14134 | 0.54897 |
| H       | -2.94966 | 3.82837 | 0.88455 |
| C       | -1.83747 | 2.05283 | 1.35122 |
| H       | -2.30558 | 1.87764 | 2.31252 |
| C       | -0.85714 | 1.19843 | 0.88760 |
| C       | 2.23713 | 0.57909 | -0.20331 |
| N       | 2.94768 | -0.70762 | 0.19969 |
| O       | 4.20356 | -0.40195 | 0.70880 |
| O       | 3.09161 | -1.48013 | -0.98094 |
|     |     |     |     |
|-----|-----|-----|-----|
| H   | 2.17772 | 1.11030 | 0.75055 |
| H   | 4.66897 | 0.08910 | 0.00179 |
| O   | 3.02739 | 1.27073 | -1.11542 |
| H   | 3.25521 | 2.14954 | -0.78879 |
| H   | 2.11500 | -1.30005 | 1.26417 |
| H   | 3.53137 | -2.29950 | -0.69783 |
| O   | -1.43624 | -1.15388 | -1.92789 |
| O   | -1.88127 | -2.00299 | 0.12858 |
| C   | -3.19588 | -2.53146 | -0.28308 |
| H   | -3.34545 | -3.37303 | 0.39062 |
| H   | -3.10117 | -2.89457 | -1.30557 |
| C   | -4.27913 | -1.48325 | 0.01752 |
| H   | -5.24406 | -1.93431 | -0.38819 |
| H   | -4.12075 | -0.64615 | -0.82433 |
| H   | -4.33891 | -1.10828 | 0.88170 |

|     |     |     |     |
|-----|-----|-----|-----|
| TS [3.1"/3.2"]  | -1086.2410391 |  |  |
|     |     |     |     |
| O   | -0.75858 | 0.20111 | 1.85642 |
| C   | -0.13567 | -0.88543 | 1.48553 |
| O   | 0.54777 | -1.51476 | 2.31787 |
| C   | -0.00186 | -1.17710 | 0.01752 |
| C   | -1.31743 | -1.30236 | -0.77931 |
| H   | 0.50326 | -2.13655 | -0.10214 |
| C   | 0.86583 | -0.00483 | -0.48378 |
| H   | 0.99958 | -0.12225 | -1.55883 |
| C   | 0.06858 | 1.25801 | -0.18529 |
| C   | 0.07398 | 2.38302 | -1.00904 |
| H   | 0.72153 | 2.40149 | -1.87927 |
| C   | -0.75993 | 3.46665 | -0.73522 |
| H   | -0.74414 | 4.33256 | -1.38674 |
| C   | -1.62186 | 3.43395 | 0.35964 |
| H   | -2.27405 | 4.27458 | 0.56605 |
| C   | -1.65101 | 2.32187 | 1.20043 |
| H   | -2.29821 | 2.27617 | 2.06818 |
| C   | -0.80835 | 1.26642 | 0.90762 |
| C   | 2.27032 | -0.01313 | 0.18969 |
| N   | 3.32132 | 0.19854 | -0.75012 |
| O   | 3.31078 | -0.72795 | -1.79633 |
| O   | 4.52494 | 0.06146 | -0.01394 |
| H   | 2.37477 | 0.73925 | 0.96842 |
| H   | 3.53697 | -1.60510 | -1.43245 |
| H   | 5.15648 | 0.66931 | -0.42699 |
| O   | 2.50974 | -1.36178 | 0.90911 |
| H   | 3.38726 | -1.32814 | 1.32795 |
| H   | 1.62903 | -1.63744 | 1.68815 |

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| Element | X    | Y    | Z    |
|---------|------|------|------|
| O       | -1.37527 | -1.07759 | -1.95633 |
| O       | -2.28336 | -1.76342 | 0.00594  |
| C       | -3.59102 | -2.06162 | -0.60815 |
| H       | -3.99125 | -2.84618 | 0.03117  |
| H       | -3.40605 | -2.46081 | -1.60449 |
| C       | -4.47604 | -0.83360 | -0.63448 |
| H       | -5.45664 | -1.11006 | -1.03071 |
| H       | -4.06480 | -0.05498 | -1.27927 |
| H       | -4.62430 | 0.04297  | 0.36912  |

