# Supporting Information

# Mechanism and Origins of Regioselecitivities of Rh-Catalyzed Alkenylation of Allylbenzenes

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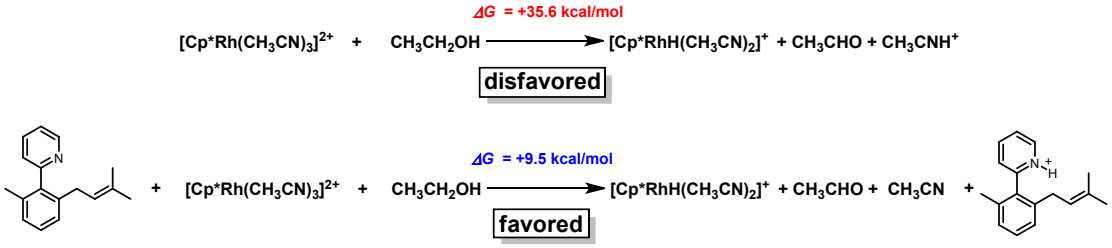


Figure S1. Transformations of the $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$

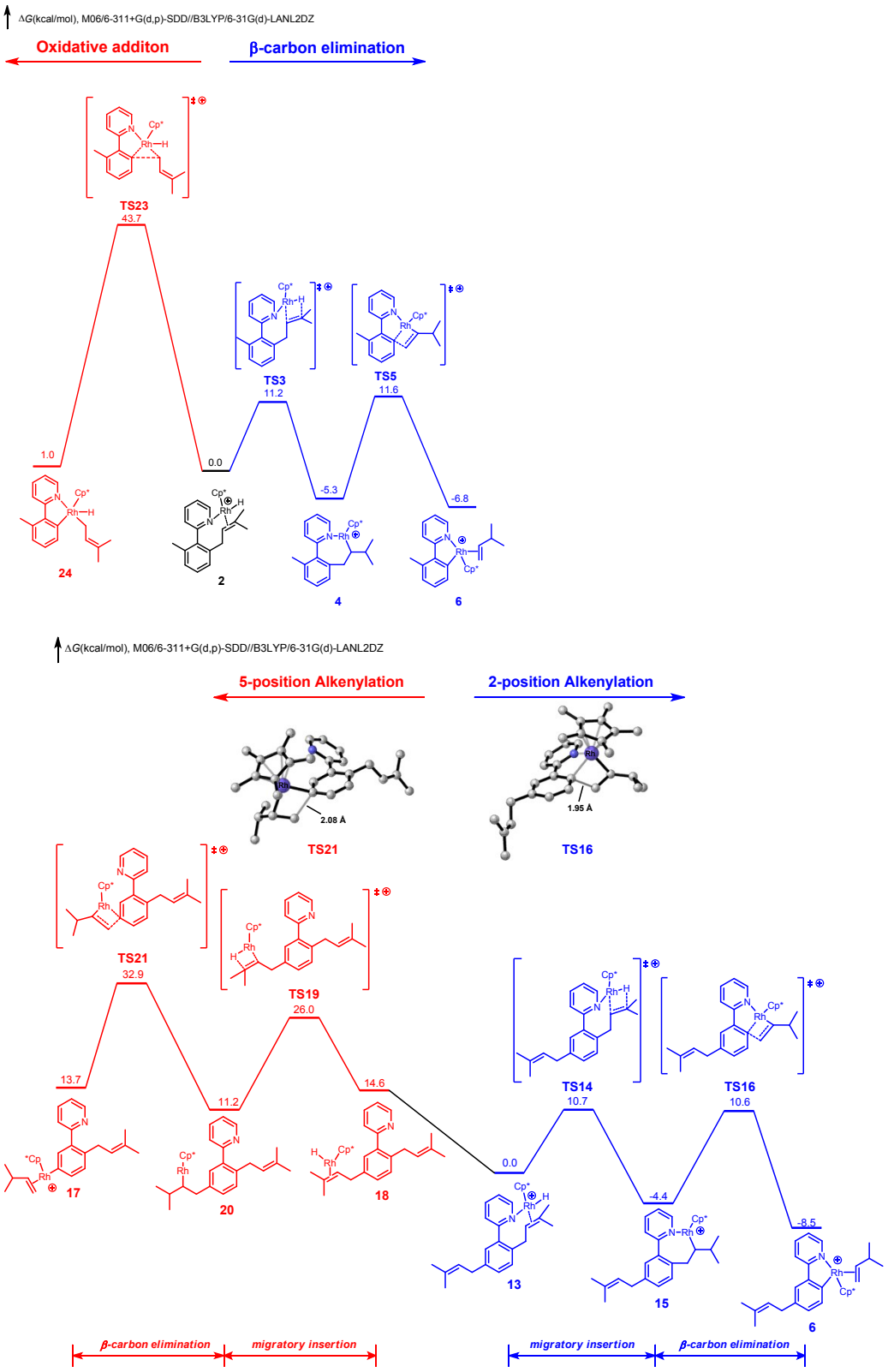


Figure S2. DFT-computed Gibbs free changes under gas phase

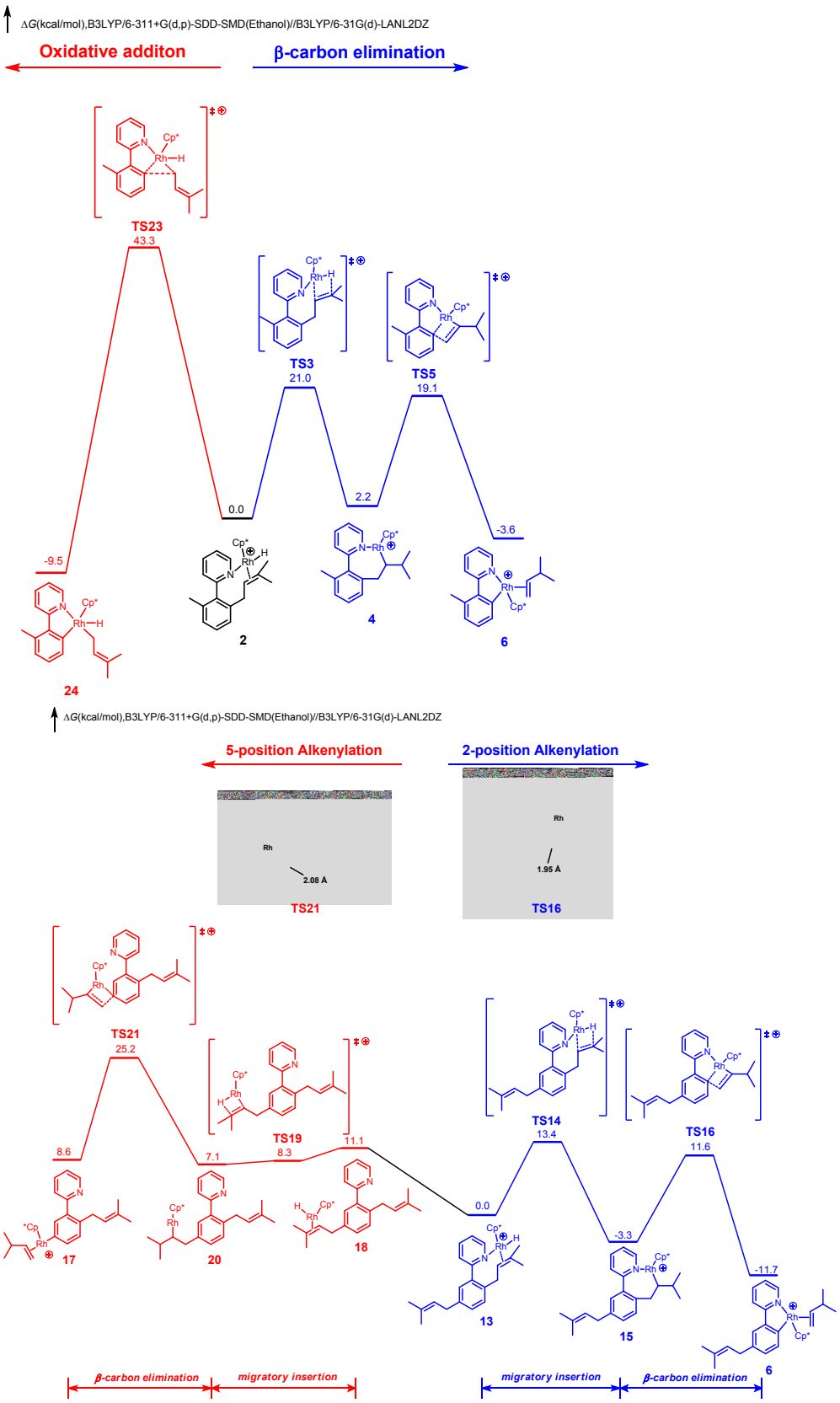


Figure S3. Solvent effects were computed with the B3LYP

1. Hong, X.; Trost, B. M.; Houk, K. N. J. Am. Chem. Soc. 2013, 135, 6588−6600.
2. Lu, G.; Fang, C.; Xu, T.; Dong, G.; Liu, P. J. Am. Chem. Soc. 2015, 137, 8274−8283.

## Cartesian coordinates (in angstrom) and solution-phase Gibbs fee energies (in Hartree) of all intermediates and transition states.

**1a**

Thermal correction to Gibbs free energy: 0.268294
SCF energy in solution: -713.622665268
Sum of electronic and thermal Energies: -713.649942
Solution-phase Gibbs free energy: -713.354371268
Coordinates:

| | | | |
|---|---|---|---|
| C | -1.68905 | -0.46954 | 0.02095 |
| C | -2.46231 | -0.80818 | 1.14234 |
| C | -3.17461 | -2.00576 | 1.14358 |
| C | -3.0958 | -2.83357 | 0.02426 |
| C | -2.29628 | -2.41917 | -1.04175 |
| C | -0.90799 | 0.81016 | -0.01886 |
| C | -1.58847 | 2.04003 | -0.14241 |
| C | -0.84275 | 3.22411 | -0.19017 |
| C | 0.54748 | 3.19627 | -0.12096 |
| C | 1.21294 | 1.97746 | -0.00636 |
| C | 0.5022 | 0.77361 | 0.04665 |
| H | -2.49151 | -0.1404 | 1.9982 |
| H | -3.77671 | -2.28814 | 2.00337 |
| H | -3.63306 | -3.77612 | -0.02342 |
| H | -2.20353 | -3.03936 | -1.93252 |
| H | -1.36272 | 4.17382 | -0.2922 |
| H | 1.11373 | 4.12337 | -0.16283 |
| H | 2.29748 | 1.9507 | 0.04042 |
| N | -1.6052 | -1.27351 | -1.05565 |
| C | -3.09773 | 2.10692 | -0.25251 |
| H | -3.47865 | 1.41567 | -1.01261 |
| H | -3.59516 | 1.8477 | 0.69027 |
| H | -3.41857 | 3.11734 | -0.52484 |
| C | 1.24169 | -0.55917 | 0.15062 |
| H | 0.65977 | -1.22829 | 0.80013 |
| H | 1.22969 | -1.04165 | -0.83282 |
| C | 2.63987 | -0.46567 | 0.70276 |
| H | 2.69642 | -0.07763 | 1.72147 |
| C | 3.79532 | -0.8112 | 0.1125 |
| C | 3.9222 | -1.35458 | -1.29027 |
| H | 4.36092 | -2.36237 | -1.27775 |
| H | 2.96923 | -1.41066 | -1.82101 |

| | | | |
|---|---|---|---|
| H | 4.60193 | -0.72898 | -1.88542 |
| C | 5.10727 | -0.67997 | 0.8513 |
| H | 5.80061 | -0.01771 | 0.31357 |
| H | 4.97021 | -0.28062 | 1.86132 |
| H | 5.61238 | -1.65281 | 0.93623 |

**2a**

Thermal correction to Gibbs free energy: 0.102269
SCF energy in solution: -309.476464729
Sum of electronic and thermal Energies:-309.501277
Solution-phase Gibbs free energy: -309.374195729
Coordinates:

| | | | |
|---|---|---|---|
| C | 2.9779 | -0.33507 | -0.00013 |
| H | 2.84078 | -1.41309 | -0.00038 |
| H | 4.00494 | 0.01704 | -0.00007 |
| C | 1.95506 | 0.52953 | 0.0001 |
| H | 2.18661 | 1.5949 | 0.00031 |
| C | 0.51535 | 0.22048 | 0.00006 |
| C | -0.40651 | 1.28162 | -0.00001 |
| C | 0.00898 | -1.09281 | 0.00008 |
| C | -1.78126 | 1.04647 | -0.00006 |
| H | -0.03503 | 2.30403 | -0.00002 |
| C | -1.36245 | -1.3299 | 0.00003 |
| H | 0.69406 | -1.93568 | 0.00015 |
| C | -2.26578 | -0.26186 | -0.00005 |
| H | -2.47243 | 1.88524 | -0.00011 |
| H | -1.73073 | -2.35258 | 0.00005 |
| H | -3.33588 | -0.45063 | -0.00008 |

**3a**

Thermal correction to Gibbs free energy: 0.108389
SCF energy in solution: -196.420884534
Sum of electronic and thermal Energies:-196.386767
Solution-phase Gibbs free energy: -196.312495534
Coordinates:

| | | | |
|---|---|---|---|
| C | -1.98856 | -0.05448 | 0.24188 |
| H | -2.92902 | -0.59403 | 0.31738 |
| H | -1.99418 | 0.97196 | 0.59854 |
| C | -0.89813 | -0.63224 | -0.26505 |
| H | -0.96972 | -1.66854 | -0.60215 |
| C | 0.47564 | -0.01907 | -0.42274 |
| C | 0.55966 | 1.44749 | 0.01558 |
| H | -0.14994 | 2.07409 | -0.53601 |
| H | 0.34339 | 1.55342 | 1.08571 |

| | | | |
|---|---|---|---|
| H | 1.56624 | 1.84301 | -0.16108 |
| C | 1.52444 | -0.87919 | 0.31214 |
| H | 1.34743 | -0.86468 | 1.39429 |
| H | 1.48827 | -1.92405 | -0.0184 |
| H | 2.53753 | -0.50275 | 0.12766 |
| H | 0.72164 | -0.06352 | -1.49674 |

**4a**

Thermal correction to Gibbs free energy: 0.351411
SCF energy in solution: -869.5657949
Sum of electronic and thermal Energies: -869.582609
Solution-phase Gibbs free energy: -869.2143839
Coordinates:

| | | | |
|---|---|---|---|
| C | 0.33774 | 1.69496 | -0.1419 |
| C | -0.61331 | 2.58164 | -0.67896 |
| C | -0.41967 | 3.95373 | -0.54684 |
| C | 0.72084 | 4.41325 | 0.11151 |
| C | 1.61875 | 3.4635 | 0.59901 |
| C | 0.12904 | 0.22076 | -0.22633 |
| C | -1.46287 | -1.63436 | 0.02076 |
| C | -0.44019 | -2.52153 | -0.32986 |
| C | 0.8369 | -2.0487 | -0.62179 |
| C | 1.155 | -0.68537 | -0.58089 |
| H | -1.47928 | 2.19179 | -1.20409 |
| H | -1.14331 | 4.65245 | -0.9587 |
| H | 0.91556 | 5.47383 | 0.23902 |
| H | 2.52672 | 3.77715 | 1.11245 |
| H | -0.64343 | -3.5895 | -0.37501 |
| H | 1.61551 | -2.75594 | -0.89882 |
| N | 1.44337 | 2.14311 | 0.48405 |
| C | 2.57489 | -0.27024 | -0.94864 |
| H | 2.89507 | -0.86947 | -1.80759 |
| H | 2.5835 | 0.77615 | -1.27012 |
| C | 3.53535 | -0.42959 | 0.2071 |
| H | 3.27955 | 0.18787 | 1.06634 |
| C | 4.6195 | -1.21686 | 0.28743 |
| C | 5.12142 | -2.13108 | -0.80485 |
| H | 4.50267 | -2.11443 | -1.70545 |
| H | 6.14519 | -1.85898 | -1.099 |
| H | 5.16962 | -3.17049 | -0.44982 |
| C | 5.4595 | -1.2349 | 1.54429 |
| H | 6.49766 | -0.93948 | 1.33364 |
| H | 5.0628 | -0.55893 | 2.30822 |
| H | 5.50695 | -2.24543 | 1.97558 |
| C | -1.1557 | -0.27239 | 0.05859 |

| | | | |
|---|---|---|---|
| H | -1.93647 | 0.42998 | 0.33877 |
| C | -2.85649 | -2.13339 | 0.37802 |
| H | -2.99537 | -2.07357 | 1.46427 |
| H | -2.91272 | -3.20286 | 0.12792 |
| C | -3.96036 | -1.39973 | -0.343 |
| H | -3.87285 | -1.42316 | -1.4303 |
| C | -5.00674 | -0.73962 | 0.17895 |
| C | -6.02179 | -0.07422 | -0.72188 |
| H | -6.0896 | 1.00329 | -0.51466 |
| H | -5.77519 | -0.20201 | -1.78067 |
| H | -7.02787 | -0.48486 | -0.55533 |
| C | -5.29676 | -0.59621 | 1.65378 |
| H | -6.25971 | -1.06255 | 1.90553 |
| H | -4.53302 | -1.04454 | 2.29346 |
| H | -5.38584 | 0.4639 | 1.92903 |

