

Driving *tert*-Butyl Axial: The Surprising Cyclopropyl Effect

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Computational Data Methods

All DFT calculations were conducted using Gaussian 16, Revision B.01, primarily on the Digital Research Alliance of Canada Cluster.¹ Structure optimizations and frequency calculations were all performed at the M06-2X/6-311++G(2d,2p) level with the default integration grid and using acetone solvation (except where noted) using the SMD model.

All stationary points were confirmed to have zero negative eigenvalues. Thermal free energies were converted to 1 M standard state using the correction of Truhlar: (free energies prior to correction are listed below).²

Conformational analysis for appropriate side chains was conducted either by examining all possible staggered conformations or through use of rotational scans using modified redundant coordinates to identify likely stable structures, which were then minimized.

A-values were calculated using a Boltzmann population analysis of all identified stable conformations using GoodVibes³.

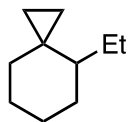
Shifts were calculated using the GIAO method at the B3LYP/6-311+G(2d,p) level with SCRF=acetone, referenced to TMS, as implemented in Gaussian and GaussView.⁴ Shifts were estimated using a Boltzmann distribution of all chair conformers.

NBO-STERIC calculations were performed as implemented in Gaussian. Energies were the total disjoint NLMO steric exchange energy from pairwise sum, as this best represents steric contacts.⁵

References:

1. Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016
2. Zhao, Y.; Truhlar, D.G. *Phys. Chem. Chem. Phys.* **2008**, *10*, 2813-2818
3. Luchini, G.; Alegre-Requena, J. V.; Funes-Ardoiz, I.; Paton, R. S. *F1000Research*, **2020**, *9*, 291
4. Wolinski, K.; Haacke, R.; Hinton, J. F.; Pulay, P. *J. Comp. Chem.* **1997**, *18*, 816-825)
5. https://nbo6.chem.wisc.edu/ex_ster.htm

Benchmarking



| Theory level | A-value |
|--------------------------|----------------|
| Experimental | -0.46 kcal/mol |
| M06-2X/6-311++G(2d,2p) | -0.89 kcal/mol |
| B3LYP-D3/6-311++G(2d,2p) | -0.85 kcal/mol |
| wB97XD/6-311++G(2d,2p) | -1.01 kcal/mol |
| MP2/6-311++G(2d,2p) | -1.07 kcal/mol |

NMR Calculation Summaries

Table 1: Predicted NMR for spirocyclobutyl-tert-butyl hexane

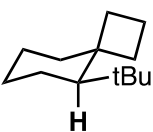
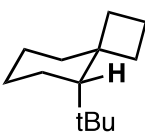
| | |
|---|--|
|  |  |
| Predicted: 1.25 ppm Observed: 1.32 ppm | 0.83 ppm 0.88 ppm |

Table 2: Predicted NMR for spirocyclobutanone-tert-butyl-hexane

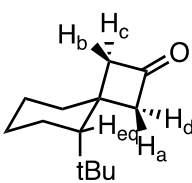
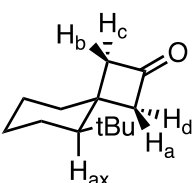
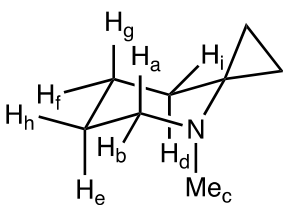
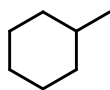
| | |
|---|--|
|  |  |
| Predicted Observed | Predicted Observed |
| H _{ax} 1.52 ppm 1.64 ppm | H _{eq} 1.34 ppm 1.36 ppm |
| H _a 3.39 ppm 3.38 ppm | H _a 3.63 ppm 3.46 ppm |
| H _b 2.72 ppm 2.75 ppm | H _b 3.19 ppm 3.04 ppm |
| H _c 2.92 ppm 2.85 ppm | H _c 2.63 ppm 2.65 ppm |
| H _d 2.46 ppm 2.52 ppm | H _d 2.43 ppm 2.51 ppm |

Table 3: Predicted NMR for spirocyclopropyl N-methyl piperidine

| | | | |
|---|--------------------|-------------------------|------|
|  | | | |
| Observed | Predicted Axial | Predicted Equatorial | |
| a | 2.79 | 3.04 | 2.22 |
| b | 2.65 | 2.77 | 2.60 |
| c | 2.29 | 2.45 | 1.95 |
| d | 2.07 | 2.20 | 1.90 |
| e | 1.73 | 1.85 | 1.60 |
| f | 1.67 | 1.70 | 1.60 |
| g | 1.48 | 1.60 | 1.41 |
| h | 1.11 | 1.02 | 1.60 |
| i | 0.53 | 0.48 | 0.81 |

Energy Summary and co-ordinates for DFT calculations

Cyclohexane Compounds



methylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -275.140397 | -274.933337 | -274.971701 |
| eq | -275.143008 | -274.93627 | -274.974815 |