**TS [2.2/4']**

-1009.3845499

| Element | X    | Y    | Z    |
|---------|------|------|------|
| O       | -1.18943 | -2.29431 | -0.24983 |
| C       | 0.09088  | -2.11347 | 0.17343  |
| O       | 0.87363  | -3.01367 | 0.09284  |
| C       | 0.41016  | -0.75205 | 0.79101  |
| H       | 0.00767  | -0.77917 | 1.80995  |
| C       | 1.92320  | -0.58410 | 0.93097  |
| C       | -0.28183 | 0.40602  | 0.01047  |
| H       | 0.18228  | 0.51059  | -0.97222 |
| C       | -1.76164 | 0.07290  | -0.12385 |
| C       | -2.76576 | 1.04570  | -0.17483 |
| H       | -2.48585 | 2.09361  | -0.10717 |
| C       | -4.10030 | 0.67321  | -0.31347 |
| H       | -4.86833 | 1.43762  | -0.35264 |
| C       | -4.44552 | -0.67493 | -0.40310 |
| H       | -5.48433 | -0.96783 | -0.51095 |
| C       | -3.45814 | -1.65437 | -0.36112 |
| H       | -3.69469 | -2.70912 | -0.44005 |
| C       | -2.13008 | -1.26904 | -0.22331 |
| C       | -0.10399 | 1.67134  | 0.78109  |
| N       | 0.46270  | 2.79085  | 0.35313  |
| O       | 1.00197  | 2.69072  | -0.95071 |
| O       | -0.73573 | 3.56609  | 0.44742  |
| H       | 1.50628  | 3.51102  | -1.04834 |
| H       | -0.43303 | 1.72062  | 1.81217  |
| O       | 2.49016  | -0.54793 | 1.99335  |
| O       | 2.50540  | -0.46075 | -0.26304 |
| C       | 3.95482  | -0.33885 | -0.27780 |
| H       | 4.37120  | -1.21424 | 0.22378  |
| H       | 4.22870  | 0.54564  | 0.30077  |
| C       | 4.39039  | -0.24166 | -1.72307 |
| H       | 5.47862  | -0.14855 | -1.77252 |
| H       | 3.95149  | 0.63161  | -2.21071 |
| H       | 4.09991  | -1.13311 | -2.28286 |
### TS [2.2/4’’]

|     | ImagFreq/IR inten: -897.0411/42.6806 |
|-----|-------------------------------------|
| O   | 0.12374 0.46193 1.71061             |
| C   | -0.32071 -0.77258 1.27250           |
| O   | -0.67531 -1.57055 2.08358           |
| C   | -0.31564 -0.99247 -0.23453          |
| H   | -0.24140 -2.07485 -0.37962          |
| C   | -1.61565 -0.53837 -0.91319          |
| C   | 0.87775  -0.32134  -0.92439         |
| H   | 0.70271  -0.33872  -2.00576         |
| C   | 0.99118  1.12512  -0.46264          |
| C   | 1.46726  2.15706  -1.27570          |
| H   | 1.76770  1.93378  -2.29515          |
| C   | 1.54118  3.46108  -0.79827          |
| H   | 1.90743  4.25378  -1.44098          |
| C   | 1.13175  3.74444   0.50661          |
| H   | 1.18457  4.75973   0.88477          |
| C   | 0.64722  2.73255   1.32759          |
| H   | 0.31885  2.92870   2.34170          |
| C   | 0.58539  1.42954   0.83885          |
| C   | 2.20301 -0.95754  -0.66948          |
| N   | 2.36864 -2.00054  -0.12613          |
| O   | 3.73346 -2.23184   0.41881          |
| O   | 1.76925 -2.95827  -0.73874          |
| H   | 3.71173 -2.77134   1.22229          |
| H   | 3.09054 -0.47134  -1.08102          |
| O   | -1.68449 -0.26350  -2.08595         |
| O   | -2.64529 -0.52909  -0.06620         |
| C   | -3.95142 -0.19790  -0.61650         |
| H   | -4.16938 -0.90278  -1.42102         |
| H   | -3.89491  0.80230  -1.05066         |
| C   | -4.95465 -0.28264   0.51255         |
| H   | -5.95221 -0.04215   0.13502         |
| H   | -4.71324  0.42263   1.31065         |
| H   | -4.98386 -1.28707   0.93955         |