**2**

Thermal correction to Gibbs free energy: 0.492222
SCF energy in solution: -1214.57465361
Sum of electronic and thermal Energies: -1213.449153
Solution-phase Gibbs free energy: -1214.08243161
Coordinates:

| | | | |
|---|---|---|---|
| C | 2.25106 | 0.80375 | 0.54915 |
| C | 3.43238 | 1.4926 | 0.86184 |
| C | 3.3923 | 2.82749 | 1.24908 |
| C | 2.15303 | 3.46142 | 1.31719 |
| C | 1.01516 | 2.72581 | 1.01267 |
| C | 2.31944 | -0.62731 | 0.12961 |
| C | 3.04576 | -0.99167 | -1.02676 |
| C | 3.12544 | -2.34971 | -1.36836 |
| C | 2.53278 | -3.32913 | -0.57816 |
| C | 1.85101 | -2.96201 | 0.58219 |
| C | 1.73382 | -1.61892 | 0.94981 |
| H | 4.37548 | 0.96079 | 0.80421 |
| H | 4.3067 | 3.35881 | 1.49521 |
| H | 2.0581 | 4.50194 | 1.60863 |
| H | 0.03192 | 3.17572 | 1.06624 |
| H | 3.67372 | -2.63595 | -2.26214 |
| H | 2.62036 | -4.37702 | -0.85047 |
| H | 1.43387 | -3.72997 | 1.22834 |
| N | 1.04638 | 1.42577 | 0.64301 |
| C | 3.76132 | 0.01221 | -1.90798 |
| H | 3.27529 | 0.99165 | -1.92326 |
| H | 4.79431 | 0.17178 | -1.57296 |

| | | | |
|---|---|---|---|
| H | 3.81779 | -0.35417 | -2.93746 |
| C | 1.1135 | -1.26545 | 2.29246 |
| H | 0.98712 | -2.1968 | 2.8578 |
| H | 1.84441 | -0.67664 | 2.85951 |
| C | -0.20389 | -0.49122 | 2.34795 |
| H | -0.14487 | 0.45575 | 2.87827 |
| C | -1.45678 | -1.06303 | 2.27543 |
| C | -1.62726 | -2.52162 | 1.92438 |
| H | -0.88443 | -2.87846 | 1.20974 |
| H | -1.5183 | -3.11391 | 2.84559 |
| H | -2.62657 | -2.73659 | 1.53756 |
| C | -2.64285 | -0.42367 | 2.95994 |
| H | -2.8586 | -0.99405 | 3.87534 |
| H | -2.44995 | 0.6139 | 3.24172 |
| H | -3.54781 | -0.46034 | 2.34761 |
| Rh | -0.90447 | 0.46237 | 0.28531 |
| C | -2.71723 | -0.27654 | -0.86826 |
| C | -2.52283 | 1.1252 | -1.09876 |
| C | -1.25489 | 1.26715 | -1.75246 |
| C | -0.78364 | -0.07747 | -2.13223 |
| C | -1.65725 | -1.01107 | -1.58294 |
| C | 0.35657 | -0.34013 | -3.06554 |
| H | 0.00922 | -0.26064 | -4.10546 |
| H | 1.16159 | 0.388 | -2.94249 |
| H | 0.77759 | -1.33849 | -2.9307 |
| C | -1.61647 | -2.4982 | -1.76775 |
| H | -2.22114 | -2.79118 | -2.63724 |
| H | -0.59804 | -2.85818 | -1.93655 |
| H | -2.02359 | -3.02987 | -0.9041 |
| C | -0.67345 | 2.54602 | -2.2794 |
| H | 0.42028 | 2.53012 | -2.26894 |
| H | -0.9878 | 2.70622 | -3.31972 |
| H | -1.00498 | 3.4117 | -1.69984 |
| C | -3.50793 | 2.22077 | -0.80303 |
| H | -3.01502 | 3.18382 | -0.64976 |
| H | -4.19782 | 2.3335 | -1.65024 |
| H | -4.10668 | 2.00578 | 0.08519 |
| C | -4.00271 | -0.88998 | -0.39798 |
| H | -4.52156 | -0.25421 | 0.32398 |
| H | -4.67848 | -1.02575 | -1.25398 |
| H | -3.85805 | -1.87475 | 0.05116 |
| H | -1.46617 | 1.53845 | 1.25672 |

**TS3**

Imaginary frequencies: -788.95
Thermal correction to Gibbs free energy: 0.49154
SCF energy in solution: -1214.55518536
Sum of electronic and thermal Energies: -1213.426946
Solution-phase Gibbs free energy: -1214.06364536
Coordinates:

| | | | |
|---|---|---|---|
| C | -2.03056 | 1.10139 | -0.06714 |
| C | -3.06506 | 2.04035 | -0.19544 |
| C | -2.88108 | 3.36399 | 0.19531 |
| C | -1.65188 | 3.73971 | 0.73314 |
| C | -0.64865 | 2.77996 | 0.80458 |
| C | -2.338 | -0.33855 | -0.40494 |
| C | -3.37151 | -0.92923 | 0.37955 |
| C | -3.81909 | -2.21921 | 0.07977 |
| C | -3.27648 | -2.94128 | -0.97815 |
| C | -2.24933 | -2.37838 | -1.72503 |
| C | -1.75632 | -1.09186 | -1.46098 |
| H | -4.01352 | 1.71689 | -0.60916 |
| H | -3.68501 | 4.08551 | 0.08431 |
| H | -1.45812 | 4.75265 | 1.06908 |
| H | 0.33906 | 3.02748 | 1.17655 |
| H | -4.60121 | -2.66037 | 0.69146 |
| H | -3.64095 | -3.93789 | -1.20949 |
| H | -1.81317 | -2.94224 | -2.54633 |
| N | -0.81602 | 1.50473 | 0.40089 |
| C | -4.00425 | -0.23842 | 1.5752 |
| H | -3.29106 | 0.36594 | 2.14385 |
| H | -4.82824 | 0.42479 | 1.28612 |
| H | -4.42395 | -0.98525 | 2.25541 |
| C | -0.62559 | -0.6537 | -2.40092 |
| H | 0.07118 | -1.4913 | -2.50856 |
| H | -1.05909 | -0.49451 | -3.40367 |
| C | 0.07551 | 0.59679 | -1.97188 |
| H | -0.61927 | 1.42798 | -1.90024 |
| C | 1.40561 | 1.07067 | -2.23225 |
| C | 2.43457 | 0.17707 | -2.89669 |
| H | 2.28799 | -0.87946 | -2.66964 |
| H | 2.34638 | 0.30664 | -3.98381 |
| H | 3.45462 | 0.4574 | -2.62046 |
| C | 1.53481 | 2.53931 | -2.65663 |
| H | 1.28977 | 2.61287 | -3.72416 |
| H | 0.84686 | 3.18529 | -2.10441 |
| H | 2.55388 | 2.91397 | -2.51937 |
| Rh | 0.98449 | 0.33744 | 0.0039 |

| | | | |
|---|---|---|---|
| C | 2.6971 | -1.09391 | 0.44751 |
| C | 2.62646 | -0.12623 | 1.52891 |
| C | 1.36646 | -0.29179 | 2.14742 |
| C | 0.68722 | -1.44426 | 1.5259 |
| C | 1.52965 | -1.95165 | 0.51686 |
| C | -0.55533 | -2.0835 | 2.06499 |
| H | -0.29562 | -2.75349 | 2.89706 |
| H | -1.2587 | -1.34409 | 2.45548 |
| H | -1.07529 | -2.6766 | 1.31007 |
| C | 1.30242 | -3.1887 | -0.30018 |
| H | 1.73902 | -4.06415 | 0.19962 |
| H | 0.23718 | -3.3888 | -0.44276 |
| H | 1.77102 | -3.12002 | -1.28684 |
| C | 0.86097 | 0.43842 | 3.35582 |
| H | -0.21966 | 0.60118 | 3.31187 |
| H | 1.06568 | -0.14614 | 4.26289 |
| H | 1.34748 | 1.41014 | 3.47709 |
| C | 3.73022 | 0.80271 | 1.94969 |
| H | 3.34453 | 1.68973 | 2.45945 |
| H | 4.41007 | 0.29396 | 2.64645 |
| H | 4.32778 | 1.14068 | 1.09887 |
| C | 3.94545 | -1.39086 | -0.33076 |
| H | 4.49537 | -0.48255 | -0.59169 |
| H | 4.61568 | -2.00996 | 0.28135 |
| H | 3.74475 | -1.94602 | -1.2495 |
| H | 1.86475 | 1.45871 | -0.82065 |

**4**

Thermal correction to Gibbs free energy: 0.495713
SCF energy in solution: -1214.58730293
Sum of electronic and thermal Energies: -1213.460063
Solution-phase Gibbs free energy: -1214.09158993
Coordinates:

| | | | |
|---|---|---|---|
| C | 2.32329 | 0.34384 | -0.79763 |
| C | 3.57605 | 0.40227 | -1.41192 |
| C | 3.75943 | -0.21766 | -2.6477 |
| C | 2.68357 | -0.87452 | -3.2459 |
| C | 1.45964 | -0.88847 | -2.58336 |
| C | 1.97099 | 0.99082 | 0.49877 |
| C | 2.66522 | 0.67673 | 1.69218 |
| C | 2.25832 | 1.29884 | 2.87654 |
| C | 1.20119 | 2.21261 | 2.89413 |
| C | 0.53182 | 2.52434 | 1.71647 |
| C | 0.89803 | 1.92835 | 0.49636 |

| | | | |
|---|---|---|---|
| H | 4.38559 | 0.9407 | -0.93199 |
| H | 4.72565 | -0.17873 | -3.1414 |
| H | 2.78205 | -1.36083 | -4.21042 |
| H | 0.58672 | -1.37001 | -3.01092 |
| H | 2.78363 | 1.06806 | 3.79959 |
| H | 0.91756 | 2.69438 | 3.82549 |
| H | -0.26407 | 3.26277 | 1.72408 |
| N | 1.29067 | -0.3027 | -1.38674 |
| C | 3.81696 | -0.30465 | 1.72918 |
| H | 3.6461 | -1.17218 | 1.08375 |
| H | 4.75693 | 0.15941 | 1.40541 |
| H | 3.97726 | -0.66784 | 2.74825 |
| C | 0.23764 | 2.4002 | -0.80746 |
| H | -0.14732 | 3.41024 | -0.63508 |
| H | 1.0103 | 2.49791 | -1.5775 |
| C | -0.89081 | 1.46023 | -1.29558 |
| H | -0.67503 | 1.11918 | -2.31366 |
| C | -2.29911 | 2.07331 | -1.30737 |
| C | -2.74744 | 2.72673 | 0.00876 |
| H | -2.59908 | 2.06592 | 0.86807 |
| H | -2.20041 | 3.65648 | 0.2065 |
| H | -3.80942 | 2.99319 | -0.03843 |
| C | -2.42057 | 3.09047 | -2.46564 |
| H | -1.73728 | 3.93806 | -2.33147 |
| H | -2.19379 | 2.62628 | -3.43232 |
| H | -3.43825 | 3.4947 | -2.5181 |
| Rh | -0.46619 | -0.2694 | -0.13382 |
| C | -2.48646 | -1.18027 | 0.29266 |
| C | -1.62895 | -2.05437 | -0.48122 |
| C | -0.57072 | -2.56552 | 0.41507 |
| C | -0.67963 | -1.88603 | 1.62598 |
| C | -1.83023 | -0.96411 | 1.53376 |
| C | 0.17531 | -2.02233 | 2.84782 |
| H | -0.40258 | -2.45628 | 3.67425 |
| H | 1.03818 | -2.6692 | 2.67207 |
| H | 0.54531 | -1.04876 | 3.18879 |
| C | -2.33685 | -0.16922 | 2.69921 |
| H | -2.74529 | -0.84546 | 3.46269 |
| H | -1.53553 | 0.40807 | 3.17133 |
| H | -3.132 | 0.52111 | 2.41085 |
| C | 0.4261 | -3.61671 | 0.03058 |
| H | 1.24612 | -3.68255 | 0.74985 |
| H | -0.05449 | -4.60258 | -0.0169 |
| H | 0.86078 | -3.42407 | -0.95628 |

| | | | |
|---|---|---|---|
| C | -1.97039 | -2.64584 | -1.81574 |
| H | -1.07895 | -2.99269 | -2.34653 |
| H | -2.62627 | -3.51829 | -1.68652 |
| H | -2.49569 | -1.93069 | -2.45478 |
| C | -3.86639 | -0.74246 | -0.09179 |
| H | -3.98729 | -0.66523 | -1.17503 |
| H | -4.59121 | -1.48838 | 0.26267 |
| H | -4.1399 | 0.21698 | 0.35198 |
| H | -3.00047 | 1.26291 | -1.53641 |

**TS5**

Imaginary frequencies: -319.11
Thermal correction to Gibbs free energy: 0.494461
SCF energy in solution: -1214.55689596
Sum of electronic and thermal Energies: -1213.432078
Solution-phase Gibbs free energy: -1214.06243496
Coordinates:

| | | | |
|---|---|---|---|
| C | 2.28656 | 1.03729 | 0.07635 |
| C | 3.37075 | 1.92942 | 0.02831 |
| C | 3.21398 | 3.19213 | -0.53395 |
| C | 1.96632 | 3.57052 | -1.03109 |
| C | 0.91671 | 2.66763 | -0.91733 |
| C | 2.30096 | -0.3154 | 0.66345 |
| C | 3.43861 | -1.15499 | 0.74405 |
| C | 3.28826 | -2.41984 | 1.33269 |
| C | 2.06281 | -2.86042 | 1.82721 |
| C | 0.93725 | -2.04508 | 1.72402 |
| C | 1.0362 | -0.78341 | 1.1271 |
| H | 4.32321 | 1.64516 | 0.45184 |
| H | 4.0547 | 3.87826 | -0.57005 |
| H | 1.79927 | 4.54564 | -1.47534 |
| H | -0.08419 | 2.92063 | -1.24918 |
| H | 4.15596 | -3.06998 | 1.3986 |
| H | 1.98448 | -3.8405 | 2.28976 |
| H | -0.01438 | -2.38332 | 2.12435 |
| N | 1.0688 | 1.44266 | -0.38595 |
| C | 4.8038 | -0.8001 | 0.19328 |
| H | 4.74622 | -0.26514 | -0.7597 |
| H | 5.38125 | -0.17858 | 0.89004 |
| H | 5.38702 | -1.7102 | 0.0281 |
| C | -0.04413 | 0.48497 | 2.15637 |
| H | -0.38086 | -0.22599 | 2.90257 |
| H | 0.86499 | 1.0035 | 2.44854 |
| C | -1.06859 | 1.2988 | 1.53615 |

| | | | |
|---|---|---|---|
| H | -0.73096 | 2.28992 | 1.23397 |
| C | -2.49786 | 1.34358 | 2.07737 |
| C | -2.95152 | 0.08335 | 2.82676 |
| H | -2.7611 | -0.83135 | 2.25683 |
| H | -2.44452 | -0.01268 | 3.7944 |
| H | -4.02548 | 0.13334 | 3.03551 |
| C | -2.64163 | 2.58106 | 2.99341 |
| H | -1.98167 | 2.5056 | 3.866 |
| H | -2.39496 | 3.50723 | 2.46193 |
| H | -3.67144 | 2.6687 | 3.35759 |
| Rh | -0.52855 | 0.03166 | -0.13657 |
| C | -2.57521 | -0.4753 | -1.10953 |
| C | -1.71879 | 0.18633 | -2.03476 |
| C | -0.58644 | -0.71102 | -2.31636 |
| C | -0.73991 | -1.8733 | -1.53455 |
| C | -1.92794 | -1.70105 | -0.71493 |
| C | 0.12043 | -3.0996 | -1.55559 |
| H | -0.37358 | -3.89914 | -2.12346 |
| H | 1.08777 | -2.90996 | -2.02723 |
| H | 0.30961 | -3.48081 | -0.54827 |
| C | -2.53422 | -2.78689 | 0.12501 |
| H | -3.0605 | -3.50501 | -0.51917 |
| H | -1.77495 | -3.34786 | 0.67685 |
| H | -3.26309 | -2.40032 | 0.8407 |
| C | 0.47244 | -0.44801 | -3.34493 |
| H | 1.37385 | -1.03859 | -3.16224 |
| H | 0.10172 | -0.70983 | -4.34496 |
| H | 0.75979 | 0.60721 | -3.37312 |
| C | -2.04369 | 1.42973 | -2.81043 |
| H | -1.14162 | 1.95298 | -3.14069 |
| H | -2.614 | 1.17835 | -3.71521 |
| H | -2.64988 | 2.12886 | -2.22662 |
| C | -3.96296 | -0.0526 | -0.73563 |
| H | -4.0948 | 1.031 | -0.7966 |
| H | -4.68064 | -0.5055 | -1.43346 |
| H | -4.24204 | -0.37611 | 0.26967 |
| H | -3.17527 | 1.50436 | 1.23055 |

