Supporting Information

Effects of Solvents on the DACBO-catalyzed vinylogous Henry reaction of isatin with 3,5-dimethyl-4-nitroisoxazole “on water” and in solution from QM/MM MC simulations

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Fig. S1 Illustration of the transition structure of the proton migration process for DACBO-catalyzed vinylogous Henry reactions of isatin with 3,5-dimethyl-4-nitroisoxazole in methanol from QM/MM calculations.
Fig. S2 Illustration of the transition structure of the proton migration process for DACBO-catalyzed vinylogous Henry reactions of isatin with 3,5-dimethyl-4-nitroisoxazole in THF from QM/MM calculations.
Path A

Path B

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Fig. S3 DFT calculated free energy profiles of three pathways for the vinylogous Henry reaction of isatin with 3,5-dimethyl-4-nitroisoxazole in water and the corresponding optimized structures. Gibbs free energies are given in kcal mol$^{-1}$. 
Fig. S4 The geometry structures of reactant, transition, intermediate for the proton migration process (rate-limiting step) in DACBO-catalyzed vinylogous Henry reactions of isatin with 3,5-dimethyl-4-nitroisoxazole by employing microsolvent models with the introducing one-, three- and six-water clusters.
Fig. S5 Computed O(solute)-CH2(THF) radial distribution functions for the rate-limiting step of DACBO-catalyzed vinylogous Henry reaction in THF: transition structure (dash red), reactants (solid red) at 25 °C and 1 atm.
Coordinates of all stationary points:

DABCO catalyzes directly the vinylogous Henry reaction of 1a and 2 in water (Path A).

**DABCO**

|         |         |         |         |
|---------|---------|---------|---------|
|         |         |         |         |
| N       | 0.00000000 | 0.00000000 | 0.00000000 |
| N       | 0.00000000 | 0.00000000 | 2.62398859 |
| C       | 1.38183719  | 0.00000000 | 0.53481518 |
| C       | 1.38013416  | -0.10564268 | 2.08863911 |
| H       | 1.92212469  | -0.84086029 | 0.08680746 |
| H       | 1.87127720  | 0.92327368 | 0.21155942 |
| H       | 1.80302223  | -1.05888849 | 2.41963610 |
| H       | 1.98344632  | 0.68882219 | 2.54085485 |
| C       | -0.70078441 | -1.18937450 | 0.53828103 |
| H       | -1.70815970 | -1.20820714 | 0.10882544 |
| H       | -0.17687755 | -2.08428390 | 0.18980601 |
| C       | -0.77595093 | -1.14709417 | 2.09383580 |
| H       | -1.81006484 | -1.05279622 | 2.43797609 |
| H       | -0.36373653 | -2.06426672 | 2.52774054 |
| C       | -0.67207450 | 1.20809022 | 0.53078384 |
| C       | -0.60282377 | 1.24685134 | 2.09012744 |
| H       | -1.60467075 | 1.34779239 | 2.52073561 |
| H       | -0.00431654 | 2.09378134 | 2.43828175 |
| H       | -1.70828157 | 1.20989390 | 0.17961811 |
| H       | -0.17373395 | 2.08368059 | 0.10163429 |

**2**

|         |         |         |         |
|---------|---------|---------|---------|
|         |         |         |         |
| C       | -1.1401  | -0.74977 | -0.00001 |
| C       | -0.00421 | 0.12669  | -0.00002 |
| C       | 1.10736  | -0.68684 | -0.00001 |
| N       | -0.73668 | -1.99708 | 0.        |
| O       | 0.6827   | -1.95143 | -0.00001 |
| N       | 0.00333  | 1.55427  | -0.00001 |
### 1a

|   |       |       |          |
|---|-------|-------|----------|
| C | -2.6007 | -0.43309 | 0.00001  |
| C | 2.57333 | -0.45079 | 0.00003  |
| H | -2.86421 | 0.16093 | -0.87895 |
| H | -3.17095 | -1.36358 | -0.00001 |
| H | -2.86418 | 0.16087 | 0.87901  |
| H | 2.86434 | 0.13265 | 0.87821  |
| H | 3.09862 | -1.40764 | -0.00025 |
| H | 2.8643 | 0.1332 | -0.8778  |
| O | -1.08712 | 2.13461 | 0.00003  |
| O | 1.10288 | 2.12258 | -0.00003 |

**Sum of electronic and zero-point Energies:** -512.999847

**Sum of electronic and thermal Energies:** -512.991865

**Sum of electronic and thermal Enthalpies:** -512.990921

**Sum of electronic and thermal Free Energies:** -513.032854

### TS1-A

|   |       |       |          |
|---|-------|-------|----------|
| C | 0.37222 | 0.6128 | 0.00001  |
| C | 0.53358 | -0.78891 | 0. |
| C | 1.80399 | -1.36632 | 0.00001 |
| C | 2.91661 | -0.51984 | 0.00002 |
| C | 2.74089 | 0.87107 | 0.00003 |
| C | 1.46614 | 1.46382 | 0.00002 |
| C | -1.7784 | -0.1508 | 0. |
| C | -0.80129 | -1.36911 | -0.00001 |
| H | 1.91658 | -2.44603 | 0. |
| H | 3.91824 | -0.93644 | 0.00002 |
| H | 3.61436 | 1.51628 | 0.00004 |
| H | 1.35321 | 2.5419 | 0.00004 |
| N | -1.00073 | 0.96565 | -0.00001 |
| O | -1.18285 | -2.53131 | -0.00002 |
| O | -3.00603 | -0.22104 | 0.00001 |
| H | -1.33736 | 1.90728 | -0.00003 |

**Sum of electronic and zero-point Energies:** -874.275212

**Sum of electronic and thermal Energies:** -874.258843

**Sum of electronic and thermal Enthalpies:** -874.257899

**Sum of electronic and thermal Free Energies:** -874.320613

|   |       |       |          |
|---|-------|-------|----------|
| C | 3.18492 | -0.7269 | 0.56278  |
| C | 2.36789 | 0.13046 | -0.25099 |
| C | 1.54269 | -0.71313 | -1.02733 |
| N | 2.90286 | -1.98037 | 0.32932  |

TS1-A
O     1.87142  -1.98363  -0.67757
N     2.35203   1.51121  -0.26345
C     4.2328    -0.3768    1.56435
C     0.48012  -0.51468  -1.93414
H     3.81006   0.24125   2.3613
H     4.6469   -1.2893    1.99859
H     5.03686   0.19511   1.09277
H     0.255  -1.39398  -2.53978
H    -0.64623  -0.337  -1.19483
H     0.53038   0.41665  -2.49369
O     3.1428   2.14904   0.48138
O     1.53642   2.1085  -1.01474
C    -1.47598  -0.60467   0.93127
C    -2.76625   -0.451   1.78735
H    -1.13566  -1.64269   0.88673
H    -0.6564    0.01199   1.30946
H    -3.11413  -1.42664   2.13638
H    -2.57129   0.1701   2.66547
C    -2.89303  -0.95502  -1.01521
H    -3.03767  -0.65014  -2.05498
H    -2.59472  -2.00655  -1.00231
C    -4.1615  -0.70127  -0.15017
H    -4.94213  -0.22077  -0.74556
H    -4.56079  -1.64602   0.22751
C    -3.36656   1.47498   0.48713
H    -4.18242   1.96158  -0.05349
H    -3.10768   2.10415   1.34268
C    -2.13468   1.28158  -0.44651
H    -2.35389   1.57585  -1.47626
H    -1.2633   1.84685  -0.10416
N    -1.76968  -0.15797  -0.45662
N    -3.85385   0.17526   1.00225

IM1-A
Sum of electronic and zero-point Energies=   -874.284935
Sum of electronic and thermal Energies=      -874.267814
Sum of electronic and thermal Enthalpies=    -874.266869
Sum of electronic and thermal Free Energies= -874.332592

C     3.12738  -0.73114   0.55627
C     2.29776   0.13282  -0.24201
C     1.47112  -0.7273  -1.04766
N     2.8615  -1.98482   0.31809
O     1.82324  -2.01932  -0.67981
|   |   |   |   |
|---|---|---|---|
| N | 2.2711 | 1.48646 | -0.24322 |
| C | 4.17757 | -0.3789 | 1.55666 |
| C | 0.51466 | -0.54086 | -1.99322 |
| H | 3.75299 | 0.22552 | 2.36307 |
| H | 4.60466 | -1.2914 | 1.97887 |
| H | 4.97345 | 0.20759 | 1.0892 |
| H | 0.09037 | -1.40336 | -2.49792 |
| H | -1.00551 | -0.31055 | -0.97578 |
| H | 0.30813 | 0.4523 | -2.36644 |
| O | 3.06545 | 2.15621 | 0.50187 |
| O | 1.43687 | 2.09597 | -0.99384 |
| C | -1.57958 | -0.62232 | 0.99084 |
| C | -2.88308 | -0.45305 | 1.80954 |
| H | -1.24624 | -1.65953 | 0.93134 |
| H | -0.75998 | -0.00495 | 1.36235 |
| H | -3.24147 | -1.42461 | 2.15623 |
| H | -2.69756 | 0.17149 | 2.68585 |
| C | -2.98696 | -0.97215 | -1.00639 |
| H | -3.0988 | -0.65322 | -2.04387 |
| H | -2.67517 | -2.01761 | -0.98554 |
| C | -4.2525 | -0.70478 | -0.15238 |
| H | -5.02314 | -0.22383 | -0.75843 |
| H | -4.65696 | -1.64617 | 0.22511 |
| C | -3.45994 | 1.47511 | 0.48865 |
| H | -4.26595 | 1.9544 | -0.07079 |
| H | -3.21707 | 2.10928 | 1.34386 |
| C | -2.21531 | 1.29426 | -0.41881 |
| H | -2.4029 | 1.57508 | -1.45648 |
| H | -1.33921 | 1.8341 | -0.05563 |
| N | -1.87168 | -0.16596 | -0.40894 |
| N | -3.94992 | 0.17508 | 0.99839 |