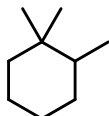
ax

| ===== | | | |
|-------|-----------|-----------|-----------|
| C | 0.334823 | -0.597813 | 1.257164 |
| C | -0.323549 | -1.184490 | -0.000000 |
| H | -0.142246 | -2.262501 | -0.000000 |
| C | 0.334823 | -0.597813 | -1.257164 |
| C | 0.334823 | 0.932564 | -1.260544 |
| H | 0.848624 | 1.299288 | -2.151042 |
| H | -0.691833 | 1.304950 | -1.315608 |
| C | 0.334823 | 0.932564 | 1.260544 |
| C | 1.003024 | 1.482481 | 0.000000 |
| H | 0.975260 | 2.573688 | 0.000000 |
| H | 2.058219 | 1.189551 | 0.000000 |
| H | 1.372008 | -0.944375 | -1.303737 |
| H | -0.691833 | 1.304950 | 1.315608 |
| H | 0.848624 | 1.299288 | 2.151042 |
| H | -0.168379 | -0.978756 | -2.149014 |
| H | -0.168379 | -0.978756 | 2.149014 |
| H | 1.372008 | -0.944375 | 1.303737 |
| C | -1.838934 | -0.978870 | -0.000000 |
| H | -2.290274 | -1.435894 | -0.882655 |
| H | -2.290274 | -1.435894 | 0.882655 |
| H | -2.110511 | 0.077093 | -0.000000 |

eq

| ===== | | | |
|-------|-----------|-----------|-----------|
| C | -0.089893 | 0.325574 | 1.254644 |
| C | 0.576846 | 0.895270 | -0.000000 |
| H | 1.623198 | 0.567789 | -0.000000 |
| C | -0.089893 | 0.325574 | -1.254644 |
| C | -0.089893 | -1.202997 | -1.259474 |
| H | -0.594959 | -1.577603 | -2.151659 |
| H | 0.943687 | -1.560853 | -1.304770 |
| C | -0.089893 | -1.202997 | 1.259474 |
| C | -0.755091 | -1.757609 | 0.000000 |
| H | -0.717680 | -2.848459 | 0.000000 |
| H | -1.812524 | -1.473944 | 0.000000 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.124372 | 0.686542 | -1.292131 |
| H | 0.943687 | -1.560853 | 1.304770 |
| H | -0.594959 | -1.577603 | 2.151659 |
| H | 0.412072 | 0.709011 | -2.146233 |
| H | 0.412072 | 0.709011 | 2.146233 |
| H | -1.124372 | 0.686542 | 1.292131 |
| C | 0.544740 | 2.418903 | -0.000000 |
| H | 1.040081 | 2.826148 | 0.883311 |
| H | 1.040081 | 2.826148 | -0.883311 |
| H | -0.487553 | 2.777811 | -0.000000 |



1,1,2-trimethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -353.754171 | -353.488235 | -353.531685 |
| eq | -353.756151 | -353.490499 | -353.534483 |