**6**

Thermal correction to Gibbs free energy: 0.492838
SCF energy in solution: -1214.58626731
Sum of electronic and thermal Energies: -1213.462115
Solution-phase Gibbs free energy: -1214.09342931
Coordinates:

| | | | |
|---|---|---|---|
| C | 2.16181 | 0.77145 | -0.69122 |
| C | 3.10705 | 1.55922 | -1.37435 |
| C | 2.71125 | 2.68322 | -2.09041 |
| C | 1.36343 | 3.03905 | -2.12502 |
| C | 0.46513 | 2.22762 | -1.44613 |
| C | 2.40527 | -0.42029 | 0.1407 |
| C | 3.67805 | -0.96395 | 0.48448 |
| C | 3.71384 | -2.07421 | 1.33581 |
| C | 2.55519 | -2.64491 | 1.85494 |
| C | 1.3097 | -2.11472 | 1.51801 |
| C | 1.22538 | -1.02102 | 0.65871 |
| H | 4.1511 | 1.29627 | -1.35391 |
| H | 3.45419 | 3.27768 | -2.6135 |
| H | 1.01176 | 3.91393 | -2.66056 |
| H | -0.59559 | 2.44936 | -1.43537 |
| H | 4.67934 | -2.49313 | 1.60359 |
| H | 2.62259 | -3.49995 | 2.52242 |
| H | 0.41171 | -2.56558 | 1.92974 |
| N | 0.84439 | 1.13097 | -0.76809 |
| C | 5.01344 | -0.42946 | 0.0122 |
| H | 5.12584 | -0.48707 | -1.07724 |
| H | 5.17726 | 0.61168 | 0.31454 |
| H | 5.82396 | -1.01983 | 0.44696 |
| C | -0.99803 | 0.21739 | 2.32486 |
| H | -0.53359 | -0.64263 | 2.79344 |
| H | -2.07622 | 0.29582 | 2.42284 |
| C | -0.24494 | 1.31336 | 1.97279 |
| H | 0.83431 | 1.21939 | 2.08179 |
| C | -0.72431 | 2.74001 | 1.81055 |
| C | -2.22853 | 2.90723 | 1.57809 |
| H | -2.5617 | 2.37286 | 0.68212 |
| H | -2.81319 | 2.54216 | 2.43054 |
| H | -2.47237 | 3.96673 | 1.44872 |
| C | -0.26911 | 3.52737 | 3.0637 |
| H | -0.76957 | 3.15385 | 3.96413 |
| H | 0.81245 | 3.45043 | 3.21977 |
| H | -0.51831 | 4.58779 | 2.95057 |
| Rh | -0.54682 | -0.21289 | 0.08808 |
| C | -2.21579 | -1.76987 | 0.11282 |
| C | -2.91375 | -0.57086 | -0.38789 |
| C | -2.30438 | -0.17701 | -1.58106 |
| C | -1.20305 | -1.11528 | -1.85002 |
| C | -1.2602 | -2.16509 | -0.87204 |
| C | -0.3875 | -1.13677 | -3.10906 |

| | | | |
|---|---|---|---|
| H | -0.95015 | -1.62498 | -3.91618 |
| H | -0.13759 | -0.1281 | -3.45 |
| H | 0.54587 | -1.6896 | -2.97525 |
| C | -0.50839 | -3.46029 | -0.92932 |
| H | -1.07404 | -4.18095 | -1.53511 |
| H | 0.47767 | -3.34412 | -1.38536 |
| H | -0.36859 | -3.9011 | 0.05965 |
| C | -2.7398 | 0.92125 | -2.50616 |
| H | -1.89556 | 1.37155 | -3.03619 |
| H | -3.41737 | 0.52428 | -3.27411 |
| H | -3.27648 | 1.71613 | -1.98004 |
| C | -4.15033 | 0.00137 | 0.23586 |
| H | -4.39331 | 0.99033 | -0.15934 |
| H | -5.00624 | -0.65548 | 0.0287 |
| H | -4.071 | 0.08066 | 1.32448 |
| C | -2.69648 | -2.60907 | 1.26097 |
| H | -3.06254 | -1.99939 | 2.09174 |
| H | -3.52759 | -3.25136 | 0.93924 |
| H | -1.91022 | -3.26522 | 1.644 |
| H | -0.19023 | 3.17612 | 0.95553 |

**7**

Thermal correction to Gibbs free energy: 0.486729
SCF energy in solution: -1327.64396743
Sum of electronic and thermal Energies: -1326.579486
Solution-phase Gibbs free energy: -1327.15723843
Coordinates:

| | | | |
|---|---|---|---|
| C | 0.97833 | 1.78915 | 0.87853 |
| C | 1.96186 | 2.39628 | 1.67989 |
| C | 2.8214 | 1.62562 | 2.45492 |
| C | 2.71497 | 0.23637 | 2.42763 |
| C | 1.7278 | -0.31918 | 1.62643 |
| C | 0.01954 | 2.43962 | -0.03034 |
| C | -0.07307 | 3.83636 | -0.30481 |
| C | -0.99845 | 4.2606 | -1.26427 |
| C | -1.80787 | 3.36307 | -1.95639 |
| C | -1.72547 | 1.99912 | -1.67947 |
| C | -0.84023 | 1.53554 | -0.70817 |
| H | 2.05986 | 3.46838 | 1.70269 |
| H | 3.57301 | 2.1115 | 3.0699 |
| H | 3.37398 | -0.4042 | 3.00281 |
| H | 1.60393 | -1.39193 | 1.55175 |
| H | -1.07442 | 5.32223 | -1.48044 |
| H | -2.50096 | 3.72659 | -2.71054 |

| | | | |
|---|---|---|---|
| H | -2.35149 | 1.30446 | -2.23093 |
| N | 0.88329 | 0.42447 | 0.89317 |
| C | 0.75838 | 4.91368 | 0.35857 |
| H | 0.62928 | 4.93153 | 1.44725 |
| H | 1.82909 | 4.80472 | 0.1473 |
| H | 0.45853 | 5.89619 | -0.01487 |
| Rh | -0.72772 | -0.42956 | -0.14991 |
| C | -2.63406 | -1.66134 | -0.48266 |
| C | -1.77282 | -2.5355 | 0.32079 |
| C | -1.51888 | -1.88937 | 1.54347 |
| C | -2.20604 | -0.5971 | 1.52374 |
| C | -2.98554 | -0.53132 | 0.31544 |
| C | -2.31629 | 0.34425 | 2.68678 |
| H | -3.13189 | 0.03552 | 3.35458 |
| H | -1.39774 | 0.36493 | 3.27984 |
| H | -2.52682 | 1.36488 | 2.35643 |
| C | -4.04576 | 0.48436 | 0.01875 |
| H | -4.97148 | 0.19805 | 0.53615 |
| H | -3.76863 | 1.48402 | 0.36081 |
| H | -4.27493 | 0.54396 | -1.04739 |
| C | -0.77298 | -2.44503 | 2.7198 |
| H | -0.2327 | -1.66798 | 3.2678 |
| H | -1.47632 | -2.90517 | 3.42666 |
| H | -0.05713 | -3.21834 | 2.42612 |
| C | -1.36248 | -3.92439 | -0.06928 |
| H | -0.46484 | -4.25393 | 0.46139 |
| H | -2.16377 | -4.63604 | 0.17184 |
| H | -1.17655 | -4.015 | -1.14419 |
| C | -3.25906 | -2.05046 | -1.79084 |
| H | -2.57142 | -2.62386 | -2.42032 |
| H | -4.14029 | -2.68326 | -1.62015 |
| H | -3.58983 | -1.17785 | -2.36082 |
| C | 0.03793 | -0.61617 | -2.30749 |
| H | 0.41994 | 0.33761 | -2.65046 |
| H | -0.86544 | -0.9562 | -2.80234 |
| C | 0.86156 | -1.52848 | -1.66907 |
| H | 0.49029 | -2.54428 | -1.55711 |
| C | 2.29315 | -1.38054 | -1.37671 |
| C | 3.01437 | -0.19826 | -1.63237 |
| C | 2.98963 | -2.49317 | -0.86826 |
| C | 4.38169 | -0.13617 | -1.38267 |
| H | 2.50674 | 0.67326 | -2.03431 |
| C | 4.36003 | -2.43137 | -0.62068 |
| H | 2.45098 | -3.42065 | -0.68527 |

| | | | |
|---|---|---|---|
| C | 5.05986 | -1.25053 | -0.87553 |
| H | 4.92566 | 0.78002 | -1.59352 |
| H | 4.88139 | -3.30473 | -0.23983 |
| H | 6.129 | -1.19953 | -0.69143 |

**TS8**

Imaginary frequencies: -307.39
Thermal correction to Gibbs free energy: 0.489229
SCF energy in solution: -1327.61933124
Sum of electronic and thermal Energies: -1326.553263
Solution-phase Gibbs free energy: -1327.13010224
Coordinates:

| | | | |
|---|---|---|---|
| C | -2.45069 | 1.26098 | -0.5423 |
| C | -3.39051 | 2.27778 | -0.78086 |
| C | -3.18904 | 3.55305 | -0.26316 |
| C | -2.03673 | 3.81725 | 0.47803 |
| C | -1.11816 | 2.78875 | 0.64571 |
| C | -2.5201 | -0.12136 | -1.04975 |
| C | -3.71612 | -0.82138 | -1.34306 |
| C | -3.61444 | -2.13634 | -1.82128 |
| C | -2.38174 | -2.75792 | -2.00797 |
| C | -1.20628 | -2.07921 | -1.69461 |
| C | -1.25977 | -0.77351 | -1.19444 |
| H | -4.26022 | 2.07759 | -1.38979 |
| H | -3.91825 | 4.33567 | -0.44934 |
| H | -1.83903 | 4.79724 | 0.89834 |
| H | -0.18756 | 2.94494 | 1.18001 |
| H | -4.52696 | -2.6803 | -2.04786 |
| H | -2.33826 | -3.7732 | -2.39261 |
| H | -0.24509 | -2.56101 | -1.85128 |
| N | -1.31564 | 1.5526 | 0.15667 |
| C | -5.10747 | -0.26302 | -1.12998 |
| H | -5.18575 | 0.33196 | -0.21482 |
| H | -5.43163 | 0.36878 | -1.96722 |
| H | -5.82971 | -1.0808 | -1.05676 |
| C | 0.17393 | 0.27564 | -2.03059 |
| H | 0.5437 | -0.51814 | -2.66974 |
| H | -0.57324 | 0.89148 | -2.52221 |
| C | 1.16669 | 1.01252 | -1.2766 |
| H | 0.92845 | 2.05984 | -1.10284 |
| Rh | 0.10659 | -0.04865 | 0.32107 |
| C | 1.84282 | -0.59685 | 1.75928 |
| C | 0.81146 | 0.09762 | 2.45068 |
| C | -0.3874 | -0.75536 | 2.45352 |

| | | | |
|---|---|---|---|
| C | -0.08764 | -1.93082 | 1.73438 |
| C | 1.26414 | -1.80028 | 1.21235 |
| C | -0.96872 | -3.13034 | 1.56952 |
| H | -0.70703 | -3.89139 | 2.3169 |
| H | -2.02485 | -2.88366 | 1.70451 |
| H | -0.85685 | -3.58756 | 0.58344 |
| C | 2.02236 | -2.88752 | 0.50922 |
| H | 2.46515 | -3.57524 | 1.24291 |
| H | 1.3725 | -3.48277 | -0.13881 |
| H | 2.83704 | -2.4849 | -0.0971 |
| C | -1.65209 | -0.45149 | 3.19984 |
| H | -2.50474 | -1.0033 | 2.79552 |
| H | -1.5479 | -0.73086 | 4.25687 |
| H | -1.89525 | 0.61473 | 3.16949 |
| C | 0.97713 | 1.34398 | 3.2693 |
| H | 0.04594 | 1.91331 | 3.34204 |
| H | 1.27457 | 1.08711 | 4.29518 |
| H | 1.7517 | 1.99997 | 2.86122 |
| C | 3.28511 | -0.20616 | 1.69286 |
| H | 3.42189 | 0.87586 | 1.75815 |
| H | 3.82279 | -0.65999 | 2.53686 |
| H | 3.76367 | -0.54824 | 0.77332 |
| C | 2.61776 | 0.77961 | -1.4278 |
| C | 3.16938 | -0.3992 | -1.96726 |
| C | 3.50218 | 1.81819 | -1.07868 |
| C | 4.54581 | -0.53127 | -2.14363 |
| H | 2.52207 | -1.21935 | -2.26478 |
| C | 4.87874 | 1.68759 | -1.25587 |
| H | 3.09893 | 2.74636 | -0.67926 |
| C | 5.40847 | 0.51014 | -1.78738 |
| H | 4.94651 | -1.44585 | -2.57194 |
| H | 5.53674 | 2.50893 | -0.98674 |
| H | 6.47948 | 0.40722 | -1.93346 |

**9**

Thermal correction to Gibbs free energy: 0.488423
SCF energy in solution: -1327.64940626
Sum of electronic and thermal Energies: -1326.581301
Solution-phase Gibbs free energy: -1327.16098326
Coordinates:

| | | | |
|---|---|---|---|
| C | 2.33897 | 0.31447 | -1.41591 |
| C | 3.40115 | 0.32193 | -2.32279 |
| C | 3.56139 | -0.75446 | -3.19495 |
| C | 2.65093 | -1.81065 | -3.14633 |

| | | | |
|---|---|---|---|
| C | 1.60963 | -1.75071 | -2.22492 |
| C | 2.03526 | 1.40994 | -0.44955 |
| C | 2.98233 | 1.80441 | 0.52682 |
| C | 2.63502 | 2.83002 | 1.4116 |
| C | 1.3929 | 3.46509 | 1.33826 |
| C | 0.47086 | 3.07617 | 0.37359 |
| C | 0.76286 | 2.0447 | -0.53622 |
| H | 4.07941 | 1.16753 | -2.34942 |
| H | 4.37967 | -0.76378 | -3.90849 |
| H | 2.73568 | -2.6628 | -3.81205 |
| H | 0.86526 | -2.53692 | -2.15591 |
| H | 3.35456 | 3.14264 | 2.1638 |
| H | 1.15725 | 4.27558 | 2.02197 |
| H | -0.47482 | 3.60342 | 0.28736 |
| N | 1.46581 | -0.71805 | -1.37787 |
| C | 4.34374 | 1.15399 | 0.6478 |
| H | 4.30359 | 0.07206 | 0.4866 |
| H | 5.0568 | 1.56347 | -0.07847 |
| H | 4.76479 | 1.33256 | 1.64119 |
| Rh | -0.01585 | -0.42683 | 0.16327 |
| C | -1.63841 | -1.36779 | 1.41496 |
| C | -0.67144 | -2.33466 | 0.93671 |
| C | 0.58904 | -2.1273 | 1.67762 |
| C | 0.44243 | -0.96833 | 2.43963 |
| C | -0.92092 | -0.44078 | 2.21744 |
| C | 1.44447 | -0.32195 | 3.34461 |
| H | 1.1067 | -0.37559 | 4.38787 |
| H | 2.42119 | -0.80805 | 3.28589 |
| H | 1.57902 | 0.7385 | 3.10315 |
| C | -1.48942 | 0.73967 | 2.9446 |
| H | -1.75975 | 0.45928 | 3.97198 |
| H | -0.76503 | 1.55731 | 3.00814 |
| H | -2.38947 | 1.11644 | 2.45347 |
| C | 1.78401 | -3.02692 | 1.58027 |
| H | 2.6724 | -2.57524 | 2.02864 |
| H | 1.59482 | -3.97503 | 2.10043 |
| H | 2.02217 | -3.27334 | 0.53979 |
| C | -0.99413 | -3.55365 | 0.12692 |
| H | -0.11665 | -3.9353 | -0.40382 |
| H | -1.34796 | -4.36042 | 0.78418 |
| H | -1.78309 | -3.35512 | -0.60357 |
| C | -3.11452 | -1.41524 | 1.18741 |
| H | -3.3694 | -1.8212 | 0.20656 |
| H | -3.57257 | -2.06305 | 1.94779 |

| | | | |
|---|---|---|---|
| H | -3.57552 | -0.42892 | 1.26464 |
| C | -0.22628 | 1.74023 | -1.67025 |
| H | 0.33493 | 1.63574 | -2.60546 |
| H | -0.87014 | 2.61573 | -1.79663 |
| C | -1.09103 | 0.47205 | -1.45215 |
| C | -2.55195 | 0.69281 | -1.27243 |
| C | -3.46297 | -0.14049 | -1.95039 |
| C | -3.08611 | 1.73626 | -0.49045 |
| C | -4.84069 | 0.05508 | -1.85444 |
| H | -3.07899 | -0.93924 | -2.58217 |
| C | -4.46316 | 1.93511 | -0.39255 |
| H | -2.41853 | 2.40585 | 0.0447 |
| C | -5.349 | 1.09442 | -1.07269 |
| H | -5.51684 | -0.59645 | -2.40124 |
| H | -4.84659 | 2.75476 | 0.20936 |
| H | -6.42063 | 1.25533 | -1.00231 |
| H | -0.93952 | -0.23234 | -2.27332 |