**IM1'-A**

Sum of electronic and zero-point Energies= -1387.286028
Sum of electronic and thermal Energies= -1387.258944
Sum of electronic and thermal Enthalpies= -1387.258000
Sum of electronic and thermal Free Energies= -1387.347797

|   |   |   |
|---|---|---|
| C | 3.11105 | -2.72463 | 0.25731 |
| C | 2.7388 | -1.66678 | -0.64525 |
| C | 1.29847 | -1.59754 | -0.61819 |
| N | 2.05901 | -3.26175 | 0.80885 |
| O | 0.9041 | -2.58056 | 0.28954 |
| N | 3.55826 | -0.89122 | -1.39087 |
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | 4.46756   | -3.23781  | 0.6105    |
| C    | 0.36053   | -0.83923  | -1.23062  |
| H    | 5.083     | -2.44019  | 1.03592   |
| H    | 4.37741   | -4.04727  | 1.33863   |
| H    | 4.9822    | -3.61177  | -0.27886  |
| H    | -0.69015  | -1.02273  | -1.03679  |
| H    | 0.64866   | -0.08852  | -1.95044  |
| C    | -0.18561  | 1.64708   | 0.47381   |
| O    | -1.29403  | 1.84501   | -0.01807  |
| O    | 4.82839   | -1.06222  | -1.36524  |
| O    | 3.05707   | 0.02666   | -2.12606  |
| H    | -2.82604  | 0.72534   | 0.02825   |
| N    | -3.75597  | 0.28588   | -0.08407  |
| C    | -4.80021  | 1.37321   | -0.06454  |
| C    | -6.18789  | 0.69317   | -0.20053  |
| H    | -4.68421  | 1.91265   | 0.87666   |
| H    | -4.57441  | 2.04549   | -0.89349  |
| H    | -6.79136  | 0.88933   | 0.68816   |
| H    | -6.71837  | 1.0941    | -1.0667   |
| C    | -3.99167  | -0.67749  | 1.0495    |
| H    | -3.18099  | -1.40615  | 1.026     |
| H    | -3.93148  | -0.10278  | 1.97452   |
| C    | -5.385    | -1.32228  | 0.83207   |
| H    | -5.28284  | -2.40179  | 0.70259   |
| H    | -6.02081  | -1.14304  | 1.70153   |
| C    | -3.80184  | -0.44855  | -1.39952  |
| C    | -5.22633  | -1.04211  | -1.55383  |
| H    | -5.16603  | -2.12287  | -1.6984   |
| H    | -5.72427  | -0.61105  | -2.42485  |
| H    | -3.0276   | -1.21608  | -1.36326  |
| H    | -3.55655  | 0.27124   | -2.18158  |
| N    | -6.05998  | -0.77114  | -0.36298  |
| C    | 1.09911   | 2.28004   | 0.21798   |
| C    | 2.02365   | 1.73512   | 1.13451   |
| C    | 1.49662   | 3.24528   | -0.71085  |
| C    | 2.83345   | 3.64735   | -0.71649  |
| C    | 3.74216   | 3.08924   | 0.19668   |
| C    | 3.35266   | 2.12683   | 1.14183   |
| C    | 0.07596   | 0.64785   | 1.64671   |
| H    | 0.78009   | 3.66138   | -1.4122   |
| H    | 3.17531   | 4.3908    | -1.42873  |
| H    | 4.77861   | 3.41196   | 0.17711   |
| H    | 4.06361   | 1.7069    | 1.84525   |
| N    | 1.38811   | 0.79821   | 1.97324   |
### TS2-A

**Sum of electronic and zero-point Energies** = -1387.278498  
**Sum of electronic and thermal Energies** = -1387.252987  
**Sum of electronic and thermal Enthalpies** = -1387.252043  
**Sum of electronic and thermal Free Energies** = -1387.335703

| Element | X     | Y     | Z     | Data     |
|---------|-------|-------|-------|----------|
| C       | 3.12037 | -2.55853 | 0.07657 |
| C       | 2.63374 | -1.51181 | -0.77805 |
| C       | 1.25061 | -1.38972 | -0.52069 |
| N       | 2.14436 | -3.04737 | 0.79574 |
| O       | 0.96263 | -2.32764 | 0.42573 |
| N       | 3.36007 | -0.80512 | -1.7242 |
| C       | 4.49735 | -3.11233 | 0.22204 |
| C       | 0.2192  | -0.53063 | -0.93456 |
| H       | 5.20147 | -2.32409 | 0.502  |
| H       | 4.50098 | -3.88903 | 0.98979 |
| H       | 4.83924 | -3.54109 | -0.72414 |
| H       | -0.7836 | -0.89334 | -0.73379 |
| H       | -2.74546| 0.70188  | -0.05335 |
| H       | 0.3704  | -0.00507 | -1.86807 |
| O       | 4.58533 | -1.05049 | -1.86673 |
| O       | 2.78122 | 0.06302  | -2.42208 |
| C       | -4.72988| 1.37099  | -0.10006|
| C       | -6.13021| 0.70931  | -0.19805|
| H       | -4.58671| 1.91658  | 0.83404 |
| H       | -4.51797| 2.03729  | -0.93775|
| H       | -6.70807| 0.91558  | 0.7054  |
| H       | -6.67834| 1.11514  | -1.05098|
| C       | -3.92453| -0.68087 | 1.00199 |
| H       | -3.12115| -1.41761 | 0.96757 |
| H       | -3.83997| -0.10411 | 1.92406 |
| C       | -5.32797| -1.31518 | 0.81846 |
| H       | -5.23833| -2.39547 | 0.68525 |
| H       | -5.94115| -1.13227 | 1.70343 |
| C       | -5.2228 | -1.03831 | -1.57025|
| H       | -5.18103| -2.11942 | -1.71937|
| H       | -5.73544| -0.59833 | -2.4284 |
| C       | -3.78757| -0.4655  | -1.44605|
| H       | -3.02427| -1.24481 | -1.42238|
| H       | -3.5468 | 0.24513  | -2.23815|
| N       | -3.70021| 0.27383  | -0.13831|
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| N       | -6.02723 | -0.75789 | -0.36045 |
| C       | 2.0522  | 1.6477  | 0.97993 |
| C       | 1.14338 | 1.99004 | -0.03684 |
| C       | 1.49145 | 2.91394 | -1.0151 |
| C       | 2.77845 | 3.46862 | -0.984  |
| C       | 3.68616 | 3.09711 | 0.01725 |
| C       | 3.3522  | 2.18269 | 1.02351 |
| C       | 0.14995 | 0.50332 | 1.53887 |
| C       | -0.11028 | 1.23476 | 0.21029 |
| H       | 0.78443 | 3.18576 | -1.79352 |
| H       | 3.07663 | 4.18755 | -1.74078 |
| H       | 4.68176 | 3.53089 | 0.02535 |
| H       | 4.03819 | 1.91592 | 1.80539 |
| N       | 1.44739 | 0.75676 | 1.89378 |
| O       | -1.27469 | 1.61169 | -0.14325 |
| O       | -0.66387 | -0.17462 | 2.17795 |
| H       | 1.919 | 0.34175 | 2.67182 |

**IM2-A**

Sum of electronic and zero-point Energies = \(-1387.294377\)

Sum of electronic and thermal Energies = \(-1387.268943\)

Sum of electronic and thermal Enthalpies = \(-1387.267999\)

Sum of electronic and thermal Free Energies = \(-1387.352063\)
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| H       | 6.44441      | 1.01762      | 0.21082      |
| H       | 6.38284      | 0.06404      | 1.69647      |
| C       | 3.83442      | 0.05615      | -1.1989      |
| H       | 3.04556      | -0.44291     | -1.76443     |
| H       | 3.85929      | 1.10934      | -1.48492     |
| C       | 5.21209      | -0.63681     | -1.36401     |
| H       | 5.10801      | -1.5678      | -1.92801     |
| H       | 5.8965       | 0.01457      | -1.91252     |
| C       | 4.93759      | -1.93906     | 0.63428      |
| H       | 4.97053      | -2.88187     | 0.08321      |
| H       | 5.34379      | -2.11652     | 1.63294      |
| C       | 3.47761      | -1.42208     | 0.72393      |
| H       | 2.79668      | -1.98418     | 0.08213      |
| H       | 3.09065      | -1.43456     | 1.74464      |
| C       | 3.45722      | 0.00143      | 0.25141      |
| N       | 3.45722      | 0.00143      | 0.25141      |
| N       | 5.81136      | -0.96088     | -0.04999     |
| C       | -1.85786     | 2.37061      | 0.23633      |
| C       | -1.23576     | 1.34599      | 0.96342      |
| C       | -1.7122      | 1.00554      | 2.22171      |
| C       | -2.82405     | 1.6936       | 2.7389       |
| C       | -3.43542     | 2.70914      | 1.99671      |
| C       | -2.95732     | 3.06804      | 0.72578      |
| C       | -0.1611      | 1.68311      | -1.13465     |
| C       | -0.03928     | 0.83005      | 0.17046      |
| H       | -1.23449     | 0.22039      | 2.80066      |
| H       | -3.20997     | 1.43515      | 3.72047      |
| H       | -4.29332     | 3.23453      | 2.40614      |
| H       | -3.42995     | 3.85962      | 0.1541       |
| N       | -1.19636     | 2.56097      | -0.9997      |
| O       | 1.17499      | 1.09758      | 0.78704      |
| O       | 0.5999       | 1.61497      | -2.10988     |
| H       | -1.45021     | 3.25963      | -1.6686      |

**TS3-A**

Sum of electronic and zero-point Energies= $-1387.296979$

Sum of electronic and thermal Energies= $-1387.271874$

Sum of electronic and thermal Enthalpies= $-1387.270930$

Sum of electronic and thermal Free Energies= $-1387.353724$

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | 3.59635      | -1.99874     | 1.01199      |
| C       | 2.67255      | -1.71567     | -0.05096     |
| C       | 1.54454      | -1.1727      | 0.54035      |
| N       | 3.06865      | -1.65115     | 2.15891      |
| O       | 1.77321      | -1.13206     | 1.85801      |
|   |        |        |        |
|---|--------|--------|--------|
| N | 1.09502| 2.33236| 1.70195|
| O | -0.68187| 1.08505| 2.48939|
| H | 1.28267| 2.85194| 2.55258|

Product

|                              |        |        |        |
|------------------------------|--------|--------|--------|
| Sum of electronic and zero-point Energies= | -1387.296498 |
| Sum of electronic and thermal Energies=   | -1387.271048 |
| Sum of electronic and thermal Enthalpies=  | -1387.270104 |
| Sum of electronic and thermal Free Energies= | -1387.354648 |
The vinylogous Henry reaction of 1a and 2 by one water auxiliary to activating the catalyst (Path B).