ax

```

=====
C  0.883008   -0.275843   0.056083
C  0.114592    0.983327   0.543919
H  0.642340    1.351753   1.429993
C -1.321345    0.630322   0.967562
C -2.097589   -0.082442  -0.140618
H -3.100880   -0.331511   0.209690
H -2.220090    0.586899  -0.996970
C  0.067038   -1.014731  -1.021378
C -1.362076   -1.344550  -0.589321
H -1.894734   -1.821515  -1.414159
H -1.347130   -2.065048   0.232914
H -1.299984   -0.012993   1.850110
H  0.025260   -0.393499  -1.921120
H  0.600615   -1.928033  -1.299102
H -1.839609    1.545472   1.262336
C  0.105384    2.122882  -0.480744
H -0.538933    2.932500  -0.133072
H  1.101861    2.537267  -0.629315
H -0.267605    1.799971  -1.453620
C  1.149476   -1.208038   1.245441
H  1.678017   -2.103934   0.912285
H  1.775739   -0.706112   1.986550
H  0.236653   -1.528928   1.744645
C  2.240813    0.110922  -0.535638
H  2.817841    0.714830   0.169381
H  2.820906   -0.786492  -0.761822
H  2.133920    0.678288  -1.460562

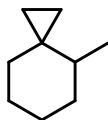
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NBO Steric Energy: 273.58

eq

| | | | |
|---|-----------|-----------|-----------|
| C | 0.623325 | -0.589989 | -0.020794 |
| C | 0.391580 | 0.894131 | -0.410204 |
| H | 0.304609 | 0.906109 | -1.503793 |
| C | -0.926709 | 1.441461 | 0.151168 |
| C | -2.131241 | 0.593131 | -0.247691 |
| H | -3.042658 | 0.995732 | 0.198120 |
| H | -2.258892 | 0.640383 | -1.334021 |
| C | -0.624089 | -1.403491 | -0.416540 |
| C | -1.927757 | -0.862331 | 0.165342 |
| H | -2.765533 | -1.474597 | -0.173601 |
| H | -1.908204 | -0.932111 | 1.256404 |
| H | -0.862372 | 1.491990 | 1.242711 |
| H | -0.702861 | -1.398381 | -1.509440 |
| H | -0.475242 | -2.444056 | -0.115796 |
| H | -1.057546 | 2.468424 | -0.198346 |
| C | 1.541360 | 1.822095 | -0.021206 |
| H | 2.501030 | 1.483503 | -0.411426 |
| H | 1.361144 | 2.824729 | -0.412809 |
| H | 1.627852 | 1.906072 | 1.063822 |
| C | 0.903572 | -0.751584 | 1.478226 |
| H | 0.967351 | -1.812439 | 1.730988 |
| H | 1.853874 | -0.290820 | 1.751195 |
| H | 0.126895 | -0.308642 | 2.101421 |
| C | 1.814237 | -1.161428 | -0.795805 |
| H | 2.754860 | -0.695368 | -0.501116 |
| H | 1.905470 | -2.233856 | -0.608170 |
| H | 1.684554 | -1.018644 | -1.871122 |

NBO Steric Energy: 270.86



4-methylspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -352.525015 | -352.282452 | -352.324709 |
| eq | -352.524767 | -352.28219 | -352.324561 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.835669 | -0.138166 | -0.053987 |
| C | -0.018318 | 1.074267 | 0.368904 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.593301 | 1.611386 | 1.128592 |
| C | -1.778128 | -0.723412 | 0.958418 |
| C | -2.311346 | 0.031195 | -0.238258 |
| C | 1.297815 | 0.603220 | 1.006227 |
| C | 2.070652 | -0.363613 | 0.105111 |
| H | 2.397010 | 0.152727 | -0.801804 |
| H | 2.974563 | -0.698909 | 0.616560 |
| C | -0.093304 | -1.111809 | -0.947682 |
| C | 1.207768 | -1.565345 | -0.282871 |
| H | 0.965611 | -2.138214 | 0.617886 |
| H | 1.760327 | -2.231142 | -0.948013 |
| C | 0.219645 | 2.035892 | -0.796222 |
| H | 0.794583 | 1.571974 | -1.598000 |
| H | -0.728755 | 2.371431 | -1.219156 |
| H | -1.848530 | -0.240991 | 1.923869 |
| H | -1.905523 | -1.797359 | 0.970914 |
| H | -2.796009 | -0.541722 | -1.017042 |
| H | -2.731255 | 1.012469 | -0.061727 |
| H | 1.067371 | 0.093497 | 1.946743 |
| H | -0.734469 | -1.968586 | -1.164589 |
| H | 0.136447 | -0.634666 | -1.905443 |
| H | 1.917623 | 1.467902 | 1.253911 |
| H | 0.769622 | 2.916826 | -0.460541 |

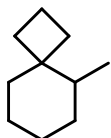
NBO Steric Energy: 240.47

eq

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.566591 | -0.531872 | -0.179370 |
| C | -0.311420 | 0.952436 | -0.431199 |
| H | -0.100645 | 1.054546 | -1.502963 |
| C | -1.355557 | -0.969825 | 1.022558 |
| C | -1.924852 | -1.137247 | -0.367585 |
| C | 0.950951 | 1.382188 | 0.327874 |
| C | 2.163426 | 0.523358 | -0.027296 |
| H | 2.409509 | 0.672812 | -1.083457 |
| H | 3.033092 | 0.842236 | 0.549977 |
| C | 0.626479 | -1.395722 | -0.545240 |
| C | 1.878500 | -0.958166 | 0.213588 |
| H | 1.724353 | -1.126299 | 1.284024 |
| H | 2.734299 | -1.565166 | -0.086858 |
| C | -1.474205 | 1.878886 | -0.093124 |
| H | -1.704257 | 1.856468 | 0.973490 |
| H | -1.210052 | 2.906290 | -0.347667 |
| H | -1.805951 | -0.218611 | 1.655135 |
| H | -1.021857 | -1.858920 | 1.540153 |
| H | -1.967285 | -2.138480 | -0.774277 |
| H | -2.750596 | -0.499110 | -0.645684 |
| H | 0.751424 | 1.304548 | 1.402634 |
| H | 0.397409 | -2.442990 | -0.337701 |
| H | 0.811060 | -1.312592 | -1.621923 |
| H | 1.159068 | 2.433880 | 0.118179 |
| H | -2.379958 | 1.627171 | -0.644305 |

NBO Steric Energy: 239.83



5-methylspiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -391.829805 | -391.556992 | -391.601179 |
| ax2 | -391.828400 | -391.555538 | -391.59993 |
| eq | -391.829132 | -391.556438 | -391.601004 |
| eq2 | -391.830131 | -391.557484 | -391.601397 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.457291 | 1.052677 | 0.486369 |
| H | 0.008698 | 1.614489 | 1.302204 |
| C | -1.648423 | 0.275623 | 1.063876 |
| C | -2.260691 | -0.687966 | 0.045464 |
| H | -3.077397 | -1.245469 | 0.507480 |
| H | -2.695327 | -0.125882 | -0.785353 |
| C | -0.001619 | -0.894244 | -1.062509 |
| C | -1.201748 | -1.651243 | -0.490710 |
| H | -1.630269 | -2.303899 | -1.253401 |
| H | -0.865609 | -2.297694 | 0.325441 |
| H | -1.305651 | -0.302583 | 1.928151 |
| H | -0.312651 | -0.336861 | -1.951353 |
| H | 0.767668 | -1.598779 | -1.389588 |
| H | -2.403422 | 0.975468 | 1.429475 |
| C | 0.598886 | 0.078578 | -0.044120 |
| C | 1.921698 | 0.706736 | -0.551778 |
| C | 1.433810 | -0.673458 | 1.032247 |
| C | 2.705747 | -0.390308 | 0.202107 |
| H | 2.085253 | 1.689935 | -0.107612 |
| H | 2.055348 | 0.775920 | -1.631820 |
| H | 1.440065 | -0.128094 | 1.977073 |
| H | 1.182557 | -1.715992 | 1.224909 |
| H | 3.596675 | -0.081380 | 0.744647 |
| H | 2.961713 | -1.226555 | -0.445924 |
| C | -0.890813 | 2.067332 | -0.572745 |
| H | -1.589542 | 2.789256 | -0.145958 |
| H | -0.032034 | 2.621670 | -0.955636 |
| H | -1.383405 | 1.594094 | -1.421952 |

ax2