**TS10**

Imaginary frequencies: -695.49

Thermal correction to Gibbs free energy: 0.485767

SCF energy in solution: -1327.62240976

Sum of electronic and thermal Energies: -1326.560517

Solution-phase Gibbs free energy: -1327.13664276

Coordinates:

| | | | |
|---|---|---|---|
| C | -2.47536 | 0.00025 | -1.02419 |
| C | -3.26754 | -0.11554 | -2.18203 |
| C | -2.99854 | 0.6353 | -3.31787 |
| C | -1.91547 | 1.51095 | -3.28835 |
| C | -1.1284 | 1.53547 | -2.14635 |
| C | -2.87948 | -0.78696 | 0.17829 |
| C | -4.24909 | -0.82249 | 0.55328 |
| C | -4.65121 | -1.68094 | 1.58668 |
| C | -3.74332 | -2.48712 | 2.26086 |
| C | -2.3902 | -2.39047 | 1.95122 |
| C | -1.9461 | -1.54496 | 0.93015 |
| H | -4.09205 | -0.81659 | -2.17855 |
| H | -3.61687 | 0.5346 | -4.20462 |
| H | -1.65759 | 2.13715 | -4.13558 |
| H | -0.24508 | 2.15582 | -2.11206 |
| H | -5.70012 | -1.69946 | 1.8695 |
| H | -4.07856 | -3.15529 | 3.04826 |
| H | -1.66434 | -2.97176 | 2.51351 |
| N | -1.36856 | 0.7951 | -1.04245 |

| | | | |
|---|---|---|---|
| C | -5.32473 | 0.06761 | -0.04308 |
| H | -4.92819 | 0.99276 | -0.46725 |
| H | -5.8965 | -0.4402 | -0.82982 |
| H | -6.04169 | 0.34056 | 0.73737 |
| C | -0.4561 | -1.42591 | 0.79079 |
| H | -0.54526 | -0.03687 | 1.43734 |
| H | 0.05324 | -1.88623 | 1.63439 |
| C | 0.2772 | -1.46029 | -0.44569 |
| H | -0.30635 | -1.38879 | -1.35799 |
| Rh | 0.37647 | 0.63684 | 0.30832 |
| C | 2.16833 | 1.03787 | 1.56273 |
| C | 2.65598 | 1.22487 | 0.20761 |
| C | 1.91304 | 2.27606 | -0.37475 |
| C | 1.00532 | 2.81427 | 0.64785 |
| C | 1.21782 | 2.09842 | 1.85313 |
| C | 0.13424 | 4.02237 | 0.47076 |
| H | 0.73748 | 4.93838 | 0.52804 |
| H | -0.36957 | 4.02874 | -0.50094 |
| H | -0.63469 | 4.08243 | 1.24472 |
| C | 0.62762 | 2.40607 | 3.19965 |
| H | 1.28047 | 3.09937 | 3.74664 |
| H | -0.35615 | 2.87526 | 3.11715 |
| H | 0.51949 | 1.5075 | 3.81258 |
| C | 2.17725 | 2.89724 | -1.71657 |
| H | 1.34953 | 3.52808 | -2.0529 |
| H | 3.05992 | 3.54859 | -1.66022 |
| H | 2.37656 | 2.14795 | -2.48885 |
| C | 3.78585 | 0.47601 | -0.42446 |
| H | 3.72852 | 0.49774 | -1.5156 |
| H | 4.74238 | 0.93138 | -0.13247 |
| H | 3.81088 | -0.56995 | -0.1098 |
| C | 2.78313 | 0.12441 | 2.58281 |
| H | 3.1608 | -0.7936 | 2.12636 |
| H | 3.63124 | 0.62218 | 3.07231 |
| H | 2.07094 | -0.14891 | 3.36692 |
| C | 1.54706 | -2.18741 | -0.64022 |
| C | 2.25202 | -2.83958 | 0.39002 |
| C | 2.05894 | -2.28315 | -1.94959 |
| C | 3.42284 | -3.54795 | 0.11989 |
| H | 1.87774 | -2.82324 | 1.40929 |
| C | 3.2281 | -2.99038 | -2.21967 |
| H | 1.52234 | -1.80069 | -2.76361 |
| C | 3.91864 | -3.62527 | -1.18434 |
| H | 3.94118 | -4.05424 | 0.92935 |

| | | | |
|---|---|---|---|
| H | 3.59602 | -3.0538 | -3.23975 |
| H | 4.82577 | -4.18461 | -1.39231 |

**11**

Thermal correction to Gibbs free energy: 0.487186
SCF energy in solution: -1327.62936974
Sum of electronic and thermal Energies: -1326.571500
Solution-phase Gibbs free energy: -1327.14218374
Coordinates:

| | | | |
|---|---|---|---|
| C | -2.39974 | 0.28536 | 1.1175 |
| C | -3.13505 | 0.62415 | 2.26754 |
| C | -2.82832 | 0.07274 | 3.50469 |
| C | -1.76584 | -0.82572 | 3.5876 |
| C | -1.03647 | -1.08242 | 2.43567 |
| C | -2.80624 | 0.84897 | -0.2003 |
| C | -4.17535 | 0.8199 | -0.57162 |
| C | -4.56595 | 1.41115 | -1.78202 |
| C | -3.64324 | 2.01309 | -2.62771 |
| C | -2.29359 | 1.99021 | -2.29155 |
| C | -1.85426 | 1.41061 | -1.09497 |
| H | -3.94303 | 1.33858 | 2.17548 |
| H | -3.40325 | 0.34303 | 4.38513 |
| H | -1.4844 | -1.29896 | 4.52204 |
| H | -0.17338 | -1.73315 | 2.46598 |
| H | -5.61458 | 1.37894 | -2.06415 |
| H | -3.96732 | 2.47204 | -3.55695 |
| H | -1.56243 | 2.42702 | -2.96631 |
| N | -1.32008 | -0.53814 | 1.23408 |
| C | -5.264 | 0.12569 | 0.22633 |
| H | -4.89194 | -0.71346 | 0.81907 |
| H | -5.77837 | 0.81216 | 0.91067 |
| H | -6.02517 | -0.26274 | -0.45684 |
| C | -0.37933 | 1.40083 | -0.89814 |
| H | -0.99873 | -0.89171 | -1.2464 |
| H | 0.157 | 1.60677 | -1.82099 |
| C | 0.31984 | 1.62049 | 0.28961 |
| H | -0.23788 | 1.62597 | 1.22006 |
| Rh | 0.20545 | -0.7103 | -0.282 |
| C | 2.57953 | -1.33249 | -0.12215 |
| C | 1.84531 | -2.33531 | 0.52956 |
| C | 0.8448 | -2.8519 | -0.40356 |
| C | 1.06803 | -2.22279 | -1.68261 |
| C | 2.05199 | -1.20058 | -1.4831 |
| C | 0.47379 | -2.63821 | -2.99887 |

| | | | |
|---|---|---|---|
| H | 1.13021 | -3.37501 | -3.48097 |
| H | -0.50954 | -3.09828 | -2.87753 |
| H | 0.36699 | -1.79336 | -3.68356 |
| C | 2.67748 | -0.36614 | -2.56178 |
| H | 3.54726 | -0.88756 | -2.98452 |
| H | 1.98098 | -0.17486 | -3.38277 |
| H | 3.0299 | 0.59399 | -2.17698 |
| C | -0.03869 | -4.03873 | -0.14893 |
| H | -0.86983 | -4.08011 | -0.85701 |
| H | 0.53269 | -4.9715 | -0.24886 |
| H | -0.46248 | -4.02358 | 0.85992 |
| C | 2.10677 | -2.87852 | 1.90414 |
| H | 1.22756 | -3.37295 | 2.32777 |
| H | 2.89938 | -3.63792 | 1.86437 |
| H | 2.43869 | -2.10294 | 2.60122 |
| C | 3.76604 | -0.59364 | 0.41035 |
| H | 3.79885 | -0.60541 | 1.50279 |
| H | 4.69195 | -1.06124 | 0.04685 |
| H | 3.7797 | 0.44872 | 0.08286 |
| C | 1.65616 | 2.22631 | 0.41599 |
| C | 2.36119 | 2.787 | -0.66725 |
| C | 2.21757 | 2.34187 | 1.70287 |
| C | 3.58756 | 3.41964 | -0.46871 |
| H | 1.93537 | 2.76554 | -1.66557 |
| C | 3.44179 | 2.97614 | 1.90145 |
| H | 1.67791 | 1.93423 | 2.55482 |
| C | 4.13468 | 3.51468 | 0.81441 |
| H | 4.10832 | 3.85786 | -1.31528 |
| H | 3.85114 | 3.05831 | 2.90413 |
| H | 5.08491 | 4.01777 | 0.96634 |

**13**

Thermal correction to Gibbs free energy: 0.573031
SCF energy in solution: -1370.517974
Sum of electronic and thermal Energies: -1369.383690
Solution-phase Gibbs free energy: -1369.944943
Coordinates:

| | | | |
|---|---|---|---|
| C | 0.85904 | 1.49253 | 1.17637 |
| C | 1.75875 | 2.50568 | 1.54405 |
| C | 1.36654 | 3.83926 | 1.5228 |
| C | 0.06228 | 4.14313 | 1.13549 |
| C | -0.7822 | 3.10079 | 0.77674 |
| C | 1.30653 | 0.07401 | 1.22378 |
| C | 3.02415 | -1.56429 | 0.60893 |

| | | | |
|---|---|---|---|
| C | 2.33255 | -2.52094 | 1.35793 |
| C | 1.16721 | -2.18292 | 2.04916 |
| C | 0.63108 | -0.89236 | 2.00156 |
| H | 2.75565 | 2.22357 | 1.86369 |
| H | 2.05969 | 4.62277 | 1.81384 |
| H | -0.30335 | 5.16401 | 1.10926 |
| H | -1.80073 | 3.2919 | 0.4631 |
| H | 2.72237 | -3.53333 | 1.42999 |
| H | 0.68686 | -2.93173 | 2.67441 |
| N | -0.40486 | 1.80305 | 0.78457 |
| C | -0.53357 | -0.52041 | 2.90279 |
| H | -0.69616 | -1.3507 | 3.60169 |
| H | -0.22242 | 0.32754 | 3.52462 |
| C | -1.88276 | -0.14055 | 2.29384 |
| H | -2.24832 | 0.83786 | 2.5951 |
| C | -2.84065 | -1.03902 | 1.87273 |
| C | -2.54214 | -2.51761 | 1.80439 |
| H | -1.51154 | -2.73179 | 1.51827 |
| H | -2.709 | -2.94987 | 2.80274 |
| H | -3.21857 | -3.04264 | 1.12539 |
| C | -4.30838 | -0.67946 | 1.90293 |
| H | -4.76684 | -1.18043 | 2.76821 |
| H | -4.47015 | 0.39591 | 2.00576 |
| H | -4.84315 | -1.03323 | 1.01728 |
| Rh | -1.83116 | 0.35088 | -0.02719 |
| C | -2.77765 | -1.0003 | -1.603 |
| C | -2.84465 | 0.369 | -2.01914 |
| C | -1.494 | 0.82719 | -2.1649 |
| C | -0.60236 | -0.34175 | -2.05505 |
| C | -1.3748 | -1.4434 | -1.69612 |
| C | 0.85341 | -0.31745 | -2.40226 |
| H | 0.97319 | -0.3251 | -3.49479 |
| H | 1.34832 | 0.58507 | -2.03264 |
| H | 1.38507 | -1.18226 | -2.00129 |
| C | -0.91011 | -2.85965 | -1.53333 |
| H | -1.02835 | -3.41312 | -2.47513 |
| H | 0.14378 | -2.91059 | -1.24754 |
| H | -1.48863 | -3.39438 | -0.77554 |
| C | -1.06874 | 2.16586 | -2.69308 |
| H | -0.10274 | 2.47605 | -2.28421 |
| H | -0.9635 | 2.12757 | -3.78593 |
| H | -1.80043 | 2.94453 | -2.46154 |
| C | -4.0933 | 1.14101 | -2.33963 |
| H | -3.95195 | 2.21704 | -2.21311 |

| | | | |
|---|---|---|---|
| H | -4.37703 | 0.96492 | -3.38604 |
| H | -4.93549 | 0.83793 | -1.71304 |
| C | -3.95508 | -1.92697 | -1.53658 |
| H | -4.86106 | -1.41851 | -1.197 |
| H | -4.16421 | -2.32346 | -2.54007 |
| H | -3.77689 | -2.78639 | -0.88704 |
| H | -2.93491 | 1.35272 | 0.41726 |
| C | 2.49634 | -0.26781 | 0.56657 |
| H | 3.03395 | 0.49447 | 0.00856 |
| C | 4.30668 | -1.91003 | -0.13504 |
| H | 4.08554 | -2.01279 | -1.20453 |
| H | 4.6379 | -2.90375 | 0.19752 |
| C | 5.41616 | -0.9108 | 0.08673 |
| H | 5.68166 | -0.76498 | 1.1345 |
| C | 6.10789 | -0.21726 | -0.83258 |
| C | 7.2171 | 0.71803 | -0.41063 |
| H | 7.02977 | 1.74058 | -0.76665 |
| H | 7.33664 | 0.74998 | 0.67662 |
| H | 8.17634 | 0.40973 | -0.8481 |
| C | 5.89894 | -0.29981 | -2.3254 |
| H | 6.80177 | -0.6863 | -2.81711 |
| H | 5.06382 | -0.94115 | -2.6184 |
| H | 5.72354 | 0.69931 | -2.7469 |

**TS14**

Imaginary frequencies: -783.05

Thermal correction to Gibbs free energy: 0.572934

SCF energy in solution: -1370.499574

Sum of electronic and thermal Energies: -1369.364113

Solution-phase Gibbs free energy: -1369.92664

Coordinates:

| | | | |
|---|---|---|---|
| C | -0.26868 | 2.0774 | 0.07194 |
| C | -0.76423 | 3.38835 | 0.19128 |
| C | 0.0226 | 4.40663 | 0.71963 |
| C | 1.31655 | 4.10626 | 1.14005 |
| C | 1.76857 | 2.8027 | 0.97843 |
| C | -1.22993 | 1.01224 | -0.392 |
| C | -3.5258 | 0.19113 | 0.05196 |
| C | -3.37691 | -0.71877 | -1.00127 |
| C | -2.18832 | -0.76577 | -1.71912 |
| C | -1.09431 | 0.07371 | -1.4489 |
| H | -1.77183 | 3.59663 | -0.14882 |
| H | -0.36909 | 5.41639 | 0.79774 |
| H | 1.97174 | 4.85831 | 1.56602 |

| | | | |
|---|---|---|---|
| H | 2.77466 | 2.51845 | 1.26438 |
| H | -4.19847 | -1.37964 | -1.26297 |
| H | -2.09966 | -1.47196 | -2.54213 |
| N | 1.014 | 1.81652 | 0.45294 |
| C | 0.09944 | -0.11156 | -2.38967 |
| H | 0.30802 | -1.18227 | -2.48539 |
| H | -0.20575 | 0.22525 | -3.39588 |
| C | 1.30882 | 0.65705 | -1.9616 |
| H | 1.08123 | 1.71436 | -1.85858 |
| C | 2.70324 | 0.45546 | -2.23712 |
| C | 3.18425 | -0.79744 | -2.94262 |
| H | 2.55449 | -1.66459 | -2.74123 |
| H | 3.16613 | -0.60789 | -4.02436 |
| H | 4.21575 | -1.04316 | -2.67539 |
| C | 3.50817 | 1.70188 | -2.62525 |
| H | 3.32059 | 1.91768 | -3.68513 |
| H | 3.21015 | 2.57752 | -2.04222 |
| H | 4.5842 | 1.54664 | -2.49947 |
| Rh | 1.99609 | -0.05499 | -0.01677 |
| C | 2.7644 | -2.16832 | 0.36383 |
| C | 3.205 | -1.32375 | 1.46138 |
| C | 2.04298 | -0.84687 | 2.10858 |
| C | 0.86693 | -1.47613 | 1.47968 |
| C | 1.32618 | -2.32003 | 0.44698 |
| C | -0.52639 | -1.39759 | 2.02506 |
| H | -0.63832 | -2.10017 | 2.86307 |
| H | -0.76091 | -0.40019 | 2.40559 |
| H | -1.276 | -1.65228 | 1.27288 |
| C | 0.49397 | -3.25305 | -0.38142 |
| H | 0.42102 | -4.23546 | 0.1047 |
| H | -0.52368 | -2.87673 | -0.51563 |
| H | 0.92875 | -3.42059 | -1.37167 |
| C | 1.99035 | 0.00317 | 3.34303 |
| H | 1.13695 | 0.68721 | 3.33193 |
| H | 1.8869 | -0.63116 | 4.23372 |
| H | 2.90077 | 0.5957 | 3.46884 |
| C | 4.63235 | -1.0896 | 1.86878 |
| H | 4.75337 | -0.14516 | 2.40612 |
| H | 4.97356 | -1.89255 | 2.53612 |
| H | 5.30634 | -1.07228 | 1.00813 |
| C | 3.68307 | -3.03081 | -0.45153 |
| H | 4.6094 | -2.51303 | -0.71493 |
| H | 3.96332 | -3.9186 | 0.13189 |
| H | 3.21599 | -3.3858 | -1.37283 |

| | | | |
|---|---|---|---|
| H | 3.30608 | 0.53007 | -0.82218 |
| C | -2.45231 | 1.03812 | 0.32075 |
| H | -2.55299 | 1.74498 | 1.14033 |
| C | -4.80234 | 0.24483 | 0.87871 |
| H | -4.7608 | 1.13464 | 1.5232 |
| H | -4.82156 | -0.6156 | 1.55811 |
| C | -6.05468 | 0.28822 | 0.03703 |
| H | -6.09777 | 1.12732 | -0.65827 |
| C | -7.09645 | -0.55963 | 0.05448 |
| C | -8.28079 | -0.33427 | -0.85605 |
| H | -8.15136 | 0.54958 | -1.48801 |
| H | -8.4463 | -1.20181 | -1.50941 |
| H | -9.20319 | -0.20449 | -0.27378 |
| C | -7.22222 | -1.76785 | 0.95049 |
| H | -6.34425 | -1.94652 | 1.57629 |
| H | -8.08926 | -1.66165 | 1.61629 |
| H | -7.4012 | -2.67246 | 0.35396 |