### TS [6.1/6.2]

|     | ImagFreq/IR inten: -2358.3760/451.6270 |
|-----|---------------------------------------|
| O   | -0.06854  0.43936   1.68772           |
| C   | -0.41342 -0.85204   1.38164           |
| O   | -0.74195 -1.59036   2.26275           |
| C   | -0.34948 -1.24175  -0.08829           |
| C   | -1.64319 -0.92246  -0.84874           |
| H   | -0.24827 -2.32896  -0.11370           |
| C   | 0.85550  -0.60347  -0.82359           |
| H   | 0.67244  -0.74156  -1.89308           |
| C   | 0.90334  0.87263  -0.50323           |

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|     | x      | y      | z      |
|-----|--------|--------|--------|
| C   | 1.40390| 1.82778| -1.39334|
| H   | 1.77491| 1.50101| -2.36017|
| C   | 1.42830| 3.17725| -1.05907|
| H   | 1.82015| 3.90380| -1.76250|
| C   | 0.94224| 3.59163| 0.18325 |
| H   | 0.05082| 2.95494| 2.05178 |
| C   | 0.41960| 1.31301| 0.73057 |
| C   | 2.18141| -1.29023| 0.52479 |
| C   | 0.42830| 3.17725| -1.05907|
| H   | 1.82015| 3.90380| -1.76250|
| C   | 0.94224| 3.59163| 0.18325 |
| H   | 0.05082| 2.95494| 2.05178 |
| C   | 0.41960| 1.31301| 0.73057 |
| C   | 2.18141| -1.29023| 0.52479 |
| O   | 1.77491| 1.50101| -2.36017|
| H   | 2.50184| -3.05935| -1.34674|
| H   | 3.71933| -1.28859| -0.76648|
| O   | -1.75442| -1.08336| -2.03937|
| O   | -2.61220| -0.47145| -0.04795|
| C   | -3.89661| -0.17664| -0.66501|
| H   | -4.26538| -1.09117| -1.13315|
| H   | -3.73486| 0.56314| -1.45156|
| C   | -4.81934| 0.32731| 0.42239 |
| H   | -5.79940| 0.55538| -0.00542|
| H   | -4.42855| 1.23747| 0.88231 |
| H   | -4.95435| -0.42234| 1.20475 |

**TS [6.2/6.3]**

-1009.4706740  ImgFreq/IR inten: -1882.8793/388.3928

|     | x      | y      | z      |
|-----|--------|--------|--------|
| O   | -0.04427| 0.29626| 1.74619 |
| C   | -0.30341| -0.95570| 1.26302|
| O   | -0.56556| -1.83733| 2.03035|
| C   | -0.19444| -1.12764| -0.24575|
| C   | -1.45031| -0.67914| -1.00602|
| H   | -0.10378| -2.20011| -0.41966|
| C   | 1.03537| -0.38098| -0.80309|
| H   | 0.96782| -0.40479| -1.89573|
| C   | 0.96566| 1.06020| -0.33394|
| C   | 1.42352| 2.13817| -1.09241|
| H   | 1.87598| 1.94810| -2.05977|
| C   | 1.31141| 3.44036| -0.61587|
| H   | 1.67420| 4.26814| -1.21507|
| C   | 0.73250| 3.67708| 0.63193 |
| H   | 0.64234| 4.69059| 1.00799 |
| C   | 0.26630| 2.61619| 1.40105 |
| H   | -0.18339| 2.77059| 2.37508 |
| C   | 0.39039| 1.32084| 0.90956 |
| C   | 2.36007| -1.00300| -0.44631|
| O   | 3.48247| -0.39776| -0.63062|