```
=====
C  0.295582    -0.976967    -1.128475
H -0.291073    -1.807728    -1.527968
C  1.522808    -1.504678    -0.384450
C  2.326874    -0.358801     0.229146
H  3.168903    -0.751808     0.801754
H  2.750821     0.253996    -0.570839
C  0.195639     1.030144     0.406927
C  1.441488     0.499082     1.135331
H  2.011772     1.339180     1.538076
H  1.129422    -0.108175     1.989183
H  1.191396    -2.175926     0.415012
H -0.452467     1.505209     1.150949
H  2.148827    -2.095668    -1.055196
C -0.591357    -0.141756    -0.211667
C -1.971094     0.281512    -0.785063
C -1.358646    -0.947950     0.878169
C -2.635069    -0.147645     0.541053
H -2.264897    -0.368782    -1.610045
H -2.093871     1.318579    -1.092687
H -1.454435    -1.997592     0.596845
H -0.986818    -0.887867     1.900358
H -3.567879    -0.703543     0.474122
H -2.776512     0.694739     1.215976
C  0.578654     2.101566    -0.616956
H  1.101566     2.922166    -0.122328
H  1.239164     1.711377    -1.391192
H -0.298171     2.520116    -1.110672
H  0.614979    -0.375315    -1.985426
```

eq

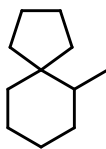
```
=====
C -0.404810     1.091508    -0.405399
H -0.664911     1.120882    -1.471568
C -1.704281     0.899591     0.386236
C -2.444652    -0.374351    -0.011461
H -3.351369    -0.489080     0.585331
H -2.757740    -0.294980    -1.057394
C -0.235547    -1.402581    -0.620587
C -1.539250    -1.592404     0.151254
H -2.046973    -2.496833    -0.188778
H -1.317809    -1.734455     1.213206
H -1.456634     0.857214     1.453679
H -0.457760    -1.344988    -1.692019
H  0.417214    -2.268008    -0.479383
H -2.346455     1.772365     0.247413
C  0.512967    -0.126268    -0.218155
C  1.913958    -0.103131    -0.884750
C  1.223348    -0.306680     1.154967
C  2.508079    -0.720707     0.401823
H  2.284083     0.906820    -1.050123
H  2.013978    -0.673764    -1.808625
H  1.355651     0.639241     1.678268
```

| | | | |
|---|-----------|-----------|-----------|
| H | 0.790318 | -1.032514 | 1.842656 |
| H | 3.446286 | -0.303272 | 0.761062 |
| H | 2.610427 | -1.801716 | 0.329561 |
| C | 0.228000 | 2.432605 | -0.041573 |
| H | 1.156408 | 2.618678 | -0.580695 |
| H | -0.460512 | 3.243835 | -0.284203 |
| H | 0.438917 | 2.495085 | 1.027478 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.643346 | -1.431547 | -0.584166 |
| H | 0.879038 | -1.349399 | -1.651657 |
| C | 1.920009 | -1.246027 | 0.232165 |
| C | 2.489568 | 0.154969 | 0.024003 |
| H | 3.378206 | 0.303341 | 0.640235 |
| H | 2.802172 | 0.262715 | -1.019562 |
| C | 0.146495 | 1.023414 | -0.454770 |
| C | 1.440024 | 1.215967 | 0.345406 |
| H | 1.837903 | 2.214861 | 0.152110 |
| H | 1.200374 | 1.175286 | 1.413986 |
| H | 1.690985 | -1.387274 | 1.293738 |
| H | 0.400382 | 1.086453 | -1.520753 |
| H | 2.656775 | -2.004710 | -0.037476 |
| C | -0.417857 | -0.392280 | -0.233693 |
| C | -1.797628 | -0.632814 | -0.902106 |
| C | -1.098742 | -0.596719 | 1.152355 |
| C | -2.484399 | -0.486158 | 0.475304 |
| H | -1.875256 | -1.647667 | -1.292997 |
| H | -2.093625 | 0.067007 | -1.683450 |
| H | -0.908858 | -1.596379 | 1.544245 |
| H | -0.871766 | 0.130975 | 1.930769 |
| H | -3.215174 | -1.248731 | 0.736820 |
| H | -2.936618 | 0.493829 | 0.613882 |
| C | -0.832653 | 2.153316 | -0.141151 |
| H | -1.747792 | 2.084477 | -0.729339 |
| H | -1.106516 | 2.156591 | 0.915936 |
| H | -0.369765 | 3.116582 | -0.362027 |
| H | 0.230557 | -2.430683 | -0.424535 |



6-methylspiro[4.5]decane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -431.162735 | -430.858789 | -430.905236 |
| ax2 | -431.162461 | -430.858567 | -430.904992 |
| ax3 | -431.161759 | -430.857667 | -430.903946 |
| eq | -431.163849 | -430.860143 | -430.906292 |
| eq2 | -431.162133 | -430.858193 | -430.905006 |
| eq3 | -431.163732 | -430.859972 | -430.906078 |
| eq4 | -431.161465 | -430.857521 | -430.904334 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.862788 | 0.977122 | 0.600827 |
| H | -0.514182 | 1.493254 | 1.501400 |
| C | -1.981633 | 0.009521 | 1.015455 |
| C | -2.425970 | -0.889745 | -0.139236 |
| H | -3.201657 | -1.577637 | 0.202032 |
| H | -2.871660 | -0.281971 | -0.931516 |
| C | -0.098892 | -0.730917 | -1.105649 |
| C | -1.239714 | -1.669190 | -0.705645 |
| H | -1.551162 | -2.258225 | -1.570371 |
| H | -0.887778 | -2.380831 | 0.046080 |
| H | -1.626747 | -0.620987 | 1.835707 |
| H | -0.423885 | -0.120532 | -1.953223 |
| H | 0.755761 | -1.313983 | -1.457038 |
| H | -2.830671 | 0.579817 | 1.399317 |
| C | -1.387225 | 2.050699 | -0.357299 |
| H | -2.269066 | 2.535301 | 0.066478 |
| H | -0.638302 | 2.823050 | -0.533392 |
| H | -1.672211 | 1.638985 | -1.325825 |
| C | 0.346550 | 0.203621 | 0.035908 |
| C | 1.470057 | 1.134220 | -0.451840 |
| C | 1.087480 | -0.590980 | 1.131090 |
| C | 2.743665 | 0.269988 | -0.468685 |
| H | 1.582036 | 1.951356 | 0.266948 |
| H | 1.252667 | 1.579492 | -1.423380 |
| C | 2.490831 | -0.860876 | 0.560823 |
| H | 0.576330 | -1.506243 | 1.426061 |
| H | 1.162402 | 0.040545 | 2.020499 |
| H | 2.908614 | -0.148937 | -1.461079 |
| H | 3.626996 | 0.857421 | -0.222528 |
| H | 2.524260 | -1.834506 | 0.072106 |
| H | 3.244085 | -0.876149 | 1.347232 |

ax2