**15**

Thermal correction to Gibbs free energy: 0.576469
SCF energy in solution: -1370.528779
Sum of electronic and thermal Energies: -1369.393494
Solution-phase Gibbs free energy: -1369.95231
Coordinates:

| | | | |
|---|---|---|---|
| C | -0.21923 | 2.44736 | 0.50676 |
| C | -0.01083 | 3.82331 | 0.62506 |
| C | -1.09547 | 4.68831 | 0.48288 |
| C | -2.36244 | 4.15715 | 0.23681 |
| C | -2.49704 | 2.77599 | 0.12419 |
| C | 0.83917 | 1.41711 | 0.653 |
| C | 3.04148 | 0.56603 | 0.0177 |
| C | 2.81338 | -0.54399 | 0.85124 |
| C | 1.63812 | -0.66227 | 1.58298 |
| C | 0.62102 | 0.31178 | 1.521 |
| H | 0.98296 | 4.19848 | 0.84477 |
| H | -0.95626 | 5.76101 | 0.57661 |
| H | -3.2337 | 4.79518 | 0.13535 |
| H | -3.45902 | 2.31126 | -0.0646 |
| H | 3.59161 | -1.29521 | 0.95393 |
| H | 1.51421 | -1.5031 | 2.25972 |
| N | -1.44815 | 1.94619 | 0.24057 |
| C | -0.55695 | 0.26318 | 2.50846 |
| H | -0.23774 | -0.3319 | 3.37008 |
| H | -0.73124 | 1.27637 | 2.88678 |

| | | | |
|---|---|---|---|
| C | -1.85464 | -0.30908 | 1.89518 |
| H | -2.66535 | 0.42177 | 1.98484 |
| C | -2.35219 | -1.62653 | 2.50694 |
| C | -1.30921 | -2.75143 | 2.58998 |
| H | -0.80296 | -2.91378 | 1.63383 |
| H | -0.53941 | -2.53609 | 3.34089 |
| H | -1.78386 | -3.69269 | 2.88963 |
| C | -2.95099 | -1.36207 | 3.90775 |
| H | -2.19287 | -0.98465 | 4.60503 |
| H | -3.76272 | -0.62685 | 3.86448 |
| H | -3.35787 | -2.28652 | 4.334 |
| Rh | -1.3416 | -0.17874 | -0.15768 |
| C | -2.34393 | -1.95639 | -1.11687 |
| C | -2.8306 | -0.69679 | -1.6378 |
| C | -1.76851 | -0.11216 | -2.48362 |
| C | -0.62801 | -0.89677 | -2.33174 |
| C | -0.95641 | -2.0122 | -1.42116 |
| C | 0.72161 | -0.70393 | -2.95204 |
| H | 0.93992 | -1.51504 | -3.65891 |
| H | 0.78807 | 0.23953 | -3.49912 |
| H | 1.5137 | -0.71136 | -2.19491 |
| C | -0.0138 | -3.14387 | -1.14092 |
| H | 0.13447 | -3.73952 | -2.05218 |
| H | 0.96953 | -2.78068 | -0.82577 |
| H | -0.39485 | -3.81417 | -0.36794 |
| C | -1.93957 | 1.11866 | -3.32154 |
| H | -0.98236 | 1.49933 | -3.6861 |
| H | -2.56728 | 0.90339 | -4.19607 |
| H | -2.43032 | 1.92474 | -2.76534 |
| C | -4.26385 | -0.25681 | -1.6498 |
| H | -4.35503 | 0.82644 | -1.77217 |
| H | -4.79578 | -0.72072 | -2.49237 |
| H | -4.78508 | -0.54455 | -0.73256 |
| C | -3.18672 | -3.04467 | -0.52585 |
| H | -4.07093 | -2.651 | -0.01857 |
| H | -3.54102 | -3.70304 | -1.33108 |
| H | -2.63319 | -3.66311 | 0.1837 |
| H | -3.17955 | -1.9803 | 1.88093 |
| C | 2.03898 | 1.53413 | -0.06721 |
| H | 2.18216 | 2.39617 | -0.71473 |
| C | 4.34166 | 0.70296 | -0.76017 |
| H | 4.34377 | -0.02351 | -1.58149 |
| H | 4.35928 | 1.69429 | -1.2345 |
| C | 5.56685 | 0.53095 | 0.10599 |

| | | | |
|---|---|---|---|
| H | 5.62495 | 1.2285 | 0.942 |
| C | 6.56941 | -0.35096 | -0.04175 |
| C | 7.73259 | -0.35277 | 0.92217 |
| H | 7.83832 | -1.33153 | 1.40954 |
| H | 8.67763 | -0.16527 | 0.39477 |
| H | 7.62226 | 0.40707 | 1.70161 |
| C | 6.67035 | -1.3814 | -1.13999 |
| H | 6.78783 | -2.38701 | -0.71461 |
| H | 5.80762 | -1.39892 | -1.81093 |
| H | 7.56362 | -1.20013 | -1.75258 |

**TS16**

Imaginary frequencies: -325.02
Thermal correction to Gibbs free energy: 0.574954
SCF energy in solution: -1370.501775
Sum of electronic and thermal Energies: -1369.367847
Solution-phase Gibbs free energy: -1369.926821
Coordinates:

| | | | |
|---|---|---|---|
| C | 0.10257 | 2.41173 | 0.36293 |
| C | 0.3598 | 3.78137 | 0.52689 |
| C | -0.69732 | 4.6822 | 0.57434 |
| C | -2.00721 | 4.20427 | 0.47695 |
| C | -2.20124 | 2.83625 | 0.3318 |
| C | 1.12703 | 1.36272 | 0.31571 |
| C | 3.4207 | 0.59743 | -0.04151 |
| C | 2.98712 | -0.71479 | 0.2067 |
| C | 1.65382 | -0.99222 | 0.503 |
| C | 0.6958 | 0.03131 | 0.55581 |
| H | 1.38162 | 4.12728 | 0.63267 |
| H | -0.50526 | 5.7434 | 0.69999 |
| H | -2.86103 | 4.87146 | 0.52172 |
| H | -3.19623 | 2.40943 | 0.26727 |
| H | 3.71379 | -1.52263 | 0.18692 |
| H | 1.36188 | -2.01542 | 0.72618 |
| N | -1.17946 | 1.96474 | 0.26361 |
| C | -0.4508 | -0.2387 | 2.11176 |
| H | 0.00472 | -1.16746 | 2.43741 |
| H | -0.00494 | 0.63472 | 2.57969 |
| C | -1.89546 | -0.23424 | 2.00575 |
| H | -2.35381 | 0.73599 | 2.19705 |
| C | -2.74746 | -1.36996 | 2.57376 |
| C | -2.04391 | -2.7312 | 2.66245 |
| H | -1.56323 | -3.01383 | 1.72075 |
| H | -1.27602 | -2.73576 | 3.44537 |

| | | | |
|---|---|---|---|
| H | -2.76514 | -3.51372 | 2.92133 |
| C | -3.26263 | -0.95223 | 3.97049 |
| H | -2.43138 | -0.80701 | 4.67094 |
| H | -3.83475 | -0.01848 | 3.92663 |
| H | -3.91834 | -1.72719 | 4.38326 |
| Rh | -1.36898 | -0.15383 | -0.09126 |
| C | -2.86054 | -1.6277 | -1.08569 |
| C | -3.00082 | -0.31957 | -1.62955 |
| C | -1.76141 | -0.00236 | -2.35776 |
| C | -0.87284 | -1.08532 | -2.20899 |
| C | -1.51225 | -2.06608 | -1.34549 |
| C | 0.47491 | -1.24836 | -2.84292 |
| H | 0.42045 | -1.96867 | -3.66985 |
| H | 0.8484 | -0.30588 | -3.25088 |
| H | 1.2168 | -1.62072 | -2.1304 |
| C | -0.96403 | -3.43896 | -1.0865 |
| H | -1.11266 | -4.07229 | -1.97219 |
| H | 0.11057 | -3.41717 | -0.88406 |
| H | -1.4609 | -3.93295 | -0.24866 |
| C | -1.5552 | 1.22878 | -3.18856 |
| H | -0.49499 | 1.4346 | -3.35631 |
| H | -2.02918 | 1.10601 | -4.17155 |
| H | -2.00103 | 2.11311 | -2.72355 |
| C | -4.27086 | 0.47681 | -1.70844 |
| H | -4.07539 | 1.55 | -1.78932 |
| H | -4.8476 | 0.19077 | -2.59877 |
| H | -4.91186 | 0.31163 | -0.83736 |
| C | -3.95709 | -2.45525 | -0.48815 |
| H | -4.72979 | -1.83981 | -0.01966 |
| H | -4.4449 | -3.03864 | -1.28115 |
| H | -3.58758 | -3.16562 | 0.25478 |
| H | -3.63283 | -1.48037 | 1.93675 |
| C | 2.47223 | 1.62324 | 0.02169 |
| H | 2.79005 | 2.64109 | -0.19115 |
| C | 4.87357 | 0.88861 | -0.38566 |
| H | 5.02713 | 1.97645 | -0.34737 |
| H | 5.05388 | 0.59836 | -1.4278 |
| C | 5.85562 | 0.2066 | 0.536 |
| H | 5.73238 | 0.46147 | 1.58921 |
| C | 6.84449 | -0.64314 | 0.21224 |
| C | 7.74938 | -1.20607 | 1.28314 |
| H | 7.71692 | -2.30415 | 1.28945 |
| H | 8.79564 | -0.92828 | 1.0968 |
| H | 7.47667 | -0.85004 | 2.28121 |

| | | | |
|---|---|---|---|
| C | 7.17635 | -1.10237 | -1.18681 |
| H | 7.17187 | -2.19918 | -1.24319 |
| H | 6.49187 | -0.72385 | -1.95009 |
| H | 8.19067 | -0.78427 | -1.46276 |

**17**

Thermal correction to Gibbs free energy: 0.573348
SCF energy in solution: -1370.532515
Sum of electronic and thermal Energies: -1369.349205
Solution-phase Gibbs free energy: -1369.959167
Coordinates:

| | | | |
|---|---|---|---|
| C | -0.12679 | -2.05233 | -1.01063 |
| C | -0.29969 | -3.32064 | -1.58744 |
| C | 0.79979 | -4.13828 | -1.8122 |
| C | 2.07282 | -3.68786 | -1.44956 |
| C | 2.18589 | -2.42605 | -0.88143 |
| C | -1.19197 | -1.1024 | -0.69136 |
| C | -3.54002 | -0.45147 | -0.51785 |
| C | -3.12269 | 0.74825 | 0.07927 |
| C | -1.76849 | 1.03085 | 0.27657 |
| C | -0.78416 | 0.12195 | -0.11701 |
| H | -1.29413 | -3.65705 | -1.85611 |
| H | 0.66846 | -5.11825 | -2.26084 |
| H | 2.95766 | -4.29661 | -1.59954 |
| H | 3.1474 | -2.03024 | -0.57476 |
| H | -3.87371 | 1.46446 | 0.40295 |
| H | -1.49578 | 1.97357 | 0.74408 |
| N | 1.1233 | -1.6271 | -0.67528 |
| C | 0.91851 | 0.55243 | 2.34293 |
| H | 1.75341 | 1.12374 | 2.73649 |
| H | -0.05393 | 1.02964 | 2.38655 |
| C | 1.022 | -0.80861 | 2.16437 |
| H | 0.09644 | -1.34392 | 1.95904 |
| C | 2.16824 | -1.70443 | 2.58414 |
| C | 3.51313 | -1.00261 | 2.79132 |
| H | 3.84868 | -0.49679 | 1.87994 |
| H | 3.46386 | -0.26023 | 3.59645 |
| H | 4.27816 | -1.73385 | 3.07212 |
| C | 1.72921 | -2.44631 | 3.87036 |
| H | 1.59355 | -1.74393 | 4.70047 |
| H | 0.78714 | -2.98618 | 3.72514 |
| H | 2.49319 | -3.17487 | 4.1619 |
| Rh | 1.22638 | 0.38181 | 0.05533 |
| C | 3.07342 | 1.97045 | 0.11634 |

| | | | |
|---|---|---|---|
| C | 3.26705 | 1.15104 | -0.9982 |
| C | 2.05927 | 1.24394 | -1.8345 |
| C | 1.19732 | 2.24172 | -1.26965 |
| C | 1.74181 | 2.59392 | 0.00491 |
| C | -0.00231 | 2.84688 | -1.9334 |
| H | 0.31599 | 3.69597 | -2.55311 |
| H | -0.51528 | 2.13425 | -2.5835 |
| H | -0.72948 | 3.22133 | -1.21024 |
| C | 1.24257 | 3.68928 | 0.90162 |
| H | 1.68977 | 4.65007 | 0.61225 |
| H | 0.15717 | 3.80424 | 0.83755 |
| H | 1.50271 | 3.51403 | 1.94918 |
| C | 1.91429 | 0.63132 | -3.19609 |
| H | 0.86543 | 0.55328 | -3.49344 |
| H | 2.42752 | 1.2493 | -3.94516 |
| H | 2.35401 | -0.36896 | -3.24175 |
| C | 4.50979 | 0.39632 | -1.36911 |
| H | 4.28352 | -0.52232 | -1.91822 |
| H | 5.14441 | 1.00673 | -2.02569 |
| H | 5.10859 | 0.13159 | -0.4929 |
| C | 4.06627 | 2.30031 | 1.18902 |
| H | 4.90114 | 1.59633 | 1.21119 |
| H | 4.4833 | 3.30077 | 1.00995 |
| H | 3.61347 | 2.32203 | 2.18513 |
| H | 2.2934 | -2.47066 | 1.80718 |
| C | -2.5589 | -1.37039 | -0.889 |
| H | -2.87092 | -2.31291 | -1.33227 |
| C | -5.01685 | -0.73306 | -0.75692 |
| H | -5.12349 | -1.7853 | -1.05738 |
| H | -5.35558 | -0.14214 | -1.61612 |
| C | -5.88163 | -0.46467 | 0.45069 |
| H | -5.59598 | -1.02833 | 1.33978 |
| C | -6.94035 | 0.35635 | 0.54833 |
| C | -7.70111 | 0.47211 | 1.84859 |
| H | -7.7113 | 1.51003 | 2.20876 |
| H | -8.7518 | 0.18067 | 1.71487 |
| H | -7.27196 | -0.15802 | 2.63361 |
| C | -7.49077 | 1.20566 | -0.57166 |
| H | -7.54046 | 2.25976 | -0.26711 |
| H | -6.90833 | 1.14982 | -1.49458 |
| H | -8.52015 | 0.90513 | -0.80927 |