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| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| N    | 2.68478 | -2.16747 | 0.07744 |
| O    | 1.80882 | -3.26024 | 0.14928 |
| H    | 3.87375 | -1.59225 | -0.16488 |
| H    | 1.77208 | -3.50534 | 1.08586 |
| O    | -1.46999 | -0.52266 | -2.20107 |
| O    | -2.50183 | -0.53356 | -0.19688 |
| C    | -3.76878 | -0.17358 | -0.81783 |
| H    | -4.03172 | -0.95854 | -1.52956 |
| H    | -3.62290 | 0.75311 | -1.37582 |
| C    | -4.79252 | -0.02979 | 0.28651 |
| H    | -5.76159 | 0.23513 | -0.14486 |
| H    | -4.50724 | 0.75510 | 0.99011 |
| H    | -4.90972 | -0.96312 | 0.84102 |

| TS [6.1/6.2]w   | ImgFreq/IR inten: -1591.9468/751.6748 |
|-----------------|--------------------------------------|
| O               | -0.27101 0.20815 1.78077             |
| C               | -0.69254 -1.01883 1.33899             |
| O               | -1.09611 -1.81964 2.13022             |
| C               | -0.57786 -1.26624 -0.15893            |
| C               | -1.77683 -0.74951 -0.96300            |
| H               | -0.56897 -2.34902 -0.29058            |
| C               | 0.73258  -0.66302  -0.73172           |
| H               | 0.67039  -0.75294  -1.81816           |
| C               | 0.75444  0.79592  -0.34169            |
| C               | 1.18873  1.81571  -1.19175            |
| H               | 1.57814  1.55669  -2.17061            |
| C               | 1.13698  3.14865  -0.79519            |
| H               | 1.48479  3.92662  -1.46624            |
| C               | 0.62748  3.48006  0.46122             |
| H               | 0.58565  4.51698  0.77744             |
| C               | 0.15411  2.48370  1.30822             |
| H               | -0.26008 2.71248  2.28330             |
| C               | 0.21331  1.15777  0.89392             |
| C               | 1.92376 -1.53849  0.25601             |
| O               | 1.66393  2.87166 -0.55637             |
| N               | 2.68769  1.36692  0.83592             |
| O               | 3.09798  -0.17379  1.11440             |
| H               | 2.20499 -3.41614  0.03587             |
| H               | 3.02713  -0.89176 -1.06058             |
| H               | 3.58101  0.33022 -0.23184             |
| O               | 3.74171  0.04715 -1.23589             |
| H               | 4.65591  -0.25590 -1.32731             |
| O               | -1.78679 -0.70227  2.16793             |
| O               | -2.79972 -0.39882  0.17791             |
| C               | -4.01476 0.04980  0.83973              |
| H               | -4.35050 -0.74484 -1.50887             |

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| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| H       | -3.76905 | 0.92166 | -1.44926 |
| C       | -5.03065 | 0.36457 | 0.23620  |
| H       | -5.96236 | 0.70125 | -0.22660 |
| H       | -4.67380 | 1.15651 | 0.89815  |
| H       | -5.24955 | -0.51692 | 0.84233 |