```
=====
C -1.507703 -1.585483 -0.663825
C -0.324517 -0.771864 -1.189178
C -0.690546 0.976836 0.598655
H -0.192419 1.427048 1.464576
C -2.536554 -0.677505 0.008193
C -1.878942 0.149848 1.113686
H -2.610667 0.816939 1.575132
H -1.535180 -0.531180 1.896940
H -2.980175 -0.015792 -0.740602
H -3.351831 -1.271595 0.425020
H -1.967390 -2.143345 -1.481765
H -1.156395 -2.323913 0.062931
C 0.355627 0.071844 -0.094245
C 1.074427 -0.858385 0.937258
C 1.512461 0.896516 -0.709995
C 2.567438 -0.493901 0.892403
H 0.946453 -1.903635 0.650934
H 0.663361 -0.752373 1.941105
C 2.761725 0.036377 -0.527055
H 1.644309 1.822459 -0.142640
H 1.315634 1.171861 -1.747028
H 2.780359 0.307349 1.604179
H 3.213598 -1.335891 1.139246
H 3.688946 0.593549 -0.659584
H 2.762414 -0.792338 -1.239580
H 0.419324 -1.433022 -1.641757
H -0.679685 -0.109643 -1.983931
C -1.174745 2.123033 -0.294166
H -1.918398 2.722490 0.234428
H -0.356538 2.785771 -0.575428
H -1.637754 1.761373 -1.212566
```

ax3