H$_2$O
Sum of electronic and zero-point Energies= -76.427052
Sum of electronic and thermal Energies= -76.424215
Sum of electronic and thermal Enthalpies= -76.423271
Sum of electronic and thermal Free Energies= -76.444714

O  -1.67183  1.37647  -0.07598
H   -0.71183  1.37647  -0.07598
H    -1.99228  2.2814  -0.07598

TS1-B
Sum of electronic and zero-point Energies= -950.698214
Sum of electronic and thermal Energies= -950.679253
Sum of electronic and thermal Enthalpies= -950.678308
Sum of electronic and thermal Free Energies= -950.747442

C    -2.75924  -1.3264  -1.20351
C     -1.88705  -0.04463  -1.25077
H     -2.13756  -2.21144  -1.35337
H     -3.51096  -1.3046  -1.99506
H     -0.81977  -0.26307  -1.31936
H    -2.16393    0.62024  -2.07033
C    -2.45024  -1.45118   1.17595
H    -2.96762  -1.58562   2.13035
H    -1.7856   -2.30738   1.0274
C    -1.63955  -0.1272    1.18818
H    -1.80832   0.45968   2.09299
H    -0.56694  -0.28733   1.06494
C    -3.5509    1.04736   0.1914
H    -3.64522   1.64646   1.09876
H    -3.83691   1.65775  -0.66667
C    -4.34586  -0.28351   0.26791
H    -4.84651  -0.37334   1.23442
H    -5.10974  -0.30982  -0.51232
N    -3.45774  -1.45275   0.09344
N    -2.09875    0.70788   0.02972
C    -2.51708  -1.20443  -0.79577
C    -2.44422  -0.07199   0.08533
C    -2.17786   1.05307  -0.72108
O    -2.08457   0.59124  -1.99064
N    -2.29932  -0.8334   -2.02977
N    -2.61436  -0.06403   1.46164
O    -2.89489  -1.13519   2.05491
O    -2.47707    1.0151    2.0887
C    -1.93791   2.43076  -0.48144
H    -2.43058   2.80542   0.41335
H    -2.11145   3.04483  -1.36705
H    -0.66208   2.60489  -0.22369
C    -2.79396  -2.63773  -0.49068
H    -3.78026  -2.74539  -0.03059
H    -2.05597  -3.03295   0.2123
H    -2.76253  -3.22318  -1.41197
O    -0.59981   2.88936   0.05224
H    -0.87832   3.49436  -0.65172
H    -1.50865   1.61785   0.00773

IM1-B

Sum of electronic and zero-point Energies= -950.714115
Sum of electronic and thermal Energies= -950.693803
Sum of electronic and thermal Enthalpies= -950.692859
Sum of electronic and thermal Free Energies= -950.766992

C    -2.80277  -1.33026  -1.25305
C    -1.95545  -0.03127  -1.28158
H    -2.16112  -2.20044  -1.40616
H    -3.54813  -1.31384  -2.05118
H   -0.8835   -0.22492   -1.35014
H   -2.24741    0.64456   -2.08702
C   -2.50657  -1.48616    1.12666
H   -3.02412  -1.6401    2.07586
H   -1.83104  -2.32941    0.96848
C   -1.70946  -0.15538    1.16435
H   -1.88353   0.41659    2.07729
H   -0.63578  -0.29914    1.03198
C   -3.64679   1.01042    0.18194
H   -3.74746   1.58539    1.104
H   -3.93457   1.63785   -0.6634
C   -4.4179  -0.33396    0.22442
H   -4.92612  -0.44932    1.18412
H   -5.17312  -0.35786   -0.56397
N   -3.50783  -1.48475    0.03787
N   -2.18705   0.69109    0.01675
C   2.42261   -1.1718   -0.83236
C   2.36117  -0.0847    0.10946
C   2.20198    1.12017   -0.66817
O   2.10789    0.68769   -1.98925
N   2.26936  -0.74264   -2.05346
N   2.45102  -0.15323    1.45651
O   2.65331  -1.27177    2.04695
O   2.32309    0.91561    2.14724
C   2.16586   2.44607   -0.39021
H   2.29414   2.79277    0.62529
H   2.12599   3.16385   -1.20297
H   0.15191   2.85294   -0.09143
C   2.63825  -2.62823   -0.5855
H   3.60609  -2.79386   -0.10347
H   1.86757  -3.02953    0.07799
H   2.61407  -3.17026   -1.53371
O  -0.78263    3.09857    0.08478
H  -1.03806    3.66731   -0.65741
H  -1.65138    1.58914    0.01149

IM1'-B
Sum of electronic and zero-point Energies=          -1463.716177
Sum of electronic and thermal Energies=             -1463.685954
Sum of electronic and thermal Enthalpies=           -1463.685010
Sum of electronic and thermal Free Energies=        -1463.782790

C    6.22879  -1.68677   -1.09488
C    5.12564  -1.72594   -0.00358
| Atoms | x     | y     | z     |
|-------|-------|-------|-------|
| H     | 5.88934 | -2.2107 | -1.99092 |
| H     | 7.13377 | -2.18088 | -0.73496 |
| H     | 4.2017 | -2.18838 | -0.35426 |
| H     | 5.45181 | -2.22683 | 0.90941 |
| N     | 6.5716 | -0.29827 | -1.46645 |
| C     | 5.34795 | 0.38095 | -1.94266 |
| H     | 5.61076 | 1.44577 | -0.51458 |
| H     | 4.97571 | -0.15811 | -2.8165 |
| C     | 6.0332 | 0.38629 | 0.88021 |
| H     | 5.73538 | 1.38656 | 1.19839 |
| H     | 6.37362 | -0.17779 | 1.75028 |
| H     | 7.31135 | 1.43488 | -0.54634 |
| H     | 8.00003 | -0.07808 | 0.0544 |
| N     | 4.79932 | -0.30402 | 0.36366 |
| H     | 4.06951 | -0.29537 | 1.11094 |
| O     | 2.81547 | -0.10604 | 2.34447 |
| H     | 2.46932 | -0.94355 | 2.68605 |
| H     | 2.05618 | 0.31817 | 1.89043 |
| O     | 0.89633 | 1.32026 | 0.84083 |
| C     | -0.32213 | 1.33719 | 0.99384 |
| C     | -1.0692 | 0.47455 | 2.06286 |
| N     | -2.37461 | 0.84898 | 1.98963 |
| C     | -0.90811 | -1.28129 | -0.78654 |
| H     | -0.01227 | -1.66722 | -0.31317 |
| H     | -0.82197 | -0.5534 | -1.57875 |
| C     | -2.11964 | -1.75196 | -0.41348 |
| O     | -2.20378 | -2.71363 | 0.59533 |
| N     | -3.57936 | -3.05507 | 0.83644 |
| C     | -3.48648 | -1.49552 | -0.8009 |
| N     | -3.89365 | -0.62876 | -1.75453 |
| O     | -5.13911 | -0.48596 | -2.02706 |
| O     | -3.02409 | 0.06325 | -2.38793 |
| C     | -4.30822 | -2.34428 | 0.0224 |
| C     | -5.79388 | -2.48714 | 0.05307 |
| H     | -6.26799 | -1.52756 | 0.27737 |
| H     | -6.17047 | -2.8211 | -0.91779 |
| H     | -6.07771 | -3.21452 | 0.81708 |
| C     | -2.57983 | 1.8053 | 0.97504 |
| C     | -3.77108 | 2.39595 | 0.58544 |
| C     | -1.35625 | 2.13278 | 0.35249 |
C  -1.30667  3.07598  -0.67778
C  -2.50011  3.67605  -1.08293
C  -3.71023  3.33277  -0.45851
H  -4.71133  2.14355   1.064
H  -0.36128  3.32359  -1.15042
H  -2.49708  4.40765  -1.88396
H  -4.62965  3.80782  -0.78717
O  -0.55569  -0.33877  2.82536
H  -3.11477  0.44293   2.55175

TS2-B
Sum of electronic and zero-point Energies=  -1463.708099
Sum of electronic and thermal Energies=     -1463.679427
Sum of electronic and thermal Enthalpies=    -1463.678482
Sum of electronic and thermal Free Energies= -1463.771580

C   6.05974  -1.69884  -1.03759
C   4.98964  -1.66108   0.08547
H   5.65181  -2.16936  -1.9353
H   6.92363  -2.28368  -0.71157
H   4.05936  -2.15475  -0.20156
H   5.34748  -2.09109   1.02278
C   5.36676   0.43026  -1.92008
H   5.70384   1.44971  -2.12468
H   5.04833  -0.01787  -2.86401
C   4.18827   0.44279  -0.91222
H   3.86425   1.45197  -0.65345
H   3.32691  -0.12902  -1.26194
C   5.88613   0.4944   0.87759
H   5.60625   1.53808  1.03404
H   6.1329    0.04347  1.84081
C   7.01565   0.3289  -0.1718
H   7.42029   1.30706  -0.44619
H   7.83109  -0.27417   0.23781
N   6.51712  -0.33838  -1.39376
N   4.6659    0.25999   0.35438
C  -4.07964  -2.3518   0.05176
C  -3.21904  -1.49032  -0.71035
C  -1.96687  -1.48976  -0.05748
O  -2.10442  -2.31758   1.01728
N  -3.43614  -2.84493  1.07701
N  -3.52487  -0.84121  -1.89608
O  -4.67889  -0.95764  -2.38254
O  -2.64187  -0.15276  -2.46487
C  -0.74762  -0.81344  -0.22358
H  -0.55336  -0.4013  -1.20516
H   0.09496  -1.24896   0.30449
H   1.87771   0.52941   1.73416
C  -5.50747  -2.71858  -0.17128
H  -6.13495  -1.82264  -0.19322
H  -5.62544  -3.23063  -1.13034
H  -5.84777  -3.37727   0.63113
O   2.66227   0.19339   2.24529
H   2.33987  -0.57934   2.73445
H   3.90683  -0.15149   1.07332
C  -3.89034   2.46658   0.60635
C  -2.71799   1.79508   0.93219
C  -1.55881   1.89479   0.14307
C  -1.5444   2.71212  -0.98267
C  -2.71548   3.40022  -1.32618
C  -3.87259   3.26957  -0.5437
H  -4.78025   2.37988   1.22233
H  -0.64709   2.8019  -1.58844
H  -2.73028   4.03829  -2.2044
H  -4.77341   3.80697  -0.82525
C  -0.5059    1.05715   0.77713
O   0.7463    1.26949   0.69938
N  -2.46397   0.96832   2.04357
C  -1.17154   0.52954   2.06413
O  -0.64117  -0.14162   2.95526
H  -3.13785   0.75832   2.77155