**TS [6.2/6.3]w**

| X         | Y         | Z         |
|-----------|-----------|-----------|
| -1085.9655039 | ImgFreq/IR inten: -1717.4712/137.0958 |
| O         | -0.61659  | 0.68170  | 1.74190  |
| C         | -0.51235  | -0.67707 | 1.60938  |
| O         | -0.65734  | -1.37194 | 2.57035  |
| C         | -0.28650  | -1.20553 | 0.19804  |
| C         | -1.62110  | -1.39657 | -0.55656 |
| H         | 0.11610   | -2.21489 | 0.31667  |
| C         | 0.65933   | -0.34555 | -0.67394 |
| H         | 0.42496   | -0.59128 | -1.71061 |
| C         | 0.37587   | 1.12462  | -0.44512 |
| C         | 0.71167   | 2.08984  | -1.40047 |
| H         | 1.20738   | 1.77242  | -2.31300 |
| C         | 0.41769   | 3.43411  | -1.19964 |
| H         | 0.68772   | 4.16639  | -1.95261 |
| C         | -0.23425  | 3.83168  | -0.03072 |
| H         | -0.47426  | 4.87695  | 0.13291  |
| C         | -0.58295  | 2.88881  | 0.92886  |
| H         | -1.08883  | 3.16941  | 1.84571  |
| C         | -0.27246  | 1.54641  | 0.71688  |
| C         | 2.13871   | -0.70278 | -0.55949 |
| O         | 2.70051   | -1.18898 | -1.61302 |
| N         | 2.87538   | -0.54246 | 0.51659  |
| O         | 2.18091   | -0.18466 | 1.68508  |
| H         | 3.87443   | -1.47578 | -1.27767 |
| H         | 2.62463   | 0.60684  | 2.01981  |
| H         | 4.07106   | -1.07996 | 0.31145  |
| O         | 4.80309   | -1.54519 | -0.51103 |
| H         | 5.09003   | -2.44579 | -0.32377 |
| O         | -1.67276  | -1.65085 | -1.73354 |
| O         | -2.67672  | -1.28244 | 0.25166  |
| C         | -3.99762  | -1.49826 | -0.32309 |
| H         | -4.59398  | -1.83495 | 0.52424  |
| H         | -3.92642  | -2.30044 | -1.05766 |
| C         | -4.55031  | -0.22274 | -0.93120 |
| H         | -5.57140  | -0.39859 | -1.28205 |
| H         | -3.95231  | 0.10148  | -1.78457 |
| H         | -4.58002  | 0.58254  | -0.19378 |

**TS [6.2/7]^w**

| X         | Y         | Z         |
|-----------|-----------|-----------|
| -1086.3392486 | ImgFreq/IR inten: -156.1182/85.2664 |
| O         | -0.03895  | 0.61962  | 1.01697  |
\[
\begin{array}{cccc}
C & 0.08204 & 1.21589 & -0.19435 \\
O & 0.78255 & 2.31514 & -0.17355 \\
C & 0.22495 & 0.28862 & -1.38262 \\
C & 1.44070 & -0.66226 & -1.36529 \\
H & 0.35559 & 0.87696 & -2.28955 \\
C & -1.09055 & -0.50942 & -1.35670 \\
H & -1.26239 & -1.13239 & -2.23281 \\
C & -1.12028 & -1.29639 & -0.05272 \\
C & -1.66032 & -2.57548 & 0.08031 \\
H & -2.07992 & -3.07127 & -0.78891 \\
C & -1.65224 & -3.21604 & 1.31659 \\
H & -2.06406 & -4.21417 & 1.40893 \\
C & -1.11225 & -2.57594 & 2.43256 \\
H & -1.10598 & -3.07444 & 3.39499 \\
C & -0.57520 & -1.29562 & 2.32226 \\
H & -0.15042 & -0.78329 & 3.17743 \\
C & -0.58685 & -0.67592 & 1.08233 \\
C & -2.14059 & 0.55690 & -1.18791 \\
O & -3.40562 & 0.33137 & -1.42602 \\
N & -1.62990 & 1.62893 & -0.67406 \\
O & -2.52376 & 2.53486 & -0.13073 \\
H & -3.96109 & 1.07937 & -1.14114 \\
H & -2.16699 & 3.41722 & -0.31875 \\
O & 0.98496 & 3.65438 & 2.08389 \\
H & 0.85549 & 2.73868 & 0.73009 \\
H & 0.94332 & 3.30070 & 2.97929 \\
H & 1.51759 & 4.45788 & 2.10538 \\
O & 1.44703 & 1.66450 & -2.03015 \\
O & 2.43361 & -0.20890 & -0.61217 \\
C & 3.67240 & -0.99818 & -0.60942 \\
H & 4.01838 & -1.07314 & -1.64100 \\
H & 3.42650 & -2.00099 & -0.25767 \\
C & 4.66298 & -0.29212 & 0.28629 \\
H & 5.59822 & -0.85693 & 0.30584 \\
H & 4.29326 & -0.21935 & 1.31138 \\
H & 4.88454 & 0.71269 & -0.07898 \\
\end{array}
\]