**18**

Thermal correction to Gibbs free energy: 0.569114

SCF energy in solution: -1370.496252
Sum of electronic and thermal Energies: -1369.358704
Solution-phase Gibbs free energy: -1369.927138
Coordinates:

| | | | |
|---|---|---|---|
| C | -3.06706 | -1.00885 | -0.68818 |
| C | -3.75673 | -1.30659 | -1.87089 |
| C | -4.67749 | -2.35383 | -1.86799 |
| C | -4.87644 | -3.07092 | -0.68922 |
| C | -4.14399 | -2.70038 | 0.43999 |
| C | -2.09228 | 1.15477 | 0.26506 |
| C | -2.02908 | 0.06699 | -0.65293 |
| C | -0.96181 | -0.02358 | -1.54663 |
| C | 0.0675 | 0.93584 | -1.59053 |
| H | -3.58424 | -0.7173 | -2.76602 |
| H | -5.23096 | -2.60159 | -2.76926 |
| H | -5.5815 | -3.89462 | -0.63996 |
| H | -4.26975 | -3.23538 | 1.37934 |
| H | -0.93215 | -0.85871 | -2.24255 |
| N | -3.26019 | -1.6952 | 0.45318 |
| C | 1.1271 | 0.8821 | -2.68353 |
| H | 1.173 | -0.13052 | -3.09302 |
| H | 0.83678 | 1.54015 | -3.51681 |
| C | 2.47042 | 1.32614 | -2.15128 |
| H | 2.54872 | 2.38783 | -1.92893 |
| C | 3.65409 | 0.63559 | -2.18479 |
| C | 3.81035 | -0.73753 | -2.78772 |
| H | 2.89444 | -1.33093 | -2.77687 |
| H | 4.12592 | -0.62578 | -3.83493 |
| H | 4.60189 | -1.30447 | -2.28863 |
| C | 4.94722 | 1.35795 | -1.89319 |
| H | 5.48615 | 1.51209 | -2.83876 |
| H | 4.78033 | 2.3344 | -1.43197 |
| H | 5.61003 | 0.77227 | -1.24974 |
| Rh | 2.17599 | 0.52929 | 0.10499 |
| C | 3.61839 | -0.71416 | 1.2106 |
| C | 2.88305 | 0.11254 | 2.13814 |
| C | 1.51635 | -0.30007 | 2.055 |
| C | 1.45122 | -1.53684 | 1.24411 |
| C | 2.72272 | -1.79192 | 0.74156 |
| C | 0.22445 | -2.37872 | 1.09913 |
| H | 0.09093 | -2.99309 | 2.00093 |
| H | -0.68681 | -1.78446 | 0.98904 |
| H | 0.2938 | -3.0601 | 0.24717 |
| C | 3.16221 | -2.99474 | -0.036 |

| | | | |
|---|---|---|---|
| H | 3.60165 | -3.74011 | 0.64107 |
| H | 2.3258 | -3.47505 | -0.55039 |
| H | 3.92525 | -2.75419 | -0.78003 |
| C | 0.38865 | 0.20327 | 2.90033 |
| H | -0.56403 | 0.16302 | 2.36743 |
| H | 0.29144 | -0.42462 | 3.79719 |
| H | 0.55597 | 1.23157 | 3.22973 |
| C | 3.46268 | 1.12779 | 3.08019 |
| H | 2.74288 | 1.91194 | 3.32537 |
| H | 3.75191 | 0.63409 | 4.01772 |
| H | 4.35361 | 1.60631 | 2.66701 |
| C | 5.10927 | -0.7378 | 1.0745 |
| H | 5.54638 | 0.25691 | 1.19186 |
| H | 5.53889 | -1.38106 | 1.85561 |
| H | 5.428 | -1.14688 | 0.11238 |
| H | 2.61093 | 2.00684 | 0.37295 |
| C | -1.06161 | 2.0897 | 0.23757 |
| H | -1.1048 | 2.94167 | 0.91142 |
| C | -3.28127 | 1.37744 | 1.18594 |
| H | -2.96819 | 2.07334 | 1.97781 |
| H | -3.55211 | 0.43981 | 1.67417 |
| C | -4.458 | 1.96971 | 0.43775 |
| H | -4.20274 | 2.81746 | -0.19929 |
| C | -5.7467 | 1.59727 | 0.49248 |
| C | -6.78996 | 2.33765 | -0.31102 |
| H | -7.31393 | 1.65709 | -0.99632 |
| H | -7.55833 | 2.76848 | 0.34523 |
| H | -6.35501 | 3.14925 | -0.90227 |
| C | -6.2903 | 0.46987 | 1.33464 |
| H | -6.83629 | -0.24918 | 0.70931 |
| H | -5.52028 | -0.07755 | 1.88239 |
| H | -7.01338 | 0.85554 | 2.06612 |
| C | 0.01113 | 2.00079 | -0.66821 |
| H | 0.69704 | 2.83712 | -0.74136 |

**TS19**

Imaginary frequencies: -577.37

Thermal correction to Gibbs free energy: 0.564833

SCF energy in solution: -1370.48725

Sum of electronic and thermal Energies: -1369.341841

Solution-phase Gibbs free energy: -1369.922417

Coordinates:

| | | | |
|---|---|---|---|
| C | 3.26824 | 1.90445 | -0.13886 |
| C | 2.51795 | 2.96321 | -0.67639 |

| | | | |
|---|---|---|---|
| C | 3.14657 | 4.17807 | -0.94265 |
| C | 4.50748 | 4.30428 | -0.67013 |
| C | 5.17685 | 3.19506 | -0.14962 |
| C | 3.19257 | -0.64765 | -0.10846 |
| C | 2.52173 | -1.79973 | 0.3247 |
| C | 1.32251 | -1.73924 | 1.02936 |
| C | 0.7309 | -0.50493 | 1.32718 |
| H | 1.46343 | 2.82609 | -0.89733 |
| H | 2.58546 | 5.00844 | -1.36273 |
| H | 5.04073 | 5.23031 | -0.8603 |
| H | 6.24152 | 3.2468 | 0.07043 |
| H | 2.96149 | -2.76964 | 0.1058 |
| H | 0.85231 | -2.66072 | 1.36563 |
| N | 4.58458 | 2.02593 | 0.11284 |
| C | -0.54028 | -0.45024 | 2.16011 |
| H | -0.99986 | -1.44485 | 2.18677 |
| H | -0.26425 | -0.2334 | 3.20641 |
| C | -1.55306 | 0.60606 | 1.74253 |
| H | -1.0945 | 1.51408 | 1.33277 |
| C | -2.77786 | 0.86019 | 2.43924 |
| C | -3.30256 | -0.1432 | 3.44739 |
| H | -3.13133 | -1.17768 | 3.14218 |
| H | -2.77839 | 0.01728 | 4.39981 |
| H | -4.37114 | -0.00399 | 3.63312 |
| C | -3.1492 | 2.3093 | 2.7357 |
| H | -2.61923 | 2.6128 | 3.64893 |
| H | -2.84391 | 2.98747 | 1.93333 |
| H | -4.22105 | 2.43549 | 2.91243 |
| Rh | -2.95109 | 0.26064 | 0.13889 |
| C | -3.84624 | -1.55405 | -0.62563 |
| C | -4.49309 | -0.48633 | -1.35618 |
| C | -3.4627 | 0.19656 | -2.05113 |
| C | -2.18774 | -0.54264 | -1.9 |
| C | -2.43478 | -1.64012 | -1.06765 |
| C | -0.90933 | -0.20068 | -2.60401 |
| H | -0.90726 | -0.6205 | -3.61917 |
| H | -0.77964 | 0.88103 | -2.70276 |
| H | -0.03917 | -0.59447 | -2.07339 |
| C | -1.51113 | -2.76271 | -0.72583 |
| H | -1.73193 | -3.62547 | -1.37001 |
| H | -0.46494 | -2.48961 | -0.86913 |
| H | -1.63758 | -3.0958 | 0.30872 |
| C | -3.61799 | 1.42275 | -2.89136 |
| H | -2.78088 | 2.11506 | -2.754 |

| | | | |
|---|---|---|---|
| H | -3.6303 | 1.14442 | -3.95448 |
| H | -4.54737 | 1.95391 | -2.67451 |
| C | -5.96212 | -0.17629 | -1.37007 |
| H | -6.15266 | 0.887 | -1.53589 |
| H | -6.45707 | -0.73154 | -2.17744 |
| H | -6.44516 | -0.45841 | -0.43135 |
| C | -4.53446 | -2.58346 | 0.21158 |
| H | -5.4333 | -2.18534 | 0.68832 |
| H | -4.84053 | -3.42723 | -0.42344 |
| H | -3.87614 | -2.9836 | 0.98746 |
| H | -3.99362 | 0.75658 | 1.2731 |
| C | 2.62143 | 0.60505 | 0.21186 |
| C | 4.48369 | -0.82531 | -0.89682 |
| H | 4.70244 | 0.08727 | -1.45944 |
| H | 4.32758 | -1.62314 | -1.63063 |
| C | 5.65763 | -1.1442 | 0.00125 |
| H | 5.8757 | -0.35882 | 0.72232 |
| C | 6.42826 | -2.24348 | -0.00112 |
| C | 7.57246 | -2.37374 | 0.97774 |
| H | 7.64907 | -1.50209 | 1.6347 |
| H | 7.45443 | -3.26693 | 1.60735 |
| H | 8.53054 | -2.48979 | 0.45212 |
| C | 6.27627 | -3.42013 | -0.9352 |
| H | 5.44142 | -3.32207 | -1.63407 |
| H | 7.19015 | -3.56128 | -1.52842 |
| H | 6.13309 | -4.34978 | -0.36688 |
| C | 1.40483 | 0.64879 | 0.91665 |
| H | 1.0178 | 1.62782 | 1.18834 |

**20**

Thermal correction to Gibbs free energy: 0.572491
SCF energy in solution: -1370.509525
Sum of electronic and thermal Energies: -1369.364387
Solution-phase Gibbs free energy: -1369.937034
Coordinates:

| | | | |
|---|---|---|---|
| C | -2.72001 | 1.83452 | -0.64471 |
| C | -2.1902 | 3.13008 | -0.52167 |
| C | -3.05937 | 4.21958 | -0.48609 |
| C | -4.43023 | 3.98884 | -0.57639 |
| C | -4.86777 | 2.66705 | -0.69106 |
| C | -2.12953 | -0.6086 | -0.14586 |
| C | -1.24256 | -1.67343 | -0.36541 |
| C | -0.09264 | -1.5509 | -1.1508 |
| C | 0.20692 | -0.31517 | -1.77813 |

| | | | |
|---|---|---|---|
| H | -1.1175 | 3.28354 | -0.45145 |
| H | -2.67104 | 5.22938 | -0.38894 |
| H | -5.14481 | 4.8053 | -0.55713 |
| H | -5.9296 | 2.44106 | -0.76329 |
| H | -1.47884 | -2.63973 | 0.07273 |
| H | 0.51313 | -2.42761 | -1.36313 |
| N | -4.04496 | 1.61518 | -0.72376 |
| C | 1.40521 | -0.16872 | -2.71783 |
| H | 1.4872 | -1.0585 | -3.35047 |
| H | 1.24615 | 0.68528 | -3.38452 |
| C | 2.63824 | 0.02793 | -1.81738 |
| H | 3.00586 | 1.05969 | -1.88023 |
| C | 3.81613 | -0.93728 | -2.02958 |
| C | 3.46551 | -2.42826 | -1.89715 |
| H | 3.02658 | -2.65888 | -0.9196 |
| H | 2.76015 | -2.75483 | -2.67077 |
| H | 4.36599 | -3.04164 | -2.01163 |
| C | 4.47859 | -0.66228 | -3.39804 |
| H | 3.79089 | -0.87416 | -4.22554 |
| H | 4.79985 | 0.38167 | -3.48615 |
| H | 5.36103 | -1.29842 | -3.53192 |
| Rh | 1.65873 | 0.00643 | 0.04625 |
| C | 3.26362 | 0.68396 | 1.37492 |
| C | 2.1252 | 1.56109 | 1.48615 |
| C | 1.05125 | 0.86293 | 2.22744 |
| C | 1.45582 | -0.45265 | 2.40199 |
| C | 2.8079 | -0.60543 | 1.80083 |
| C | 0.71552 | -1.5691 | 3.07009 |
| H | 1.17164 | -1.80137 | 4.04167 |
| H | -0.33218 | -1.31561 | 3.24612 |
| H | 0.74705 | -2.48667 | 2.47356 |
| C | 3.63614 | -1.84595 | 1.91913 |
| H | 4.08123 | -1.89907 | 2.92306 |
| H | 3.03555 | -2.7497 | 1.78279 |
| H | 4.45226 | -1.86337 | 1.19321 |
| C | -0.22443 | 1.50739 | 2.67549 |
| H | -0.95806 | 0.76754 | 3.00366 |
| H | -0.03503 | 2.18351 | 3.5198 |
| H | -0.68509 | 2.10349 | 1.88159 |
| C | 2.11898 | 3.02458 | 1.17664 |
| H | 1.12345 | 3.37339 | 0.88793 |
| H | 2.41504 | 3.59097 | 2.0715 |
| H | 2.8223 | 3.2766 | 0.37908 |
| C | 4.65411 | 1.08117 | 0.9806 |

| | | | |
|---|---|---|---|
| H | 4.65863 | 1.80718 | 0.16225 |
| H | 5.16456 | 1.54497 | 1.83498 |
| H | 5.25115 | 0.22044 | 0.67149 |
| H | 4.56533 | -0.70564 | -1.26127 |
| C | -1.82899 | 0.64126 | -0.74342 |
| C | -3.34683 | -0.8819 | 0.72682 |
| H | -3.01903 | -1.47747 | 1.58575 |
| H | -3.74538 | 0.05874 | 1.11589 |
| C | -4.43425 | -1.6039 | -0.03832 |
| H | -4.82882 | -1.02968 | -0.87381 |
| C | -4.94574 | -2.82165 | 0.20414 |
| C | -6.04906 | -3.36995 | -0.67079 |
| H | -5.75045 | -4.32165 | -1.13168 |
| H | -6.95087 | -3.58088 | -0.07992 |
| H | -6.32135 | -2.67461 | -1.47026 |
| C | -4.52945 | -3.74339 | 1.3251 |
| H | -4.19423 | -4.71057 | 0.92601 |
| H | -3.72885 | -3.34309 | 1.95314 |
| H | -5.38435 | -3.96183 | 1.97906 |
| C | -0.65437 | 0.7676 | -1.51355 |
| H | -0.45988 | 1.71021 | -2.01742 |

**TS21**

Imaginary frequencies: -291.76
Thermal correction to Gibbs free energy: 0.568795
SCF energy in solution: -1370.470502
Sum of electronic and thermal Energies: -1369.330741
Solution-phase Gibbs free energy: -1369.901707
Coordinates:

| | | | |
|---|---|---|---|
| C | -2.71601 | 1.28363 | -0.56617 |
| C | -4.04531 | 1.59988 | -0.25072 |
| C | -4.61852 | 2.74191 | -0.80934 |
| C | -3.85356 | 3.53608 | -1.66093 |
| C | -2.53366 | 3.15284 | -1.90491 |
| C | -2.54515 | -1.19823 | 0.1116 |
| C | -2.00438 | 0.10332 | 0.00856 |
| C | -0.68434 | 0.33063 | 0.44489 |
| C | 0.12941 | -0.71377 | 0.88919 |
| H | -4.60967 | 0.97333 | 0.43138 |
| H | -5.645 | 3.00875 | -0.57448 |
| H | -4.25989 | 4.43193 | -2.11954 |
| H | -1.89928 | 3.75043 | -2.55702 |
| H | -0.31372 | 1.35091 | 0.39516 |
| N | -1.96781 | 2.06289 | -1.3761 |

| | | | |
|---|---|---|---|
| C | 1.44366 | -0.23509 | 2.43215 |
| H | 0.61637 | 0.32372 | 2.8573 |
| H | 1.53405 | -1.24598 | 2.81783 |
| C | 2.63822 | 0.47705 | 2.09393 |
| H | 3.5644 | -0.07936 | 2.24862 |
| C | 2.81186 | 1.97839 | 2.32197 |
| C | 1.63773 | 2.85022 | 1.8556 |
| H | 1.46589 | 2.75787 | 0.77599 |
| H | 0.70371 | 2.60005 | 2.37291 |
| H | 1.84713 | 3.90458 | 2.06424 |
| C | 3.12614 | 2.23018 | 3.81345 |
| H | 2.26855 | 1.96887 | 4.44492 |
| H | 3.98506 | 1.63899 | 4.14993 |
| H | 3.35894 | 3.28743 | 3.98185 |
| Rh | 2.04037 | -0.19094 | 0.1399 |
| C | 4.06269 | -0.32545 | -0.84272 |
| C | 3.4711 | -1.63968 | -0.63569 |
| C | 2.33748 | -1.79941 | -1.55915 |
| C | 2.11911 | -0.55727 | -2.16246 |
| C | 3.17563 | 0.37599 | -1.69167 |
| C | 1.03788 | -0.16748 | -3.12312 |
| H | 1.47194 | 0.18401 | -4.06763 |
| H | 0.37917 | -1.0089 | -3.34789 |
| H | 0.41311 | 0.64163 | -2.72404 |
| C | 3.31748 | 1.78133 | -2.18656 |
| H | 3.77777 | 1.7818 | -3.18448 |
| H | 2.34442 | 2.27327 | -2.28003 |
| H | 3.94919 | 2.38478 | -1.53012 |
| C | 1.57632 | -3.07289 | -1.75713 |
| H | 0.65529 | -2.90905 | -2.3201 |
| H | 2.18607 | -3.79911 | -2.31022 |
| H | 1.30224 | -3.5347 | -0.80328 |
| C | 4.07877 | -2.75262 | 0.15737 |
| H | 3.31969 | -3.44587 | 0.53013 |
| H | 4.76101 | -3.32911 | -0.48382 |
| H | 4.66162 | -2.38318 | 1.00498 |
| C | 5.36849 | 0.15645 | -0.28443 |
| H | 5.57072 | -0.25997 | 0.7067 |
| H | 6.1955 | -0.14781 | -0.93934 |
| H | 5.39767 | 1.24629 | -0.20382 |
| H | 3.69785 | 2.282 | 1.74707 |
| C | -1.72811 | -2.21679 | 0.63468 |
| H | -2.13926 | -3.22055 | 0.71669 |
| C | -3.95258 | -1.57716 | -0.32253 |

| | | | |
|---|---|---|---|
| H | -3.89772 | -2.57961 | -0.77315 |
| H | -4.29674 | -0.90837 | -1.11553 |
| C | -4.93828 | -1.60991 | 0.83201 |
| H | -4.51261 | -1.9265 | 1.78454 |
| C | -6.25401 | -1.34126 | 0.79393 |
| C | -7.10073 | -1.46967 | 2.03835 |
| H | -7.5972 | -0.51941 | 2.27787 |
| H | -7.9002 | -2.2089 | 1.89343 |
| H | -6.51037 | -1.77473 | 2.90774 |
| C | -7.01235 | -0.93154 | -0.44506 |
| H | -7.59092 | -0.01605 | -0.26279 |
| H | -6.37213 | -0.76228 | -1.31436 |
| H | -7.74192 | -1.70634 | -0.7176 |
| C | -0.40724 | -1.99807 | 1.01802 |
| H | 0.19067 | -2.82244 | 1.39867 |