IM2-B
Sum of electronic and zero-point Energies=          -1463.722027
Sum of electronic and thermal Energies=             -1463.693519
Sum of electronic and thermal Enthalpies=           -1463.692575
Sum of electronic and thermal Free Energies=        -1463.785730

C     6.271  -1.64675  -1.06447
C     5.18007  -1.66542   0.04012
H     5.90361  -2.13983  -1.96708
H      7.16  -2.18169  -0.72343
H     4.26287  -2.16168  -0.2811
H     5.5278  -2.1238   0.96731
C     5.47463   0.45229  -1.92456
H     5.76752   1.47791  -2.15931
H     5.15069  -0.02751  -2.85058
C     4.32164   0.44687  -0.88767
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 4.00764   | 1.45109   | -0.59953  |
| H    | 3.44999   | -0.11391  | -1.22854  |
| C    | 6.03366   | 0.48519   | 0.88813   |
| H    | 5.72436   | 1.50886   | 1.10561   |
| H    | 6.31749   | -0.00637  | 1.8202    |
| C    | 7.14356   | 0.41386   | -0.19317  |
| H    | 7.4732    | 1.41989   | -0.46126  |
| H    | 8.00771   | -0.13603  | 0.18611   |
| N    | 6.66226   | -0.2657   | -1.41451  |
| N    | 4.82602   | -0.23772  | 0.35467   |
| C    | -4.02241  | -2.14294  | 0.06395   |
| C    | -3.18858  | -1.21248  | -0.64513  |
| C    | -1.93679  | -1.23514  | -0.03572  |
| O    | -2.012    | -2.16458  | 0.93634   |
| N    | -3.32609  | -2.72244  | 1.00941   |
| N    | -3.55918  | -0.4591   | -1.77938  |
| O    | -4.73102  | -0.54197  | -2.19057  |
| O    | -2.70152  | 0.24798   | -2.33417  |
| C    | -0.66825  | -0.47212  | -0.14623  |
| H    | -0.5043   | -0.16097  | -1.17677  |
| H    | 0.1446    | -1.11505  | 0.19709   |
| H    | 1.97184   | 0.35613   | 1.67161   |
| C    | -5.46415  | -2.48232  | -0.11866  |
| H    | -6.0801   | -1.58374  | -0.02504  |
| H    | -5.63789  | -2.9034   | -1.11273  |
| H    | -5.76784  | -3.20846  | 0.63809   |
| O    | 2.76233   | 0.02456   | 2.20923   |
| H    | 2.4608    | -0.78851  | 2.63905   |
| H    | 4.06548   | -0.21166  | 1.07744   |
| C    | -3.7145   | 2.5034    | 0.76819   |
| C    | -2.57485  | 1.74647   | 1.01273   |
| C    | -1.4367   | 1.8145    | 0.19634   |
| C    | -1.38767  | 2.73777   | -0.84105  |
| C    | -2.51721  | 3.53667   | -1.09214  |
| C    | -3.67191  | 3.39901   | -0.31205  |
| H    | -4.59648  | 2.41504   | 1.39517   |
| H    | -0.50001  | 2.82689   | -1.46137  |
| H    | -2.49931  | 4.2569    | -1.90472  |
| H    | -4.54595  | 4.0053    | -0.53144  |
| C    | -0.44726  | 0.75347   | 0.66484   |
| O    | 0.86181   | 1.07608   | 0.68163   |
| N    | -2.33841  | 0.8377    | 2.06772   |
| C    | -1.07372  | 0.33008   | 2.02153   |
| O    | -0.54865  | -0.39186  | 2.87676   |
|     |      |      |      |
|-----|------|------|------|
| H   | -2.98293 | 0.66939 | 2.83276 |

**TS3-B**

- Sum of electronic and zero-point Energies: -1463.724188
- Sum of electronic and thermal Energies: -1463.696399
- Sum of electronic and thermal Enthalpies: -1463.695455
- Sum of electronic and thermal Free Energies: -1463.786097

|     |      |      |      |
|-----|------|------|------|
| C   | 5.52844 | 1.80972 | -0.41557 |
| C   | 4.37171 | 0.94559 | -0.98357 |
| H   | 5.1376  | 2.73706 | 0.00915 |
| H   | 6.22689 | 2.07428 | -1.21276 |
| H   | 3.40031 | 1.43612 | -0.89739 |
| H   | 4.53354 | 0.66323 | -2.02575 |
| N   | 6.27538 | 1.08623 | 0.63771 |
| C   | 5.35508 | 0.78241 | 1.75533 |
| H   | 5.90504 | 0.1975  | 2.49616 |
| H   | 5.04834 | 1.72012 | 2.22423 |
| C   | 4.10807 | 0.00042 | 1.26405 |
| H   | 3.96741 | -0.94277 | 1.79526 |
| H   | 3.19045 | 0.58686 | 1.33739 |
| C   | 6.75852 | -0.19335 | 0.06842 |
| C   | 5.57715 | -1.10063 | -0.36523 |
| H   | 5.49296 | -1.99998 | 0.24796 |
| H   | 5.63712 | -1.39465 | -1.41476 |
| H   | 7.36601 | -0.70445 | 0.81864 |
| H   | 7.39972 | 0.03357 | -0.78649 |
| N   | 4.30607 | -0.32408 | -0.18711 |
| H   | 3.4691  | -0.92217 | -0.53922 |
| O   | 2.3086  | -1.81954 | -1.02969 |
| H   | 2.06623 | -1.56696 | -1.93209 |
| H   | 1.24551 | -1.85019 | -0.37954 |
| O   | 0.30281 | -1.94915 | 0.32419 |
| C   | -0.85157 | -1.31567 | -0.15452 |
| C   | -1.33959 | -2.02361 | -1.46423 |
| N   | -2.5626 | -2.56536 | -1.22301 |
| C   | -3.0086 | -2.2982  | 0.08789 |
| C   | -2.0398 | -1.54775 | 0.76796 |
| C   | -0.54104 | 0.1983 | -0.42691 |
| C   | -1.70689 | 1.03163 | -0.81328 |
| C   | -2.47502 | 2.00897 | -0.20695 |
| C   | -3.48147 | 2.38741 | -1.15994 |
|   |   |   |   |
|---|---|---|---|
| O | -2.20858 | 0.83893 | -2.03752 |
| N | -3.33106 | 1.69168 | -2.25933 |
| N | -2.29752 | 2.54714 | 1.09249 |
| O | -3.09698 | 3.4149 | 1.47849 |
| O | -1.35897 | 2.13734 | 1.79306 |
| H | -0.09872 | 0.60537 | 0.48071 |
| H | 0.19578 | 0.24192 | -1.23623 |
| C | -4.5781 | 3.38997 | -1.05303 |
| H | -5.245 | 3.13614 | -0.22429 |
| H | -4.16803 | 4.38466 | -0.85801 |
| H | -5.14926 | 3.41096 | -1.98339 |
| C | -4.19902 | -2.69421 | 0.68479 |
| C | -2.25301 | -1.18111 | 2.09027 |
| C | -3.44859 | -1.57012 | 2.7177 |
| C | -4.40634 | -2.31448 | 2.01975 |
| H | -4.93665 | -3.27593 | 0.14088 |
| H | -1.50882 | -0.60588 | 2.63291 |
| H | -3.63033 | -1.29083 | 3.75104 |
| H | -5.32635 | -2.60831 | 2.51655 |
| O | -0.70871 | -2.10917 | -2.52335 |
| H | -3.07562 | -3.11325 | -1.9053 |

Product

Sum of electronic and zero-point Energies= -1463.722027
Sum of electronic and thermal Energies= -1463.693519
Sum of electronic and thermal Enthalpies= -1463.692575
Sum of electronic and thermal Free Energies= -1463.785730
| Element | x   | y   | z   |
|---------|-----|-----|-----|
| H       | 7.4732 | 1.41989 | -0.46126 |
| H       | 8.00771 | -0.13603 | 0.18611 |
| N       | 6.66226 | -0.2657 | -1.41451 |
| N       | 4.82602 | -0.23772 | 0.35467 |
| C       | -4.02241 | -2.14294 | 0.06395 |
| C       | -3.18858 | -1.21248 | -0.64513 |
| C       | -1.93679 | -1.23514 | -0.03572 |
| O       | -2.012 | -2.16458 | 0.93634 |
| N       | -3.32609 | -2.72244 | 1.00941 |
| N       | -3.55918 | -0.4591 | -1.77938 |
| O       | -4.73102 | -0.54197 | -2.19057 |
| O       | -2.70152 | 0.24798 | -2.33417 |
| C       | -0.66825 | -0.16097 | -1.17677 |
| H       | -0.1446 | -1.11505 | 0.19709 |
| H       | 1.97184 | 0.35613 | 1.67161 |
| C       | -5.46415 | -2.48232 | -0.11866 |
| H       | -6.0801 | -1.58374 | -0.02504 |
| H       | -5.63789 | -2.9034 | -1.11273 |
| H       | -5.76784 | -3.20846 | 0.63809 |
| O       | 2.76233 | 0.02456 | 2.20923 |
| H       | 2.4608 | -0.78851 | 2.63905 |
| H       | 4.06548 | -0.21166 | 1.07744 |
| C       | -3.7145 | 2.5034 | 0.76819 |
| C       | -2.57485 | 1.74647 | 1.01273 |
| C       | -1.93679 | 1.8145 | 0.19634 |
| C       | -1.38767 | 2.73777 | -0.84105 |
| C       | -2.51721 | 3.53667 | -1.09214 |
| C       | -3.67191 | 3.39901 | -0.31205 |
| H       | -4.59648 | 2.41504 | 1.39517 |
| H       | -0.50001 | 2.82689 | -1.46137 |
| H       | 2.49931 | 4.2569 | -1.90472 |
| H       | -4.54595 | 4.0053 | -0.53144 |
| C       | -0.44726 | 0.75347 | 0.66484 |
| O       | 0.86181 | 1.07608 | 0.68163 |
| N       | -2.33841 | 0.8377 | 2.06772 |
| C       | -1.07372 | 0.33008 | 2.02153 |
| O       | -0.54865 | -0.39186 | 2.87676 |
| H       | -2.98293 | 0.66939 | 2.83276 |

The three water molecules auxiliary without catalyst (Path C).