```
=====
C -0.744658 -0.923489 1.190507
H -0.294128 -1.794846 1.672934
C -1.992128 -1.334233 0.409759
C -2.600682 -0.127095 -0.300418
H -3.474698 -0.425412 -0.882186
H -2.948285 0.593405 0.445868
C -0.291824 0.951952 -0.462525
C -1.565204 0.526465 -1.214432
H -1.993045 1.401244 -1.709118
H -1.306036 -0.182132 -2.004858
H -1.726026 -2.092347 -0.333593
H 0.437375 1.261706 -1.217033
H -2.720461 -1.790929 1.082402
C 0.318511 -0.246223 0.318302
C 1.537818 0.170272 1.157645
C 0.991541 -1.223011 -0.669971
C 2.650505 0.417901 0.133684
```

| | | | |
|---|-----------|-----------|-----------|
| H | 1.808474 | -0.676345 | 1.795499 |
| H | 1.348156 | 1.020767 | 1.811185 |
| C | 2.361919 | -0.592281 | -1.006204 |
| H | 0.396099 | -1.415774 | -1.560914 |
| H | 1.136610 | -2.181002 | -0.164386 |
| H | 2.594630 | 1.440685 | -0.241549 |
| H | 3.642708 | 0.287699 | 0.563244 |
| H | 2.334442 | -0.087108 | -1.971179 |
| H | 3.135903 | -1.355801 | -1.071468 |
| C | -0.567328 | 2.172473 | 0.421321 |
| H | -1.115723 | 2.928934 | -0.143051 |
| H | -1.163194 | 1.919342 | 1.299364 |
| H | 0.357359 | 2.632086 | 0.769715 |
| H | -1.040984 | -0.240560 | 1.993117 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.875905 | 0.967191 | 0.498203 |
| C | 0.599683 | 1.099248 | -0.337125 |
| H | 0.909684 | 1.195375 | -1.385291 |
| C | 0.629245 | -1.374393 | -0.719295 |
| H | 0.048554 | -2.297826 | -0.637178 |
| H | 0.860519 | -1.241912 | -1.782196 |
| C | 2.735079 | -0.204294 | 0.028765 |
| C | 1.937149 | -1.505775 | 0.060300 |
| H | 2.529974 | -2.325545 | -0.350095 |
| H | 1.722767 | -1.765745 | 1.100372 |
| H | 3.069302 | -0.010185 | -0.995444 |
| H | 3.631511 | -0.293408 | 0.645167 |
| H | 2.443512 | 1.899198 | 0.442778 |
| H | 1.603828 | 0.826829 | 1.550551 |
| C | -0.157099 | 2.373986 | 0.030232 |
| H | 0.475058 | 3.245099 | -0.151175 |
| H | -1.065401 | 2.497098 | -0.560410 |
| H | -0.436012 | 2.390227 | 1.085118 |
| C | -0.250002 | -0.193505 | -0.267482 |
| C | -0.839842 | -0.461919 | 1.148455 |
| C | -1.499403 | -0.094820 | -1.189623 |
| C | -2.307405 | -0.844207 | 0.922349 |
| H | -0.795549 | 0.439101 | 1.761901 |
| H | -0.289592 | -1.235421 | 1.683105 |
| C | -2.710154 | 0.033908 | -0.261254 |
| H | -1.594053 | -1.019071 | -1.765018 |
| H | -1.416741 | 0.722933 | -1.906576 |
| H | -2.380967 | -1.896307 | 0.634597 |
| H | -2.925718 | -0.697230 | 1.807749 |
| H | -3.643194 | -0.272910 | -0.733690 |
| H | -2.826425 | 1.067197 | 0.074595 |

eq2

```
=====
```

| | | | |
|---|-----------|----------|-----------|
| C | -0.911758 | 1.050052 | -0.354252 |
| H | -1.158386 | 1.071849 | -1.423449 |
| C | -2.139542 | 0.501065 | 0.385509 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.527880 | -0.900610 | -0.074932 |
| H | -3.387153 | -1.262373 | 0.492831 |
| H | -2.832257 | -0.860965 | -1.125791 |
| C | -0.126077 | -1.312071 | -0.669441 |
| C | -1.347680 | -1.857078 | 0.067131 |
| H | -1.605311 | -2.842643 | -0.325399 |
| H | -1.116474 | -1.992694 | 1.127321 |
| H | -1.923807 | 0.483981 | 1.459498 |
| H | -0.358887 | -1.263092 | -1.738767 |
| H | 0.712307 | -2.003933 | -0.564811 |
| H | -2.976537 | 1.189430 | 0.246170 |
| C | -0.661230 | 2.490187 | 0.094062 |
| H | 0.215891 | 2.935801 | -0.373451 |
| H | -1.521113 | 3.109333 | -0.167355 |
| H | -0.535681 | 2.552280 | 1.176294 |
| C | 0.299979 | 0.099775 | -0.214505 |
| C | 1.517298 | 0.530846 | -1.052872 |
| C | 0.919055 | 0.053940 | 1.195974 |
| C | 2.710074 | -0.248144 | -0.465897 |
| H | 1.689804 | 1.600456 | -0.932132 |
| H | 1.367469 | 0.339030 | -2.116871 |
| C | 2.312472 | -0.570993 | 0.998328 |
| H | 0.314724 | -0.494450 | 1.917855 |
| H | 1.029030 | 1.073201 | 1.570047 |
| H | 2.884639 | -1.167091 | -1.024555 |
| H | 3.628782 | 0.334031 | -0.518977 |
| H | 2.273686 | -1.649147 | 1.152527 |
| H | 3.031014 | -0.174826 | 1.714381 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.881962 | -1.511115 | 0.315147 |
| C | -0.609378 | -1.465538 | -0.524719 |
| H | -0.892447 | -1.468367 | -1.582769 |
| C | -0.607831 | 1.046505 | -0.488988 |
| H | -0.857272 | 1.051741 | -1.557704 |
| C | -2.731679 | -0.274895 | 0.034794 |
| C | -1.927532 | 0.995738 | 0.293299 |
| H | -2.521661 | 1.877437 | 0.041456 |
| H | -1.705971 | 1.067175 | 1.363561 |
| H | -3.053468 | -0.293929 | -1.011384 |
| H | -3.635443 | -0.279325 | 0.646967 |
| H | -2.444054 | -2.420934 | 0.096686 |
| H | -1.625553 | -1.542626 | 1.378781 |
| C | 0.253240 | -0.220599 | -0.253527 |
| C | 0.856116 | -0.270215 | 1.182395 |
| C | 1.493797 | -0.254984 | -1.192197 |
| C | 2.350897 | 0.025247 | 1.021635 |
| H | 0.736425 | -1.277127 | 1.589765 |
| H | 0.363592 | 0.412215 | 1.874480 |
| C | 2.683010 | -0.648123 | -0.309335 |
| H | 1.675629 | 0.729336 | -1.624956 |
| H | 1.341268 | -0.945435 | -2.022542 |
| H | 2.516605 | 1.102074 | 0.937605 |

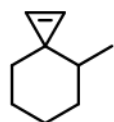
| | | | |
|---|-----------|-----------|-----------|
| H | 2.948048 | -0.341660 | 1.856469 |
| H | 3.642529 | -0.342818 | -0.726235 |
| H | 2.708251 | -1.732135 | -0.171062 |
| H | -0.000699 | -2.358488 | -0.356821 |
| C | 0.112359 | 2.355262 | -0.163485 |
| H | 1.043441 | 2.476815 | -0.715891 |
| H | -0.528764 | 3.203956 | -0.408559 |
| H | 0.343319 | 2.418405 | 0.902041 |

eq4