**22**

Thermal correction to Gibbs free energy: 0.567787
SCF energy in solution: -1370.489346
Sum of electronic and thermal Energies: -1369.332526
Solution-phase Gibbs free energy: -1369.921559
Coordinates:

| | | | |
|---|---|---|---|
| C | -2.87547 | 1.38926 | 0.55693 |
| C | -4.13473 | 1.12304 | 1.11504 |
| C | -4.77725 | 2.12285 | 1.84445 |
| C | -4.1489 | 3.35614 | 2.00277 |
| C | -2.88678 | 3.52456 | 1.43101 |
| C | -2.64715 | -0.49964 | -1.18342 |
| C | -2.10175 | 0.36884 | -0.21274 |
| C | -0.71065 | 0.34548 | 0.01615 |
| C | 0.1435 | -0.53482 | -0.65007 |
| H | -4.59086 | 0.14654 | 0.99462 |
| H | -5.75121 | 1.93509 | 2.28761 |
| H | -4.61391 | 4.164 | 2.55878 |
| H | -2.35585 | 4.46876 | 1.54014 |
| H | -0.32916 | 1.06598 | 0.73372 |
| N | -2.25635 | 2.57666 | 0.73064 |
| C | 2.22623 | -2.55687 | -0.0917 |
| H | 1.21733 | -2.95035 | -0.1112 |
| H | 2.84788 | -2.78981 | -0.95178 |
| C | 2.79634 | -2.10557 | 1.08226 |
| H | 3.87463 | -1.94952 | 1.09695 |
| C | 2.14415 | -2.08962 | 2.45593 |
| C | 0.69065 | -2.58002 | 2.48418 |

| | | | |
|---|---|---|---|
| H | 0.03754 | -1.99324 | 1.8304 |
| H | 0.62438 | -3.63161 | 2.18184 |
| H | 0.29623 | -2.50489 | 3.50244 |
| C | 3.02868 | -2.91766 | 3.41801 |
| H | 3.06235 | -3.96787 | 3.10706 |
| H | 4.0563 | -2.53881 | 3.45445 |
| H | 2.61779 | -2.87674 | 4.43169 |
| Rh | 2.08067 | -0.26702 | -0.10478 |
| C | 4.25987 | 0.49846 | -0.60512 |
| C | 3.30626 | 0.40101 | -1.72986 |
| C | 2.30127 | 1.44338 | -1.55883 |
| C | 2.50912 | 2.00206 | -0.27522 |
| C | 3.7492 | 1.43298 | 0.29717 |
| C | 1.71065 | 3.10111 | 0.35275 |
| H | 1.7815 | 3.07967 | 1.44391 |
| H | 2.10023 | 4.0742 | 0.02148 |
| H | 0.65251 | 3.05723 | 0.07829 |
| C | 4.33832 | 1.86378 | 1.60535 |
| H | 4.75873 | 2.87444 | 1.51969 |
| H | 3.58336 | 1.8986 | 2.39797 |
| H | 5.14123 | 1.19825 | 1.93045 |
| C | 1.2885 | 1.87514 | -2.57486 |
| H | 0.3915 | 2.28161 | -2.10253 |
| H | 1.72107 | 2.65789 | -3.21248 |
| H | 0.98144 | 1.04861 | -3.21955 |
| C | 3.54622 | -0.36868 | -2.98987 |
| H | 2.61162 | -0.59843 | -3.50724 |
| H | 4.16567 | 0.23027 | -3.67301 |
| H | 4.07981 | -1.30434 | -2.80308 |
| C | 5.53696 | -0.27924 | -0.50907 |
| H | 5.40838 | -1.32045 | -0.82288 |
| H | 6.29705 | 0.15986 | -1.1687 |
| H | 5.94325 | -0.27771 | 0.50541 |
| H | 2.16795 | -1.05059 | 2.82663 |
| C | -1.77156 | -1.3727 | -1.85339 |
| H | -2.18123 | -2.0329 | -2.615 |
| C | -4.1126 | -0.52372 | -1.59137 |
| H | -4.14672 | -0.68124 | -2.67981 |
| H | -4.5721 | 0.45195 | -1.41425 |
| C | -4.89764 | -1.63051 | -0.91064 |
| H | -4.32829 | -2.54097 | -0.72135 |
| C | -6.19656 | -1.62393 | -0.56775 |
| C | -6.83075 | -2.84055 | 0.06464 |
| H | -7.26347 | -2.59634 | 1.04451 |

| | | | |
|---|---|---|---|
| H | -7.65691 | -3.21785 | -0.55334 |
| H | -6.11174 | -3.65396 | 0.20242 |
| C | -7.13983 | -0.46762 | -0.79443 |
| H | -7.66385 | -0.20421 | 0.13416 |
| H | -6.64699 | 0.43085 | -1.17382 |
| H | -7.91832 | -0.7479 | -1.51718 |
| C | -0.40219 | -1.40912 | -1.5984 |
| H | 0.22254 | -2.10165 | -2.1564 |

**TS23**

Imaginary frequencies: -317.59
Thermal correction to Gibbs free energy: 0.486305
SCF energy in solution: -1214.49724017
Sum of electronic and thermal Energies: -1213.384431
Solution-phase Gibbs free energy: -1214.01093517
Coordinates:

| | | | |
|---|---|---|---|
| C | 1.80413 | 0.05634 | 1.12471 |
| C | 2.99432 | -0.27529 | 1.79475 |
| C | 3.10259 | -1.4809 | 2.47707 |
| C | 2.0218 | -2.36469 | 2.47905 |
| C | 0.88982 | -2.01432 | 1.75749 |
| C | 1.53313 | 1.29986 | 0.39114 |
| C | 2.1219 | 2.55454 | 0.70052 |
| C | 1.74366 | 3.67215 | -0.05415 |
| C | 0.80691 | 3.57568 | -1.07972 |
| C | 0.21146 | 2.34897 | -1.36501 |
| C | 0.54259 | 1.20507 | -0.62888 |
| H | 3.83598 | 0.40086 | 1.7618 |
| H | 4.02346 | -1.7318 | 2.99485 |
| H | 2.05811 | -3.31296 | 3.00389 |
| H | 0.03745 | -2.67893 | 1.68517 |
| H | 2.19049 | 4.63506 | 0.17573 |
| H | 0.53976 | 4.45589 | -1.65841 |
| H | -0.4981 | 2.28515 | -2.18442 |
| N | 0.78432 | -0.84602 | 1.09701 |
| C | 3.09902 | 2.78449 | 1.83489 |
| H | 2.83371 | 2.22606 | 2.73792 |
| H | 4.1252 | 2.5067 | 1.56128 |
| H | 3.12063 | 3.84597 | 2.09637 |
| C | 0.75177 | -0.27156 | -2.16771 |
| H | 0.27821 | -1.23505 | -2.30449 |
| H | 0.32161 | 0.45423 | -2.84791 |
| C | 2.21205 | -0.33084 | -2.16353 |
| H | 2.72532 | 0.62107 | -2.28512 |

| | | | |
|---|---|---|---|
| C | 2.97122 | -1.44806 | -2.0644 |
| C | 2.43448 | -2.84228 | -1.87431 |
| H | 1.36067 | -2.87919 | -1.67653 |
| H | 2.63565 | -3.45255 | -2.76524 |
| H | 2.94996 | -3.33635 | -1.04054 |
| C | 4.47135 | -1.35624 | -2.17082 |
| H | 4.84181 | -1.98085 | -2.99456 |
| H | 4.81269 | -0.33099 | -2.33933 |
| H | 4.95049 | -1.73566 | -1.25759 |
| Rh | -0.84448 | -0.39548 | -0.16181 |
| C | -2.95235 | -1.01649 | -0.59526 |
| C | -2.7089 | -1.08558 | 0.82633 |
| C | -2.6426 | 0.2859 | 1.33672 |
| C | -2.73947 | 1.16537 | 0.24804 |
| C | -2.85581 | 0.3612 | -0.96998 |
| C | -2.7982 | 2.66053 | 0.28892 |
| H | -3.79168 | 3.01141 | -0.01919 |
| H | -2.60763 | 3.04606 | 1.29316 |
| H | -2.06648 | 3.1162 | -0.38598 |
| C | -3.14386 | 0.91118 | -2.33629 |
| H | -4.22757 | 1.03206 | -2.47218 |
| H | -2.69142 | 1.89492 | -2.48462 |
| H | -2.78961 | 0.24616 | -3.12919 |
| C | -2.51573 | 0.63867 | 2.78828 |
| H | -2.19205 | 1.67228 | 2.93099 |
| H | -3.48069 | 0.51787 | 3.29842 |
| H | -1.79911 | -0.0121 | 3.29982 |
| C | -2.86101 | -2.30469 | 1.69008 |
| H | -2.22451 | -2.25524 | 2.57891 |
| H | -3.89734 | -2.39442 | 2.04307 |
| H | -2.61921 | -3.22211 | 1.14647 |
| C | -3.36681 | -2.14757 | -1.4932 |
| H | -3.01453 | -3.11378 | -1.12456 |
| H | -4.46283 | -2.19189 | -1.5497 |
| H | -2.99211 | -2.01869 | -2.51222 |
| H | -0.53994 | -1.85523 | -0.62199 |

**24**

Thermal correction to Gibbs free energy: 0.48104
SCF energy in solution: -1214.56796246
Sum of electronic and thermal Energies: -1213.455274
Solution-phase Gibbs free energy: -1214.08692246
Coordinates:

| | | | |
|---|---|---|---|
| C | -1.52391 | -1.18961 | 1.17328 |

| | | | |
|---|---|---|---|
| C | -2.56295 | -1.37442 | 2.10033 |
| C | -2.78937 | -0.4415 | 3.10829 |
| C | -1.98437 | 0.69253 | 3.19397 |
| C | -0.95663 | 0.82265 | 2.26991 |
| C | -1.18378 | -2.02596 | 0.00568 |
| C | -1.90153 | -3.16558 | -0.45048 |
| C | -1.4842 | -3.77268 | -1.64403 |
| C | -0.41192 | -3.28854 | -2.38555 |
| C | 0.30561 | -2.18282 | -1.92441 |
| C | -0.06106 | -1.55861 | -0.73377 |
| H | -3.19881 | -2.24165 | 2.04156 |
| H | -3.59649 | -0.60138 | 3.81691 |
| H | -2.13654 | 1.45187 | 3.95277 |
| H | -0.28938 | 1.67646 | 2.2877 |
| H | -2.02701 | -4.64356 | -1.99991 |
| H | -0.13029 | -3.77523 | -3.31549 |
| H | 1.14257 | -1.81288 | -2.50722 |
| N | -0.72247 | -0.08823 | 1.31114 |
| C | -3.09796 | -3.7829 | 0.24145 |
| H | -2.86442 | -4.12066 | 1.25815 |
| H | -3.94728 | -3.09169 | 0.3013 |
| H | -3.4388 | -4.65937 | -0.31556 |
| C | -1.15749 | 1.79083 | -1.98897 |
| H | -0.75889 | 2.80793 | -2.03086 |
| H | -0.94791 | 1.29245 | -2.94306 |
| C | -2.61111 | 1.72437 | -1.64035 |
| H | -3.05 | 0.7295 | -1.71864 |
| C | -3.42122 | 2.73455 | -1.27561 |
| C | -2.99924 | 4.17597 | -1.13215 |
| H | -1.93693 | 4.34507 | -1.32411 |
| H | -3.56914 | 4.81258 | -1.82209 |
| H | -3.2219 | 4.54314 | -0.12116 |
| C | -4.88401 | 2.48139 | -0.99979 |
| H | -5.51716 | 3.06516 | -1.68156 |
| H | -5.14755 | 1.42549 | -1.11387 |
| H | -5.15412 | 2.7959 | 0.01772 |
| Rh | 0.88439 | 0.08381 | -0.02632 |
| C | 2.59459 | 1.74729 | 0.00784 |
| C | 2.5864 | 1.1112 | 1.24933 |
| C | 2.71864 | -0.33652 | 1.00693 |
| C | 3.00543 | -0.52918 | -0.40877 |
| C | 2.80378 | 0.72142 | -1.04033 |
| C | 3.5046 | -1.80144 | -1.02279 |
| H | 4.56841 | -1.92567 | -0.78033 |

| | | | |
|---|---|---|---|
| H | 2.97207 | -2.67855 | -0.64708 |
| H | 3.41925 | -1.79317 | -2.11154 |
| C | 2.97902 | 1.03759 | -2.49514 |
| H | 3.97835 | 1.45722 | -2.67435 |
| H | 2.87733 | 0.14767 | -3.12094 |
| H | 2.24995 | 1.77737 | -2.83897 |
| C | 2.89142 | -1.37295 | 2.07354 |
| H | 2.65671 | -2.37351 | 1.7024 |
| H | 3.93407 | -1.38039 | 2.42169 |
| H | 2.25687 | -1.17181 | 2.94086 |
| C | 2.49207 | 1.74102 | 2.60639 |
| H | 1.89006 | 1.1413 | 3.29566 |
| H | 3.49236 | 1.8294 | 3.05062 |
| H | 2.06606 | 2.74741 | 2.56444 |
| C | 2.4662 | 3.21281 | -0.2746 |
| H | 2.09604 | 3.76659 | 0.59162 |
| H | 3.44353 | 3.63459 | -0.54523 |
| H | 1.79142 | 3.40492 | -1.11493 |
| H | -0.54454 | 1.23802 | -1.23102 |