3H₂O
Sum of electronic and zero-point Energies= -229.284549
| Element | X         | Y         | Z       |
|---------|-----------|-----------|---------|
| H       | -2.3152   | -0.87219  | -1.29211|
| O       | -3.1995   | -1.27694  | -1.3874 |
| H       | -3.08013  | -2.19768  | -1.11062|
| H       | -4.32711  | -0.46811  | -0.27219|
| O       | -4.942    | -0.03278  | 0.36531 |
| H       | -5.54475  | 0.49427   | -0.17898|
| O       | -3.37539  | 1.59311   | 1.99615 |
| H       | -3.96563  | 1.04382   | 1.43051 |
| H       | -3.96599  | 2.05088   | 2.61112 |

TS1-C

| Element | X         | Y         | Z       |
|---------|-----------|-----------|---------|
| H       | -1.23878  | -1.94754  | 0.08984 |
| C       | -0.28795  | -1.74517  | 1.25591 |
| C       | 0.81241   | -1.14784  | 0.65332 |
| C       | 1.15386   | 0.181     | 0.27058 |
| C       | 2.40967   | 0.10029   | -0.42585|
| N       | 2.82445   | -1.13481  | -0.48107|
| O       | 1.83273   | -1.93448  | 0.20087 |
| N       | 0.40373   | 1.30077   | 0.50573 |
| C       | 3.22681   | 1.18627   | -1.03987|
| H       | 3.49491   | 1.93329   | -0.28764|
| H       | 4.13762   | 0.76477   | -1.47047|
| H       | 2.66073   | 1.69576   | -1.82478|
| H       | -0.15284  | -2.77527  | 1.58144 |
| H       | -0.91595  | -1.11173  | 1.87283 |
| O       | 0.79157   | 2.42961   | 0.09778 |
| O       | -0.69225  | 1.18166   | 1.13747 |
| H       | -2.21899  | 1.88879   | 0.38375 |
| O       | -3.12332  | 2.01485   | 0.02552 |
| H       | -3.03252  | 2.66571   | -0.68576|
| H       | -3.57358  | 0.47737   | -0.57982|
| O       | -3.82563  | -0.42316  | -0.91868|
| H       | -4.59956  | -0.69477  | -0.40247|
| O       | -1.9742   | -2.15019  | -0.76173|
| H       | -2.72973  | -1.43505  | -0.78078|

Sum of electronic and thermal Energies= -229.275965
Sum of electronic and thermal Enthalpies= -229.275021
Sum of electronic and thermal Free Energies= -229.317771

Sum of electronic and zero-point Energies= -758.354420
Sum of electronic and thermal Energies= -758.338151
Sum of electronic and thermal Enthalpies= -758.337206
Sum of electronic and thermal Free Energies= -758.398878
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | -2.38851 | -3.01672 | -0.60318 |
| IM1-C|
| Sum of electronic and zero-point Energies= | -758.358355 |
| Sum of electronic and thermal Energies= | -758.341554 |
| Sum of electronic and thermal Enthalpies= | -758.340609 |
| Sum of electronic and thermal Free Energies= | -758.405685 |
| H    | 1.36275 | 1.99944 | -0.24039 |
| C    | 0.05316 | 1.75885 | 1.49442 |
| C    | -0.90139 | 1.14954 | 0.7531 |
| C    | -1.13834 | -0.20048 | 0.29532 |
| C    | -2.34515 | -0.15669 | -0.49286 |
| N    | -2.82608 | 1.05211 | -0.54011 |
| O    | -1.95313 | 1.89866 | 0.22757 |
| N    | -0.36418 | -1.27059 | 0.54638 |
| C    | -3.04748 | -1.2613 | -1.2092 |
| H    | -3.32493 | -2.05723 | -0.5127 |
| H    | -3.94804 | -0.87416 | -1.69118 |
| H    | -2.39535 | -1.70058 | -1.96959 |
| H    | -0.02454 | 2.82121 | 1.7008 |
| H    | 0.84212 | 1.18052 | 1.95225 |
| O    | -0.63063 | -2.42457 | 0.06631 |
| O    | 0.68283 | -1.11968 | 1.29058 |
| H    | 2.13286 | -1.59623 | 0.55237 |
| O    | 3.03415 | -1.74008 | 0.15326 |
| H    | 2.93874 | -2.46017 | -0.48948 |
| H    | 3.4644 | -0.56924 | -0.47341 |
| O    | 3.8073 | 0.32851 | -0.9575 |
| H    | 4.59267 | 0.66014 | -0.489 |
| O    | 1.99946 | 2.0987 | -0.9813 |
| H    | 3.07301 | 1.06465 | -0.93186 |
| H    | 2.37336 | 2.98918 | -0.88774 |

| IM1’-C|
| Sum of electronic and zero-point Energies= | -1271.360944 |
| Sum of electronic and thermal Energies= | -1271.334626 |
| Sum of electronic and thermal Enthalpies= | -1271.333682 |
| Sum of electronic and thermal Free Energies= | -1271.419817 |
| C    | -0.67018 | 3.17076 | 0.02844 |
| C    | -1.24165 | 1.94755 | 0.53588 |
| C    | -0.23046 | 1.34475 | 1.37641 |
| N    | 0.54075 | 3.33976 | 0.47633 |
TS2-C

Sum of electronic and zero-point Energies= -1271.352166
Sum of electronic and thermal Energies= -1271.327205
Sum of electronic and thermal Enthalpies= -1271.326261
Sum of electronic and thermal Free Energies= -1271.407641
| Atm  | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 3.94929 | -1.50809| -0.93612|
| C    | 2.63592 | -1.71114| -0.39355|
| C    | 1.77424 | -0.82115| -1.07327|
| N    | 3.92076 | -0.58125| -1.85789|
| O    | 2.55994 | -0.144  | -1.95723|
| N    | 2.26446 | -2.63406| 0.56951 |
| C    | 5.23913 | -2.17114| -0.59002|
| C    | 0.42206 | -0.46414| -0.99158|
| H    | 5.17851 | -3.24759| -0.77264|
| H    | 6.04436 | -1.74869| -1.19481|
| H    | 5.47084 | -2.02738| 0.46908 |
| H    | -0.24659| -1.16855| -0.5141 |
| H    | 0.03914 | 0.07246 | -1.85285|
| O    | 3.1319  | -3.4084 | 1.05024 |
| O    | 1.06565 | -2.67967| 0.94297 |
| C    | 2.06306 | 1.68871 | 1.16151 |
| C    | 1.22047 | 2.0356  | 0.0892  |
| C    | 1.6324  | 2.97352 | -0.85168|
| C    | 2.90123 | 3.55431 | -0.70956|
| C    | 3.73289 | 3.19033 | 0.35736 |
| C    | 3.32407 | 2.24842 | 1.31568 |
| C    | 0.14794 | 0.48447 | 1.55736 |
| C    | -0.03504| 1.25502 | 0.23337 |
| H    | 0.98465 | 3.24542 | -1.68002|
| H    | 3.24253 | 4.28892 | -1.43228|
| H    | 4.71299 | 3.64814 | 0.45297 |
| H    | 3.96447 | 1.97763 | 2.14928 |
| N    | 1.41137 | 0.75731 | 1.99389 |
| O    | -1.18455| 1.61241 | -0.1743 |
| O    | -0.703  | -0.19638| 2.13925 |
| H    | 1.80085 | 0.38445 | 2.85258 |
| H    | -2.31614| -0.01905| -0.50727|
| H    | 0.11229 | -2.62427| 2.34093 |
| O    | -0.52375| -2.47036| 3.09264 |
| H    | -0.08919| -1.84957| 3.69802 |
| H    | -1.70631| -1.92891| 2.59186 |
| O    | -2.63913| -1.49199| 2.11478 |
| H    | -2.5772 | -0.55159| 2.35571 |
| O    | -2.85547| -0.81714| -0.31669|
| H    | -2.73323| -1.25213| 1.10791 |
| H    | -2.52606| -1.505  | -0.91658|

**Product**

Sum of electronic and zero-point Energies: \(-1271.394266\)

532
Sum of electronic and thermal Energies = -1271.368293
Sum of electronic and thermal Enthalpies = -1271.367349
Sum of electronic and thermal Free Energies = -1271.451289