```

=====
C  0.885978   -1.447456   -0.537338
H  1.148006   -1.392720   -1.600143
C  2.153119   -1.258979    0.292393
C  2.752592    0.121842    0.042105
H  3.636937    0.276926    0.662917
H  3.078864    0.184649   -1.001008
C  0.424061    1.007667   -0.485118
C  1.718872    1.211616    0.311010
H  2.132225    2.193221    0.066366
H  1.484198    1.232474    1.380172
H  1.913120   -1.363863    1.355157
H  0.692993    1.026904   -1.548462
H  2.877765   -2.039309    0.052467
C -0.195022   -0.394002   -0.243968
C -1.419258   -0.635397   -1.158694
C -0.782590   -0.570473    1.174923
C -2.698198   -0.326687   -0.349679
H -1.425387   -1.683529   -1.463573
H -1.351142   -0.041256   -2.071783
C -2.250650   -0.119553    1.114530
H -0.219011   -0.034652    1.939181
H -0.739368   -1.631986    1.433292
H -3.208021    0.558765   -0.727763
H -3.404480   -1.152510   -0.427478
H -2.342096    0.928728    1.391986
H -2.868111   -0.685356    1.811566
H  0.462984   -2.440437   -0.366159
C -0.522819    2.178144   -0.227914
H -1.473837    2.067247   -0.750260
H -0.728321    2.288254    0.838287
H -0.063815    3.108124   -0.568270

```



4-methylspiro[2.5]oct-1-ene

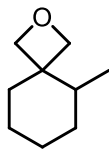
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -351.254596 | -351.037496 | -351.079864 |
| eq | -351.256967 | -351.040048 | -351.082201 |

ax

```
=====
C -0.891776 -0.169449 -0.037705
C -0.079749 1.057162 0.384117
H -0.655149 1.579746 1.152024
C -1.951226 -0.708202 0.886711
C -2.386029 -0.072772 -0.150239
C 1.255137 0.618249 1.006594
C 2.042145 -0.333262 0.103666
H 2.343987 0.183752 -0.811460
H 2.960183 -0.642956 0.606153
C -0.112727 -1.132209 -0.926228
C 1.200254 -1.554829 -0.262838
H 0.974053 -2.120155 0.647141
H 1.760323 -2.220236 -0.922313
C 0.122769 2.027416 -0.781843
H 0.690232 1.575648 -1.595826
H -0.838932 2.349039 -1.186235
H -2.157897 -1.254269 1.791637
H -3.217191 0.290273 -0.730862
H 1.047386 0.106471 1.951476
H -0.731907 -2.003755 -1.143200
H 0.112357 -0.652021 -1.884333
H 1.855898 1.498849 1.246384
H 0.663869 2.916985 -0.454000
```

eq