**25**

Thermal correction to Gibbs free energy: 0.423922
SCF energy in solution: -967.579428557
Sum of electronic and thermal Energies: -966.414179
Solution-phase Gibbs free energy: -967.155506557
Coordinates:

| | | | |
|---|---|---|---|
| C | 3.19979 | 0.33454 | -0.82121 |
| C | 3.85006 | 0.09963 | 0.38732 |
| C | 3.39898 | 0.70026 | 1.57502 |
| C | 2.28778 | 1.53434 | 1.56996 |
| C | 1.61222 | 1.80614 | 0.36529 |
| H | 4.73501 | -0.53112 | 0.40794 |
| H | 3.93733 | 0.52443 | 2.50248 |
| H | 1.95675 | 2.00952 | 2.48964 |
| C | 3.7126 | -0.23488 | -2.12094 |
| H | 2.90027 | -0.65918 | -2.72171 |
| H | 4.18594 | 0.54743 | -2.72794 |
| H | 4.45981 | -1.01533 | -1.95127 |
| C | 0.48822 | 2.8333 | 0.32575 |
| H | 0.08216 | 2.96285 | 1.3323 |
| H | 0.8925 | 3.81247 | 0.02728 |
| C | -0.58452 | 2.42279 | -0.65752 |
| H | -0.30065 | 2.49203 | -1.70508 |
| C | -1.92434 | 2.26398 | -0.41524 |

| | | | |
|---|---|---|---|
| C | -2.56727 | 2.47768 | 0.9313 |
| H | -1.88987 | 2.32661 | 1.7735 |
| H | -2.93751 | 3.51168 | 0.98052 |
| H | -3.44253 | 1.83416 | 1.06298 |
| C | -2.88563 | 2.15951 | -1.57412 |
| H | -3.44092 | 3.10437 | -1.65802 |
| H | -2.37315 | 1.97885 | -2.52214 |
| H | -3.63131 | 1.37411 | -1.42003 |
| Rh | -0.32396 | 0.02844 | -0.41605 |
| C | -1.98331 | -1.36127 | 0.02383 |
| C | -0.97872 | -2.03632 | -0.76251 |
| C | 0.20657 | -2.07356 | 0.03707 |
| C | -0.14101 | -1.62158 | 1.40306 |
| C | -1.46603 | -1.19747 | 1.39743 |
| C | 0.79928 | -1.6942 | 2.56223 |
| H | 1.00397 | -2.74267 | 2.8167 |
| H | 1.76144 | -1.2258 | 2.32853 |
| H | 0.39188 | -1.20876 | 3.45202 |
| C | -2.28644 | -0.7588 | 2.57203 |
| H | -2.91205 | -1.58964 | 2.92557 |
| H | -1.66181 | -0.43959 | 3.40998 |
| H | -2.96242 | 0.06274 | 2.32306 |
| C | 1.48495 | -2.77136 | -0.31004 |
| H | 2.34948 | -2.27441 | 0.13697 |
| H | 1.46054 | -3.8013 | 0.07277 |
| H | 1.63882 | -2.82349 | -1.39044 |
| C | -1.18027 | -2.6716 | -2.10769 |
| H | -0.25127 | -2.71408 | -2.68054 |
| H | -1.53936 | -3.70114 | -1.97588 |
| H | -1.92008 | -2.13496 | -2.70608 |
| C | -3.42566 | -1.2292 | -0.35464 |
| H | -3.55497 | -1.08402 | -1.42996 |
| H | -3.96122 | -2.14913 | -0.08007 |
| H | -3.91574 | -0.40545 | 0.17039 |
| H | -0.26671 | 0.1638 | -1.97243 |
| C | 2.06841 | 1.18794 | -0.8209 |
| H | 1.66992 | 1.4962 | -1.78177 |

**TS26**

Imaginary frequencies: -554.20
Thermal correction to Gibbs free energy: 0.419746
SCF energy in solution: -967.574449327
Sum of electronic and thermal Energies: -966.401728
Solution-phase Gibbs free energy: -967.154703327

Coordinates:

| | | | |
|---|---|---|---|
| C | 4.03159 | -0.62193 | -0.74519 |
| C | 4.82693 | -0.65058 | 0.40732 |
| C | 4.51292 | 0.15378 | 1.50333 |
| C | 3.39507 | 0.98593 | 1.46625 |
| C | 2.5704 | 1.02485 | 0.33296 |
| H | 5.70049 | -1.29673 | 0.44216 |
| H | 5.14066 | 0.13114 | 2.38975 |
| H | 3.16168 | 1.61291 | 2.32446 |
| C | 4.39934 | -1.44655 | -1.95779 |
| H | 3.54486 | -1.5868 | -2.62848 |
| H | 5.19147 | -0.95725 | -2.53894 |
| H | 4.77557 | -2.43527 | -1.67372 |
| C | 1.38817 | 1.98507 | 0.34106 |
| H | 0.96052 | 2.01262 | 1.35031 |
| H | 1.77971 | 3.0037 | 0.1741 |
| C | 0.29758 | 1.7617 | -0.68921 |
| H | 0.66942 | 1.47316 | -1.67757 |
| C | -0.89462 | 2.55366 | -0.749 |
| C | -1.25723 | 3.49125 | 0.38743 |
| H | -1.04766 | 3.06628 | 1.37114 |
| H | -0.66042 | 4.40789 | 0.2831 |
| H | -2.31166 | 3.77808 | 0.34778 |
| C | -1.37284 | 3.0119 | -2.1227 |
| H | -0.80948 | 3.91545 | -2.39302 |
| H | -1.1872 | 2.26213 | -2.89793 |
| H | -2.43656 | 3.26557 | -2.12861 |
| Rh | -1.20317 | 0.22691 | -0.39456 |
| C | -1.7254 | -0.67559 | 1.49172 |
| C | -2.76278 | -1.11112 | 0.56549 |
| C | -2.10822 | -1.84432 | -0.44642 |
| C | -0.67895 | -2.01361 | -0.07585 |
| C | -0.46403 | -1.35735 | 1.14059 |
| C | 0.30211 | -2.8401 | -0.8482 |
| H | 0.17895 | -3.90376 | -0.60196 |
| H | 0.15294 | -2.74184 | -1.92784 |
| H | 1.33229 | -2.55775 | -0.61935 |
| C | 0.76218 | -1.38165 | 1.99528 |
| H | 0.63556 | -2.13062 | 2.78971 |
| H | 1.65578 | -1.63993 | 1.42523 |
| H | 0.94519 | -0.42066 | 2.48186 |
| C | -2.73091 | -2.45652 | -1.66051 |
| H | -2.09819 | -2.33256 | -2.54557 |
| H | -2.86136 | -3.53709 | -1.50976 |

| | | | |
|---|---|---|---|
| H | -3.7123 | -2.02852 | -1.87653 |
| C | -4.23234 | -0.83216 | 0.6907 |
| H | -4.72986 | -0.82746 | -0.28213 |
| H | -4.70965 | -1.6073 | 1.30436 |
| H | -4.42464 | 0.13125 | 1.16942 |
| C | -1.95662 | 0.08163 | 2.75874 |
| H | -2.79416 | 0.77801 | 2.67047 |
| H | -2.19654 | -0.62385 | 3.56747 |
| H | -1.06729 | 0.63776 | 3.06737 |
| H | -2.18816 | 1.49166 | -0.59073 |
| C | 2.9064 | 0.21752 | -0.76079 |
| H | 2.2999 | 0.23395 | -1.66241 |

**27**

Thermal correction to Gibbs free energy: 0.425228
SCF energy in solution: -967.594039724
Sum of electronic and thermal Energies: -966.422035
Solution-phase Gibbs free energy: -967.168811724
Coordinates:

| | | | |
|---|---|---|---|
| C | -2.93177 | -1.65306 | -0.33707 |
| C | -3.0657 | -1.56466 | 1.05685 |
| C | -1.96186 | -1.72427 | 1.8936 |
| C | -0.69644 | -2.00426 | 1.35864 |
| C | -0.53473 | -2.154 | -0.04152 |
| H | -4.04558 | -1.37831 | 1.48868 |
| H | -2.08572 | -1.66153 | 2.97104 |
| H | 0.13963 | -2.20786 | 2.02135 |
| C | -4.13277 | -1.53082 | -1.2423 |
| H | -3.84948 | -1.22322 | -2.25385 |
| H | -4.64789 | -2.49623 | -1.32986 |
| H | -4.86125 | -0.8129 | -0.85208 |
| C | 0.81511 | -2.55229 | -0.64293 |
| H | 1.29688 | -3.29613 | -0.0004 |
| H | 0.65601 | -3.02431 | -1.61803 |
| C | 1.63844 | -1.25657 | -0.76061 |
| H | 1.75507 | -0.96226 | -1.81087 |
| C | 3.01755 | -1.24626 | -0.08092 |
| C | 3.00452 | -1.573 | 1.42127 |
| H | 2.35701 | -0.88956 | 1.98282 |
| H | 2.6661 | -2.59785 | 1.61605 |
| H | 4.01514 | -1.49089 | 1.83597 |
| C | 3.97759 | -2.19858 | -0.82825 |
| H | 3.6421 | -3.24039 | -0.76003 |
| H | 4.05551 | -1.93874 | -1.88989 |

| | | | |
|---|---|---|---|
| H | 4.9828 | -2.14732 | -0.39458 |
| Rh | 0.17954 | 0.09287 | -0.06469 |
| C | 1.11542 | 2.00936 | -0.5689 |
| C | -0.16837 | 1.89538 | -1.21385 |
| C | -1.23136 | 2.0481 | -0.19353 |
| C | -0.61573 | 2.07317 | 1.04937 |
| C | 0.8527 | 1.96473 | 0.83921 |
| C | -1.257 | 2.19021 | 2.39689 |
| H | -1.10233 | 3.19734 | 2.8065 |
| H | -2.33373 | 2.01188 | 2.35235 |
| H | -0.8245 | 1.48334 | 3.11228 |
| C | 1.86223 | 2.09566 | 1.93545 |
| H | 1.97715 | 3.15496 | 2.20647 |
| H | 1.55245 | 1.56217 | 2.83851 |
| H | 2.84348 | 1.72189 | 1.63466 |
| C | -2.69331 | 2.14595 | -0.50329 |
| H | -3.30938 | 1.92408 | 0.37147 |
| H | -2.94589 | 3.16101 | -0.83778 |
| H | -2.98528 | 1.46123 | -1.30506 |
| C | -0.40868 | 1.91268 | -2.69015 |
| H | -1.30123 | 1.34253 | -2.96285 |
| H | -0.56776 | 2.94774 | -3.02539 |
| H | 0.44244 | 1.51233 | -3.24629 |
| C | 2.43419 | 2.22203 | -1.24852 |
| H | 2.52581 | 1.63168 | -2.16486 |
| H | 2.54148 | 3.27896 | -1.52597 |
| H | 3.27381 | 1.96852 | -0.59771 |
| H | 3.42334 | -0.23261 | -0.19382 |
| C | -1.65673 | -1.91682 | -0.86836 |
| H | -1.54518 | -2.03468 | -1.94406 |

**TS28**

Imaginary frequencies: -308.64

Thermal correction to Gibbs free energy: 0.422248

SCF energy in solution: -967.555393252

Sum of electronic and thermal Energies: -966.384995

Solution-phase Gibbs free energy: -967.133145252

Coordinates:

| | | | |
|---|---|---|---|
| C | 3.84514 | -0.50686 | 0.39158 |
| C | 4.09263 | -0.98799 | -0.90542 |
| C | 3.05354 | -1.45718 | -1.70669 |
| C | 1.73839 | -1.46176 | -1.22938 |
| C | 1.46621 | -0.92897 | 0.04102 |
| H | 5.11336 | -1.01752 | -1.27789 |

| | | | |
|---|---|---|---|
| H | 3.26647 | -1.85168 | -2.69648 |
| H | 0.94923 | -1.88927 | -1.8422 |
| C | 4.98334 | -0.04149 | 1.26909 |
| H | 4.62288 | 0.36519 | 2.21889 |
| H | 5.66533 | -0.86893 | 1.49899 |
| H | 5.57743 | 0.73433 | 0.77223 |
| C | 0.07866 | -1.98509 | 1.12106 |
| H | 0.47841 | -2.88013 | 0.65568 |
| H | 0.50894 | -1.77409 | 2.09506 |
| C | -1.30827 | -1.68 | 0.91654 |
| H | -1.81619 | -1.25093 | 1.78172 |
| C | -2.2337 | -2.54328 | 0.05973 |
| C | -1.66315 | -2.93906 | -1.3097 |
| H | -1.42237 | -2.05801 | -1.91981 |
| H | -0.75798 | -3.55138 | -1.21926 |
| H | -2.39622 | -3.53103 | -1.86736 |
| C | -2.65739 | -3.7931 | 0.86225 |
| H | -1.79751 | -4.44453 | 1.05883 |
| H | -3.10194 | -3.52114 | 1.82587 |
| H | -3.39857 | -4.37361 | 0.30197 |
| Rh | -0.44213 | 0.03338 | -0.02441 |
| C | -2.05071 | 1.53124 | 0.46421 |
| C | -0.79329 | 1.83405 | 1.14069 |
| C | 0.1738 | 2.31577 | 0.14467 |
| C | -0.39946 | 2.11248 | -1.1127 |
| C | -1.78039 | 1.59519 | -0.91963 |
| C | 0.20215 | 2.39624 | -2.45341 |
| H | -0.23277 | 3.31001 | -2.88028 |
| H | 1.28364 | 2.53495 | -2.3931 |
| H | 0.00521 | 1.58586 | -3.16293 |
| C | -2.74536 | 1.35315 | -2.03865 |
| H | -3.15454 | 2.30884 | -2.39453 |
| H | -2.26206 | 0.87257 | -2.89479 |
| H | -3.58597 | 0.72935 | -1.7251 |
| C | 1.51648 | 2.89199 | 0.46698 |
| H | 2.14262 | 2.97958 | -0.42349 |
| H | 1.40563 | 3.89512 | 0.89888 |
| H | 2.05765 | 2.27903 | 1.19417 |
| C | -0.6082 | 1.94016 | 2.62067 |
| H | 0.43126 | 1.76822 | 2.91296 |
| H | -0.87589 | 2.95454 | 2.95012 |
| H | -1.24643 | 1.24089 | 3.16686 |
| C | -3.36499 | 1.24964 | 1.12871 |
| H | -3.24112 | 0.7267 | 2.0814 |

| | | | |
|---|---|---|---|
| H | -3.88805 | 2.19111 | 1.34189 |
| H | -4.02046 | 0.64626 | 0.49527 |
| H | -3.13963 | -1.9476 | -0.1194 |
| C | 2.5221 | -0.48482 | 0.84956 |
| H | 2.32031 | -0.12662 | 1.85708 |

**29**

Thermal correction to Gibbs free energy: 0.421655
SCF energy in solution: -967.575225629
Sum of electronic and thermal Energies: -966.402517
Solution-phase Gibbs free energy: -967.153570629
Coordinates:

| | | | |
|---|---|---|---|
| C | -3.53237 | -1.10292 | 0.5752 |
| C | -3.99928 | -1.43237 | -0.70479 |
| C | -3.18549 | -1.26505 | -1.82372 |
| C | -1.88534 | -0.76318 | -1.68842 |
| C | -1.39671 | -0.4399 | -0.41931 |
| H | -5.00788 | -1.82009 | -0.82371 |
| H | -3.5621 | -1.5216 | -2.81067 |
| H | -1.27088 | -0.63122 | -2.57645 |
| C | -4.42118 | -1.26093 | 1.78729 |
| H | -3.86157 | -1.13401 | 2.71943 |
| H | -5.22947 | -0.51893 | 1.78288 |
| H | -4.89415 | -2.24918 | 1.80877 |
| C | 0.8594 | 2.26612 | -1.02558 |
| H | 1.3576 | 2.02825 | -1.96134 |
| H | 1.45984 | 2.78088 | -0.27971 |
| C | -0.51015 | 2.22841 | -0.94438 |
| H | -1.06136 | 1.88685 | -1.81715 |
| C | -1.35995 | 2.87368 | 0.13062 |
| C | -0.63517 | 3.1033 | 1.46286 |
| H | -0.23999 | 2.16466 | 1.87914 |
| H | 0.19962 | 3.80669 | 1.36255 |
| H | -1.32749 | 3.5212 | 2.20035 |
| C | -1.92712 | 4.19655 | -0.43631 |
| H | -1.12552 | 4.9162 | -0.63717 |
| H | -2.47944 | 4.03175 | -1.36757 |
| H | -2.61628 | 4.64524 | 0.28674 |
| Rh | 0.53176 | 0.18092 | -0.08375 |
| C | 1.96784 | -1.13925 | -0.99849 |
| C | 2.87715 | -0.2395 | -0.25906 |
| C | 2.5503 | -0.33754 | 1.09169 |
| C | 1.47094 | -1.34698 | 1.23752 |
| C | 1.21857 | -1.929 | -0.0329 |

| | | | |
|---|---|---|---|
| C | 0.91085 | -1.79756 | 2.5495 |
| H | 1.57903 | -2.54164 | 3.00504 |
| H | 0.81875 | -0.96862 | 3.25739 |
| H | -0.07106 | -2.26108 | 2.4298 |
| C | 0.39682 | -3.14531 | -0.32818 |
| H | 1.04345 | -4.03275 | -0.31155 |
| H | -0.3936 | -3.28834 | 0.41141 |
| H | -0.0767 | -3.08973 | -1.31054 |
| C | 3.1562 | 0.40149 | 2.24275 |
| H | 2.38841 | 0.80211 | 2.91309 |
| H | 3.78028 | -0.27591 | 2.84079 |
| H | 3.78655 | 1.2298 | 1.91217 |
| C | 3.95288 | 0.59091 | -0.88972 |
| H | 4.27944 | 1.40375 | -0.23653 |
| H | 4.8307 | -0.03305 | -1.10378 |
| H | 3.63268 | 1.02754 | -1.84031 |
| C | 2.0419 | -1.41043 | -2.46604 |
| H | 2.32093 | -0.51842 | -3.03329 |
| H | 2.80896 | -2.17461 | -2.65877 |
| H | 1.0937 | -1.78967 | -2.85499 |
| H | -2.21006 | 2.20464 | 0.31106 |
| C | -2.22021 | -0.61354 | 0.70149 |
| H | -1.86107 | -0.36437 | 1.69931 |