C   0.60156  3.21037  -0.1896
C   1.13876  1.88934  -0.35668
C   0.11027  1.10626  -0.84761
N  -0.65682  3.22007  -0.55197
O  -0.96259  1.89123  -0.96534
N   2.47095  1.48228  -0.08902
C   1.25166  4.4606   0.29152
C  -0.03274 -0.3167  -1.25935
H   2.10498  4.71442  -0.34331
H    0.5301  5.2797   0.27019
H   1.62236  4.33132  -1.31173
H   0.96003 -0.7621  -1.31086
H  -0.48383 -0.33788  -2.25686
O   3.25056  2.311    0.39948
O   2.80528  0.31616  -0.35842
C  -0.92604 -1.21166  -0.34515
C  -2.36698  0.75099  -0.22745
C  -2.65158 -0.47894  -1.11415
C  -3.34939 -0.60349  -1.19527
C  -4.62365 -0.16891  -0.79639
C  -4.88994  0.10714  -0.54969
C  -3.90178  0.44311  -1.53401
C  -0.45925  1.1591   1.14937
H  -3.13739 -0.8139  -2.23929
H  -5.40647  0.04378  -1.53757
H  -5.87953  0.44475  -0.84312
H  -4.10688  0.167    2.57833
N  -1.50106  0.72024  -1.89578
O  -0.8925  -2.54277  -0.82917
O   2.65339 -0.14751  -1.58521
H  -1.45678 -0.61979   2.90505
H   0.03299  2.8409   -1.03085
H   4.4909  -0.53918   0.23191
O   5.04587 -1.32269   0.40137
H   5.49342 -1.14482   1.24202
H   4.26707 -2.46782   0.63178
O   2.84573  3.04301   0.73148
H   2.12276  2.53525   1.03131
O   1.49367  3.67428  -1.53351
H   2.10036 -3.45644  -0.78041
Microsolvant models
One-water
TS1-1W

| Atom | x    | y    | z    |
|------|------|------|------|
| C    | 1.52077 | 0.2467 | 0.89623 |
| C    | 2.73244 | 0.80366 | 1.69823 |
| H    | 0.78928 | 1.02714 | 0.67075 |
| H    | 1.01454 | -0.5627 | 1.42879 |
| H    | 2.59235 | 1.86603 | 1.91409 |
| H    | 2.83642 | 0.27726 | 2.65055 |
| N    | 3.99134 | 0.64332 | 0.93749 |
| C    | 3.85311 | 1.35143 | -0.3553 |
| C    | 2.66053 | 0.78399 | -1.18057 |
| H    | 2.98877 | 0.35726 | -2.13202 |
| H    | 1.90266 | 1.54523 | -1.38555 |
| H    | 4.78997 | 1.24036 | -0.90738 |
| H    | 3.70513 | 2.41507 | -0.15153 |
| C    | 4.19063 | -0.79746 | 0.66076 |
| H    | 5.12105 | -0.91076 | 0.09839 |
| H    | 4.30683 | -1.3191 | 1.61416 |
| C    | 2.99149 | -1.38648 | -0.14023 |
| H    | 3.30611 | -1.79031 | -1.10618 |
| H    | 2.47725 | -2.17614 | 0.41383 |
| N    | 2.01232 | -0.299  | -0.3968 |
| H    | 0.92802 | -0.76861 | -1.08207 |
| C    | -0.12501 | -1.16985 | -1.82288 |
| C    | -1.20035 | -1.39844 | -0.93845 |
| C    | -2.13818 | -0.5763 | -0.27268 |
| C    | -2.89587 | -1.43462 | 0.59698 |
| N    | -2.48051 | -2.66789 | 0.49201 |
| O    | -1.41624 | -2.65792 | -0.48146 |
| N    | -2.25664 | 0.78849 | -0.41624 |
| C    | -4.00601 | -1.10035 | 1.53462 |
| H    | -4.84741 | -0.66266 | 0.99023 |
| H    | -4.33976 | -2.00412 | 2.04869 |
| H    | -3.67241 | -0.36717 | 2.27422 |
| H    | 0.22918 | -2.07185 | -2.32355 |
| H    | -0.25099 | -0.30907 | -2.47629 |
O       -3.14889   1.40445   0.23676
O       -1.4715    1.40244  -1.18197
H       -3.0446    3.27574   0.09975
O       -3.07011   4.25436   0.10902
H       -2.34542   4.52371  -0.47313

IM1-1W

Sum of electronic and zero-point Energies=      -950.715004
Sum of electronic and thermal Energies=          -950.694594
Sum of electronic and thermal Enthalpies=        -950.693650
Sum of electronic and thermal Free Energies=     -950.766935

C       -1.53933   0.30176  -0.87272
C       -2.75154   0.8341   -1.68026
H       -0.83434   1.08754  -0.59785
H       -1.00538  -0.49831  -1.38715
H       -2.62585   1.89916  -1.88553
H       -2.82526   0.31067  -2.63572
N       -4.01926   0.64319  -0.94304
C       -3.92633   1.34483   0.35579
C       -2.76084   0.79207   1.21833
H       -3.10322   0.32539   2.14307
H       -2.01079   1.54824   1.4537
H       -4.8746    1.22213   0.88324
H       -3.77852   2.40949   0.16362
C       -4.21239  -0.80109  -0.69029
H       -5.14781  -0.93073  -0.14216
H       -4.30705  -1.31287  -1.65009
C       -3.03044  -1.40165   0.11716
H       -3.34137  -1.8191    1.07607
H       -2.47484  -2.15716  -0.44037
N       -2.07206  -0.2784   0.41275
H       -1.27161  -0.64563   0.95844
C       0.50002  -1.17016   2.1349
C       1.3265  -1.38924   1.08485
C       2.16103   -0.56    0.24802
C       2.7897  -1.4424   -0.70201
N       2.41184  -2.67482  -0.51437
O       1.49523  -2.68319   0.59517
N       2.30674   0.77525   0.3575
C       3.75178  -1.12543  -1.79814
H       4.65457  -0.65806  -1.39555
H       4.02817  -2.0428   -2.32285
H       3.30761  -0.42405  -2.51013
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | 0.00463| -2.00866| 2.61339|
| H    | 0.39809| -0.17861| 2.55182|
| O    | 3.09525| 1.41689 | -0.43498|
| O    | 1.65397| 1.41371 | 1.25074|
| H    | 3.09271| 3.20931 | -0.1202 |
| O    | 3.16216| 4.1886  | -0.05501|
| H    | 2.62224| 4.42277 | 0.71309 |

Three-water
TS1-3W

Sum of electronic and zero-point Energies= -1103.563745
Sum of electronic and thermal Energies= -1103.538196
Sum of electronic and thermal Enthalpies= -1103.537252
Sum of electronic and thermal Free Energies= -1103.622694

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -1.85324| -1.16506| -4.02026|
| C    | -3.34782| -0.92444| -3.66207|
| H    | -1.55665| -2.2053 | -3.86304|
| H    | -1.18473| -0.52336| -3.44044|
| H    | -3.82796| -1.86147| -3.36866|
| H    | -3.43126| -0.22755| -2.82417|
| N    | -4.08914| -0.3652 | -4.81572|
| C    | -4.02504| -1.34169| -5.9271 |
| C    | -2.55019| -1.67788| -6.29363|
| H    | -2.33046| -1.46418| -7.34289|
| H    | -2.31019| -2.726  | -6.09695|
| H    | -4.54683| -0.91372| -6.78691|
| H    | -4.55919| -2.24646| -5.62593|
| C    | -3.41143| 0.87821 | -5.24832|
| H    | -3.97983| 1.31151 | -6.07527|
| H    | -3.43492| 1.58653 | -4.41617|
| C    | -1.94409| 0.59548 | -5.68774|
| H    | -1.78861| 0.80138 | -6.75005|
| H    | -1.22187| 1.18132 | -5.11251|
| N    | -1.64939| -0.84233| -5.45736|
| H    | -0.35123| -1.09243| -5.75753|
| C    | 0.92165 | -1.33709| -6.1349 |
| C    | 1.71037 | -1.56437| -4.90665|
| C    | 2.11635 | -2.68238| -4.19939|
| C    | 2.87413 | -2.20753| -3.07687|
| N    | 2.92163 | -0.89907| -3.10252|
| O    | 2.18317 | -0.49768| -4.2629 |
| N    | 1.82356 | -4.01758| -4.53927|
| C    | 3.5517  | -2.96432| -1.98788|
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 4.30059 | -3.64288| -2.40585|
| H    | 4.03867 | -2.26803| -1.3025 |
| H    | 2.82632 | -3.56761| -1.43478|
| H    | 1.21008 | -0.37741| -6.56688|
| H    | 0.93965 | -2.24788| -6.74122|
| O    | 2.25599 | -4.92229| -3.80441|
| O    | 1.14612 | -4.2331 | -5.55954|
| H    | 2.04561 | -6.87984| -3.92175|
| O    | 2.07307 | -7.85136| -3.84816|
| H    | 1.44214 | -8.06729| -3.14572|
| H    | 0.23625 | -5.73891| -6.51189|
| O    | -0.18575| -6.3728 | -7.11796|
| H    | -1.11705| -6.39201| -6.85254|
| H    | 0.62043 | -7.97982| -6.65118|
| O    | 1.09421 | -8.77568| -6.32997|
| H    | 1.44415 | -8.50505| -5.45439|

**IM1-3W**

**Sum of electronic and zero-point Energies=** -1103.575774

**Sum of electronic and thermal Energies=** -1103.549838

**Sum of electronic and thermal Enthalpies=** -1103.548893

**Sum of electronic and thermal Free Energies=** -1103.635297

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -2.25049| -0.13616| 1.03292 |
| C    | -3.41821| -0.78686| 1.83282 |
| H    | -1.33032| -0.71607| 1.10302 |
| H    | -2.05141| 0.88714 | 1.35581 |
| H    | -3.0736 | -1.69394| 2.33162 |
| H    | -3.78124| -0.0947 | 2.59875 |
| N    | -4.54524| -1.1385 | 0.94716 |
| C    | -4.0562 | -2.08374| -0.0763 |
| C    | -2.89335| -1.4677 | -0.90509|
| H    | -3.13473| -1.39654| -1.96532|
| H    | -1.96353| -2.02883| -0.79156|
| H    | -4.88881| -2.34701| -0.73278|
| H    | -3.71919| -2.99362| 0.42584 |
| C    | -5.00972| 0.08866 | 0.26746 |
| H    | -5.85038| -0.17289| -0.38288|
| H    | -5.37658| 0.78338 | 1.02354 |
| C    | -3.87186| 0.74268 | -0.56727|
| H    | -4.10379| 0.77943 | -1.62913|
| H    | -3.63309| 1.75114 | -0.22148|
| N    | -2.63094| -0.07799| -0.41186|
| H    | -1.88913| 0.30692 | -0.91138|
Six-water
TS1-6W

Sum of electronic and zero-point Energies= -1332.850827
Sum of electronic and thermal Energies= -1332.816160
Sum of electronic and thermal Enthalpies= -1332.815216
Sum of electronic and thermal Free Energies= -1332.922091