TS [7/8]**w**

| TS [7/8]**w** | ImgFreq/IR inten: -1839.7895/970.5662 |
|---------------|----------------------------------------|
| -1086.2689347 |                                        |
| O             | 0.08406                                |
| C             | -0.28746                               |
| O             | 0.07164                                |
| C             | 0.22071                                |
| C             | 1.70454                                |
| H             | -0.05454                               |
| C             | -0.69001                               |
| H             | -0.77698                               |

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|   |   |   |   |
|---|---|---|---|
| C  | -0.19270  | 1.40713  | 0.38806  |
| C  | -0.11509  | 2.72247  | 0.84643  |
| H  | -0.44738  | 2.95874  | 1.85166  |
| C  | 0.40878   | 3.72345  | 0.02974  |
| H  | 0.47286   | 4.73992  | 0.40083  |
| C  | 0.85841   | 3.41860  | -1.25372 |
| H  | 1.26763   | 4.20001  | -1.88631 |
| C  | 0.78350   | 2.11384  | -1.74295 |
| H  | 1.11288   | 1.86521  | -2.74687 |
| C  | 0.26119   | 1.14065  | -0.91179 |
| C  | -2.01762  | -0.24462 | 0.70225  |
| O  | -3.14873  | 0.26095  | 1.01149  |
| N  | -1.76152  | -1.20566 | -0.15642 |
| O  | -2.66400  | -1.72984 | -1.03926 |
| H  | -3.97845  | -0.10447 | 0.54178  |
| H  | -2.16188  | -2.44549 | -1.48395 |
| H  | 0.54867   | -1.17193 | -1.84882 |
| O  | -5.32543  | -0.56003 | -0.03372 |
| H  | -5.43594  | -1.19739 | -0.74801 |
| H  | -6.18968  | -0.23300 | 0.24249  |
| O  | 2.07253   | -0.17786 | 2.26541  |
| O  | 2.47453   | -1.10819 | 0.24462  |
| C  | 3.92581   | -0.95481 | 0.42198  |
| H  | 4.20092   | -1.47367 | 1.34082  |
| H  | 4.13295   | 0.10801  | 0.55418  |
| C  | 4.60070   | -1.53612 | -0.79811 |
| H  | 5.68416   | -1.44880 | -0.68617 |
| H  | 4.31530   | -1.00308 | -1.70785 |
| H  | 4.35886   | -2.59345 | -0.92156 |

| TS [7/8]^2w |   |   |
|---|---|---|
| -1086.3192152 | ImgFreq/IR inten: -241.5133/103.9918 |

| O     | 1.12946  | -0.32845  | 1.23109  |
| C     | 1.04494  | -1.39068  | 0.09142  |
| O     | 1.32662  | -2.52020  | 0.52634  |
| C     | -0.18667 | -1.01586  | -0.77318 |
| C     | -1.53165 | -1.02251  | -0.06197 |
| H     | -0.25155 | -1.76060  | -1.57295 |
| C     | 0.24861  | 0.35502   | -1.36575 |
| H     | -0.31872 | 0.67145   | -2.23613 |
| C     | 0.27109  | 1.39336   | -0.25631 |
| C     | -0.10878 | 2.72419   | -0.44094 |
| H     | -0.45332 | 3.04948   | -1.41684 |
| C     | -0.05195 | 3.62649   | 0.61636  |
| H     | -0.35786 | 4.65561   | 0.46734  |
| C     | 0.39782  | 3.20050   | 1.86537  |
| H     | 0.44650  | 3.90037   | 2.69119  |