C   -0.57577  0.88977  -1.89986
C    0.26976  1.62534  -1.10571
C    1.32614  1.32216  -0.18598
C    1.75317  2.57837   0.38102
N    1.05358  3.56525  -0.10822
O    0.12103  2.98705  -1.04579
N    1.77946   0.07927   0.11074
C    2.82624  2.84892   1.37979
H    3.79087  2.49263   1.00785
H    2.88849   3.92204   1.57216
H    2.61758   2.32615   2.31743
H   -1.14512  1.45234  -2.64441
H   -0.23062  -0.09846  -2.2049
O    2.71781  -0.07254   0.95643
O    1.24934  -0.93207  -0.44641
H    4.55972  -0.26369   0.46843
O    5.4993   -0.44308   0.25495
H    5.96928  -0.341   1.09593
H    2.05438  -2.60715  -0.2077
O    2.43279  -3.51325  -0.25779
H    2.23802  -3.9202   0.59882
H    4.26094  -3.31151  -0.40029
O    5.23106  -3.18388  -0.47607
H    5.37735  -2.25025  -0.21746

C   -1.14852  -1.99676   1.02962
C   -1.90909  -3.06671   1.86769
H   -0.08736  -2.23815   0.92225
H   -1.23405  -0.9997   1.47031
H   -1.20515  -3.77932   2.30518
H   -2.46116  -2.5943   2.68431
N   -2.87552  -3.80902   1.02703
C   -2.14196  -4.3809  -0.12575
C   -1.52891  -3.25687  -1.00881
H   -2.00626  -3.2014  -1.99071
H   -0.45383  -3.39265  -1.15496
H   -2.83275  -4.99255  -0.71195
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -1.35905 | -5.03713 | 0.26319 |
| C    | -3.88 | -2.85059 | 0.51314 |
| H    | -4.55291 | -3.39087 | -0.15777 |
| H    | -4.47007 | -2.47756 | 1.35409 |
| C    | -3.19441 | -1.66831 | -0.23444 |
| H    | -3.5867 | -1.54423 | -1.24725 |
| H    | -3.31308 | -0.72404 | 0.30372 |
| N    | -1.73936 | -1.95145 | -0.33217 |
| H    | -1.07999 | -0.96597 | -1.05512 |
| C    | -0.42458 | -0.11154 | -1.83121 |
| C    | 0.02694 | 0.9542 | -1.02451 |
| C    | 1.1267 | 1.16293 | -0.16204 |
| C    | 0.93996 | 2.45078 | 0.44694 |
| N    | -0.16786 | 2.99053 | 0.01598 |
| O    | -0.74667 | 2.06394 | -0.91592 |
| N    | 2.15841 | 0.27858 | 0.06171 |
| C    | 1.78991 | 3.17673 | 1.43264 |
| H    | 2.79154 | 3.33683 | 1.02462 |
| H    | 1.33692 | 4.14138 | 1.66988 |
| H    | 1.89381 | 2.59041 | 2.34981 |
| H    | -1.16956 | 0.18824 | -2.56934 |
| H    | 0.36992 | -0.74353 | -2.22277 |
| O    | 3.0915 | 0.59544 | 0.84818 |
| O    | 2.14031 | -0.84137 | -0.51576 |
| H    | 4.86938 | 1.01873 | 0.21074 |
| O    | 5.77057 | 1.19992 | -0.11704 |
| H    | 6.23478 | 1.59903 | 0.63357 |
| H    | 3.49071 | -2.08297 | -0.09734 |
| O    | 4.15875 | -2.79551 | -0.02299 |
| H    | 4.15254 | -3.05273 | 0.91061 |
| H    | 5.76861 | -1.96315 | -0.37169 |
| O    | 6.60146 | -1.47941 | -0.56093 |
| H    | 6.37559 | -0.53819 | -0.40597 |
| O    | -3.73551 | 1.99724 | -1.2917 |
| H    | -2.76962 | 1.96271 | -1.17973 |
| H    | -4.0633 | 1.20911 | -0.83272 |
| O    | -1.71255 | 5.36504 | 0.68409 |
| H    | -1.16695 | 4.59501 | 0.4135 |
| H    | -1.5173 | 6.05727 | 0.03581 |
| O    | -4.31338 | 4.35645 | 0.20975 |
| H    | -4.12941 | 3.55587 | -0.32375 |
| H    | -3.42711 | 4.73159 | 0.40067 |

IM1-6W
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -1.41353  | -1.77325  | 1.09206   |
| C       | -2.14538  | -2.90674  | 1.85714   |
| H       | -0.35815  | -1.98916  | 0.92026   |
| H       | -1.50994  | -0.80146  | 1.57836   |
| H       | -1.4692   | -3.74619  | 2.03251   |
| H       | -2.48891  | -2.53959  | 2.82636   |
| N       | -3.31139  | -3.40206  | 1.09636   |
| C       | -2.84202  | -3.98955  | -0.17505  |
| C       | -1.996    | -2.97447  | -0.98567  |
| H       | -2.37852  | -2.81162  | -1.99428  |
| H       | -0.94144  | -3.24769  | -1.04077  |
| H       | -3.71658  | -4.30215  | -0.74959  |
| H       | -2.24607  | -4.87746  | 0.04574   |
| C       | -4.20539  | -2.26505  | 0.79675   |
| H       | -5.10222  | -2.64216  | 0.30124   |
| H       | -4.50524  | -1.80775  | 1.74196   |
| C       | -3.50278  | -1.21931  | -0.1103   |
| H       | -3.92647  | -1.17489  | -1.11476  |
| H       | -3.49499  | -0.21893  | 0.32544   |
| N       | -2.06684  | -1.65364  | -0.26082  |
| H       | -1.55371  | -0.95129  | -0.81442  |
| C       | -0.07194  | 0.14782   | -2.24698  |
| C       | 0.28574   | 0.93637   | -1.21848  |
| C       | 1.23935   | 0.84903   | -0.13985  |
| C       | 1.10497   | 2.05724   | 0.62983   |
| N       | 0.18456   | 2.82112   | 0.12016   |
| O       | -0.34636  | 2.16627   | -1.03808  |
| N       | 2.06997   | -0.16478  | 0.08095   |
| C       | 1.84362   | 2.49912   | 1.84818   |
| H       | 2.91697   | 2.54804   | 1.64597   |
| H       | 1.48885   | 3.48431   | 2.15789   |
| H       | 1.69274   | 1.78853   | 2.66575   |
| H       | -0.83182  | 0.48436   | -2.94372  |
| H       | 0.42557   | -0.7967   | -2.41204  |
| O       | 2.88646   | -0.15094  | 1.0617    |
| O       | 2.03307   | -1.1717   | -0.69596  |
| H       | 4.57512   | 0.50647   | 0.79065   |
| O       | 5.49854   | 0.80144   | 0.63083   |
| H       | 5.88128   | 0.92593   | 1.51164   |
H     3.41387 -2.34051 -0.69669
O     4.12368 -3.00286 -0.85737
H     4.04021 -3.64694 -0.13947
H     5.71408 -2.08509 -0.67223
O     6.53274 -1.55531 -0.56579
H     6.22757 -0.72369 -0.14614
O    -3.21802  2.38471 -1.52338
H    -2.2728  2.22957 -1.34364
H    -3.67143  1.60093 -1.17699
O    -0.93125  5.44277  0.48445
H    -0.50039  4.56487  0.37086
H    -0.64737  5.96430 -0.2809
O    -3.63096  4.63657  0.17876
H    -3.54571  3.85873 -0.41099
H    -2.71242  4.96771  0.27843

The first sep for DABCO catalyzes directly the vinylogous Henry reaction of 1a and 2 in CH₃OH.

2
Sum of electronic and zero-point Energies= -529.103355
Sum of electronic and thermal Energies= -529.094135
Sum of electronic and thermal Enthalpies= -529.093191
Sum of electronic and thermal Free Energies= -529.138030

C     -1.1401  -0.74977  -0.00001
C     -0.00421  0.12669  -0.00002
C     1.10736  -0.68684  -0.00001
N    -0.73668  -1.99708   0.
O     0.6827  -1.95143  -0.00001
N     0.00333  1.55427  -0.00001
C    -2.60007  -0.43309  0.00001
C     2.57333  -0.45079  0.00003
H    -2.86421  0.16093  -0.87895
H    -3.17095  -1.36358  -0.00001
H    -2.86418  0.16087  0.87901
H     2.86434  0.13265  0.87821
H     3.09862  -1.40764  -0.00025
H     2.8643  0.1332  -0.8778
O    -1.08712  2.13461  0.00003
O     1.10288  2.12258  -0.00003

DABCO
Sum of electronic and zero-point Energies= -345.187531
Sum of electronic and thermal Energies= -345.181234
|   | Sum of electronic and thermal Enthalpies= | -345.180290 |
|---|------------------------------------------|-------------|
|   | Sum of electronic and thermal Free Energies= | -345.217838 |

|   | C | 0.78284 | 1.37853 | -0.14177 |
|---|---|---------|---------|----------|
|   | C | 0.78288 | 1.37848 | -0.14202 |
|   | H | -1.18609 | 1.79416 | -1.07252 |
|   | H | -1.18566 | 1.97537 | 0.68478  |
|   | H | 1.1859  | 1.79481 | -1.07257 |
|   | H | 1.18598 | 1.97464 | 0.68488  |
| N | -1.28869 | 0.00021 | 0.00059 |
|   | C | -0.78354 | -0.81231 | -1.12223 |
|   | H | -1.18623 | -1.82633 | -1.01609 |
|   | H | -1.18743 | -0.39548 | -2.0522  |
| C | 0.78224 | -0.812   | -1.12333 |
|   | H | 1.18552 | -1.82592 | -1.01849 |
|   | H | 1.18463 | -0.39438 | -2.0536  |
| N | 1.28869 | 0.00003 | -0.00075 |
|   | C | 0.78356 | -0.5667 | 1.26422  |
|   | H | 1.18624 | -1.5811 | 1.36678  |
|   | H | 1.18731 | 0.03104 | 2.08964  |
| C | -0.78231 | -0.56613 | 1.26524  |
|   | H | -1.18563 | -1.58015 | 1.36902  |
|   | H | -1.18451 | 0.03248 | 2.09078  |

|   | TS1 |
|---|-----|
|   | Sum of electronic and zero-point Energies= | -874.277897 |
|   | Sum of electronic and thermal Energies= | -874.261532 |
|   | Sum of electronic and thermal Enthalpies= | -874.260588 |
|   | Sum of electronic and thermal Free Energies= | -874.323469 |

|   | C | 3.20921 | -0.70673 | 0.56683 |
|---|---|---------|---------|---------|
|   | C | 2.37674 | 0.12944 | -0.25309 |
|   | C | 1.55706 | -0.73469 | -1.01337 |
|   | N | 2.94338 | -1.96692 | 0.34941  |
|   | O | 1.90705 | -1.99641 | -0.65229 |
|   | N | 2.3418 | 1.50939 | -0.2826  |
|   | C | 4.25435 | -0.3302 | 1.56171  |
|   | C | 0.48078 | -0.55818 | -1.90817 |
|   | H | 3.82394 | 0.29008 | 2.35284  |
|   | H | 4.68305 | -1.2316 | 2.00486  |
|   | H | 5.04874 | 0.24863 | 1.08235  |
|   | H | 0.24806 | -1.4482 | -2.49452 |
|   | H | -0.63426 | -0.36932 | -1.15387 |
|   | H | 0.51359 | 0.36644 | -2.48005 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| O       | 3.12991 | 2.16812 | 0.44726 |
| O       | 1.51285 | 2.08563 | -1.03502 |
| N       | -1.76891 | -0.17469 | -0.43795 |
| C       | -1.49918 | -0.59384 | 0.96295 |
| C       | -2.80121 | -0.41775 | 1.79583 |
| H       | -1.16197 | -1.63342 | 0.94475 |
| H       | -0.68363 | 0.02776 | 1.3416 |
| H       | -3.15657 | -1.38443 | 2.16174 |
| H       | -2.61538 | 0.22176 | 2.66254 |
| C       | -2.88564 | -0.97971 | -0.99811 |
| H       | -3.01531 | -0.6936 | -2.04512 |
| H       | -2.58933 | -2.03123 | -0.96148 |
| C       | -4.16685 | -0.70828 | -0.15705 |
| H       | -4.93927 | -0.2409 | -0.77318 |
| H       | -4.57106 | -1.64475 | 0.2357 |
| C       | -2.13003 | 1.26624 | -0.46198 |
| C       | -3.38045 | 1.4799 | 0.44186 |
| H       | -4.1865 | 1.94921 | -0.12795 |
| H       | -3.13974 | 2.13283 | 1.28478 |
| H       | -2.32469 | 1.54361 | -1.50132 |
| H       | -1.26477 | 1.83387 | -0.1087 |
| N       | -3.87655 | 0.19327 | 0.98127 |

**IM1**

- Sum of electronic and zero-point Energies= -874.286889
- Sum of electronic and thermal Energies= -874.269691
- Sum of electronic and thermal Enthalpies= -874.268747
- Sum of electronic and thermal Free Energies= -874.335144
The first step for DABCO catalyzes directly the vinylogous Henry reaction of 1a and 2 in THF.

2

| Element | X   | Y    | Z    |
|---------|-----|------|------|
| O       | 1.57069 | 1.94943 | -1.37728 |
| C       | -1.44622 | -0.50074 | 1.02231 |
| C       | -2.73485 | -0.19782 | 1.82885 |
| H       | -1.10205 | -1.52897 | 1.14176 |
| H       | -0.62923 | 0.18149 | 1.26039 |
| H       | -3.11355 | -1.10794 | 2.29859 |
| H       | -2.51545 | 0.52469 | 2.61749 |
| C       | -2.9337 | -1.18084 | -0.82469 |
| H       | -3.05833 | -1.09687 | -1.90516 |
| H       | -2.65464 | -2.20533 | -0.5731 |
| C       | -4.17187 | -0.68171 | 0.24307 |
| H       | -4.90752 | -0.2471 | -0.71483 |
| H       | -4.64348 | -1.51726 | 0.48686 |
| C       | -3.26974 | 1.52925 | 0.24307 |
| H       | -4.07818 | 1.98242 | -0.33439 |
| H       | -2.93412 | 2.25626 | 0.9857 |
| C       | -2.10213 | 1.14269 | -0.70075 |
| H       | -2.36691 | 1.21852 | -1.75643 |
| H       | -1.19431 | 1.71971 | -0.51841 |
| N       | -1.77255 | -0.30355 | -0.43571 |
| N       | -3.79883 | 0.34883 | 0.95894 |

The sum of electronic and zero-point Energies is -529.105086
The sum of electronic and thermal Energies is -529.095727
The sum of electronic and thermal Enthalpies is -529.094783
The sum of electronic and thermal Free Energies is -529.140265
O | -1.08712 | 2.13461 | 0.00003
O | 1.10288 | 2.12258 | -0.00003

DABCO
Sum of electronic and zero-point Energies= -345.183109
Sum of electronic and thermal Energies= -345.176748
Sum of electronic and thermal Enthalpies= -345.175804
Sum of electronic and thermal Free Energies= -345.213514

C | -0.78284 | 1.37853 | -0.14177
C | 0.78288 | 1.37848 | -0.14202
H | -1.18609 | 1.79416 | -1.07252
H | -1.18566 | 1.97537 | 0.68478
H | 1.1859 | 1.79481 | -1.07257
H | 1.18598 | 1.97464 | 0.68488
N | -1.28869 | 0.00021 | 0.00059
C | -0.78354 | -0.81231 | -1.12223
H | -1.18623 | -1.82633 | -1.01609
H | -1.18743 | -0.39548 | -2.0522
C | 0.78224 | -0.812 | -1.12333
H | 1.18552 | -1.82592 | -1.01849
H | 1.18463 | -0.39438 | -2.0536
N | 1.28869 | 0.00003 | -0.00075
C | 0.78356 | -0.5667 | 1.26422
H | 1.18624 | -1.5811 | 1.36678
H | 1.18731 | 0.03104 | 2.08964
C | -0.78231 | -0.56613 | 1.26524
H | -1.18563 | -1.58015 | 1.36902
H | -1.18451 | 0.03248 | 2.09078

TS1
Sum of electronic and zero-point Energies= -874.272544
Sum of electronic and thermal Energies= -874.256004
Sum of electronic and thermal Enthalpies= -874.255060
Sum of electronic and thermal Free Energies= -874.319247

C | 3.20921 | -0.70673 | 0.56683
C | 2.37674 | 0.12944 | -0.25309
C | 1.55706 | -0.73469 | -1.01337
N | 2.94338 | -1.96692 | 0.34941
O | 1.90705 | -1.99641 | -0.65229
N | 2.3418 | 1.50939 | -0.2826
C | 4.25435 | -0.3302 | 1.56171
C | 0.48078 | -0.55818 | -1.90817
H    3.82394  0.29008  2.35284
H    4.68305 -1.2316   2.00486
H    5.04874  0.24863  1.08235
H    0.24806 -1.4482 - 2.49452
H   -0.63426 -0.36932 -1.15387
H    0.51359  0.36644 -2.48005
O    3.12991  2.16812  0.44726
O    1.51285  2.08563 -1.03502
N   -1.76891 -0.17469 -0.43795
C   -1.49918 -0.59384  0.96295
C   -2.80121 -0.41775  1.79583
H   -1.16197 -1.63342  0.94475
H   -0.68363  0.02776  1.3416
H   -3.15657 -1.38443  2.16174
H   -2.61538  0.22176  2.66254
C   -2.88564 -0.97971 -0.99811
H   -3.01531 -0.6936  -2.04512
H   -2.58933 -2.03123 -0.96148
C   -4.16685 -0.70828 -0.15705
H  -4.93927 -0.2409  -0.77318
H  -4.57106 -1.64475  0.2357
C  -2.13003  1.26624 -0.46198
C  -3.38045  1.4799  0.44186
H  -4.1865  1.94921 -0.12795
H  -3.13974  2.13283  1.28478
H  -2.32469  1.54361 -1.50132
H  -1.26477  1.83387 -0.1087
N  -3.87655  0.19327  0.98127

IM1
Sum of electronic and zero-point Energies=  -874.273827
Sum of electronic and thermal Energies=       -874.256631
Sum of electronic and thermal Enthalpies=      -874.255687
Sum of electronic and thermal Free Energies=   -874.321865

C    3.04923 -0.59339  0.76684
C    2.33987  0.13084 -0.25534
C    1.71199 -0.85921 -1.09691
N    2.90499 -1.87982  0.61569
O    2.07476 -2.08646 -0.54373
N    2.26354  1.47041 -0.41441
C    3.86659 -0.07136  1.90177
C    0.91581 -0.82563 -2.1926
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | 3.26323 | 0.57675 | 2.54355 |
| H    | 4.25141 | -0.90513 | 2.49346 |
| H    | 4.70624 | 0.5224 | 1.52989 |
| H    | 0.59717 | -1.75401 | -2.65491 |
| H    | -0.94103 | -0.56091 | -0.99661 |
| H    | 0.66116 | 0.11734 | -2.65407 |
| O    | 2.87076 | 2.26458 | 0.38745 |
| O    | 1.57069 | 1.94943 | -1.37728 |
| C    | -1.44622 | -0.50074 | 1.02231 |
| C    | -2.73485 | -0.19782 | 1.82885 |
| H    | -1.10205 | -1.52897 | 1.14176 |
| H    | -0.62923 | 0.18149 | 1.26039 |
| H    | -3.11355 | -1.10794 | 2.29859 |
| H    | -2.51545 | 0.52469 | 2.61749 |
| C    | -2.9337 | -1.18084 | -0.82469 |
| H    | -3.05833 | -1.09687 | -1.90516 |
| H    | -2.65464 | -2.20533 | -0.5731 |
| C    | -4.17187 | -0.68171 | -0.03469 |
| H    | -4.90752 | -0.2471 | -0.71483 |
| H    | -4.64348 | -1.51726 | 0.48686 |
| C    | -3.26974 | 1.52925 | 0.24307 |
| H    | -4.07818 | 1.98242 | -0.33439 |
| H    | -2.93412 | 2.25626 | 0.9857 |
| C    | -2.10213 | 1.14269 | -0.70075 |
| H    | -2.36691 | 1.21852 | -1.75643 |
| H    | -1.19431 | 1.71971 | -0.51841 |
| N    | -1.77255 | -0.30355 | -0.43571 |
| N    | -3.79883 | 0.34883 | 0.95894 |