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| Element | x1  | y1  | z1  | x2  | y2  | z2  |
|---------|-----|-----|-----|-----|-----|-----|
| C       | 0.79580 | 1.88177 | 2.06552 |
| H       | 1.16621 | 1.54967 | 3.02949 |
| C       | 0.72880 | 0.98223 | 1.00505 |
| C       | 1.69573 | 0.07247 | -1.71632 |
| O       | 2.34889 | 0.74196 | -2.6240 |
| N       | 2.14074 | -0.84886 | -0.93741 |
| O       | 3.42832 | -1.26955 | -0.88320 |
| H       | 3.29221 | 0.50633 | -2.67057 |
| H       | 3.37496 | -2.11070 | -0.38158 |
| O       | 0.53154 | -2.80744 | 2.42565 |
| H       | 0.60697 | -1.26384 | 2.51646 |
| C       | 3.00000 | 0.00000 | 0.00000 |
| C       | 0.00000 | 0.00000 | 0.00000 |
| O       | 0.00000 | 0.00000 | 0.00000 |
| H       | 0.00000 | 0.00000 | 0.00000 |
| C       | 0.00000 | 0.00000 | 0.00000 |
| C       | 0.00000 | 0.00000 | 0.00000 |
| O       | 0.00000 | 0.00000 | 0.00000 |
| H       | 0.00000 | 0.00000 | 0.00000 |

**TS [8+2w:8:H3O+]**

| Element | x1  | y1  | z1  | x2  | y2  | z2  |
|---------|-----|-----|-----|-----|-----|-----|
| O       | 0.84579 | 0.90551 | 1.45784 |
| C       | 1.09635 | -1.93547 | 0.02528 |
| O       | 1.28568 | -2.90840 | 0.70111 |
| C       | -0.12253 | -1.32698 | -0.62093 |
| C       | -1.34129 | -1.30988 | 0.31559 |
| H       | -0.37555 | -1.96054 | -1.47510 |
| C       | 0.36048 | 0.08689 | -1.14785 |
| H       | 0.22617 | 0.12211 | -2.23224 |
| C       | -0.34045 | 1.29120 | -0.54810 |
| C       | -1.27778 | 2.02020 | -1.28600 |
| H       | -1.47004 | 1.75683 | -2.32216 |
| C       | -1.98545 | 3.06456 | -0.69726 |
| H       | -2.71679 | 3.61806 | -1.27582 |
| C       | -1.74970 | 3.39308 | 0.63755 |
| H       | -2.29492 | 4.20712 | 1.10234 |
| C       | -0.80710 | 2.68763 | 1.38199 |
| H       | -0.60850 | 2.95155 | 2.41636 |
| C       | -0.11116 | 1.64000 | 0.78741 |
| C       | 1.86881 | 0.08940 | -0.88648 |
| N       | 2.67072 | 0.99953 | -1.12165 |
| O       | 2.18315 | -1.11810 | -0.35624 |
| O       | 3.43940 | -1.46087 | 0.11094 |

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| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | 3.93901 | 1.00447 | -0.53374|
| H       | 3.27435 | -2.27699| 0.63278 |
| H       | 0.58282 | 0.75597 | 2.37450 |
| O       | 4.80041 | 0.75920 | 0.09365 |
| H       | 4.59312 | -0.16152| 0.38487 |
| H       | 5.67203 | 0.80771 | -0.32973|
| O       | -2.45079| -1.45929| -0.39987|
| O       | -1.27683| -1.17520| 1.50946 |
| C       | -3.72170| -1.43995| 0.33299 |
| C       | -4.83078| -1.66448| -0.66834|
| H       | -3.79861| -0.47491| 0.83613 |
| H       | -3.67691| -2.22109| 1.09285 |
| H       | -5.79330| -1.64531| -0.15130|
| H       | -4.73301| -2.63382| -1.16111|
| H       | -4.84311| -0.88402| -1.43189|