```
=====
C -0.585312 -0.583981 -0.181831
C -0.362639 0.910786 -0.435337
H -0.144511 1.026377 -1.504495
C -1.478683 -1.041017 0.941012
C -1.954524 -1.195228 -0.249653
C 0.875744 1.380251 0.339223
C 2.117064 0.557851 -0.003168
H 2.369958 0.715290 -1.056582
H 2.971030 0.901628 0.583388
C 0.643546 -1.409327 -0.541229
C 1.873314 -0.931574 0.233658
H 1.709791 -1.104053 1.302282
H 2.752216 -1.511798 -0.053326
C -1.573236 1.767771 -0.096676
H -1.816857 1.693757 0.965974
H -1.373192 2.815728 -0.324041
H -1.600476 -1.155784 2.004751
H -2.755402 -1.530098 -0.887075
H 0.666097 1.292515 1.411556
H 0.448219 -2.463842 -0.340700
H 0.841732 -1.312138 -1.614816
H 1.056006 2.438666 0.136443
H -2.456245 1.460557 -0.659354
```



5-methyl-2-oxaspiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -427.736566 | -427.487337 | -427.531803 |
| eq | -427.737042 | -427.487872 | -427.532074 |

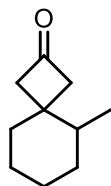
ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.380042 | 1.056762 | 0.474856 |
| H | 0.137267 | 1.592185 | 1.276712 |
| C | -1.593477 | 0.339249 | 1.082057 |
| C | -2.273981 | -0.599430 | 0.083576 |
| H | -3.102395 | -1.116820 | 0.570198 |
| H | -2.704150 | -0.022087 | -0.738850 |
| C | -0.062696 | -0.914538 | -1.089840 |
| C | -1.275740 | -1.613594 | -0.475012 |
| H | -1.754999 | -2.255162 | -1.215969 |
| H | -0.939038 | -2.264568 | 0.338142 |
| H | -1.258340 | -0.250820 | 1.941618 |
| H | -0.370970 | -0.345686 | -1.971706 |
| H | 0.672488 | -1.649297 | -1.428032 |
| H | -2.304985 | 1.076358 | 1.460366 |
| C | 0.599516 | 0.025359 | -0.085247 |
| C | 1.962018 | 0.560332 | -0.553088 |
| C | 1.444873 | -0.736315 | 0.954983 |
| H | 2.163061 | 1.592782 | -0.254851 |
| H | 2.207827 | 0.425494 | -1.607831 |
| H | 1.400666 | -0.316457 | 1.963531 |
| H | 1.317378 | -1.818835 | 0.999667 |
| O | 2.672795 | -0.370337 | 0.290574 |
| C | -0.784506 | 2.088275 | -0.578999 |
| H | -1.414614 | 2.859561 | -0.133179 |
| H | 0.094097 | 2.579038 | -1.002609 |
| H | -1.341444 | 1.640415 | -1.401513 |

eq

| | | | |
|---|-----------|----------|-----------|
| C | -0.133031 | 1.034055 | -0.458981 |
| H | -0.380317 | 1.101828 | -1.525421 |
| C | -1.429250 | 1.219329 | 0.338046 |
| C | -2.473733 | 0.155447 | 0.009610 |
| H | -3.366291 | 0.302142 | 0.620167 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.779529 | 0.261344 | -1.035977 |
| C | -0.623855 | -1.434770 | -0.586518 |
| C | -1.903847 | -1.244584 | 0.224443 |
| H | -2.638148 | -2.005050 | -0.045304 |
| H | -1.677708 | -1.381303 | 1.287423 |
| H | -1.190314 | 1.172923 | 1.406978 |
| H | -0.855141 | -1.360789 | -1.654497 |
| H | -0.206239 | -2.429509 | -0.416026 |
| H | -1.828870 | 2.218074 | 0.149512 |
| C | 0.420559 | -0.383114 | -0.236252 |
| C | 1.823542 | -0.621396 | -0.816842 |
| C | 1.135848 | -0.579429 | 1.115614 |
| H | 2.214629 | 0.119185 | -1.514917 |
| H | 1.956282 | -1.622897 | -1.234432 |
| H | 1.013570 | 0.192750 | 1.875372 |
| H | 0.961254 | -1.561715 | 1.562997 |
| O | 2.433366 | -0.518100 | 0.486715 |
| C | 0.853376 | 2.152612 | -0.129422 |
| H | 1.785367 | 2.064096 | -0.686822 |
| H | 0.410286 | 3.118814 | -0.375374 |
| H | 1.096589 | 2.166009 | 0.934412 |



5-methylspiro[3.5]nonan-2-one

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -465.858517 | -465.604807 | -465.651331 |
| eq | -465.859121 | -465.605416 | -465.651585 |
| eq2 | -465.858138 | -465.6044 | -465.651052 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.810458 | 1.024636 | 0.513141 |
| H | -0.366033 | 1.597630 | 1.332975 |
| C | -1.913259 | 0.130106 | 1.096368 |
| C | -2.467761 | -0.855829 | 0.065713 |
| H | -3.219089 | -1.494379 | 0.533161 |
| H | -2.973292 | -0.312389 | -0.736621 |
| C | -0.235254 | -0.839342 | -1.110503 |
| C | -1.347378 | -1.710756 | -0.526759 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.741017 | -2.376943 | -1.296033 |
| H | -0.931680 | -2.347009 | 0.260478 |
| H | -1.499805 | -0.438106 | 1.935673 |
| H | -0.614194 | -0.289168 | -1.976260 |
| H | 0.587321 | -1.463359 | -1.472084 |
| H | -2.715329 | 0.752856 | 1.498187 |
| C | -1.362306 | 2.027979 | -0.500408 |
| C | 0.301314 | 0.154863 | -0.079643 |
| C | 1.549881 | 0.921295 | -0.609225 |
| C | 1.208322 | -0.564487 | 0.972528 |
| H | 1.632251 | 1.922372 | -0.178693 |
| H | 1.718706 | 0.963961 | -1.684597 |
| H | 1.167053 | -0.086898 | 1.954117 |
| H | 1.128461 | -1.644883 | 1.083041 |
| C | 2.397762 | -0.055524 | 0.181502 |
| O | 3.552139 | -0.382266 | 0.124731 |
| H | -1.830407 | 1.537754 | -1.353766 |
| H | -0.570863 | 2.674717 | -0.882765 |
| H | -2.114377 | 2.664319 | -0.030943 |

eq

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=====
```

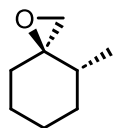
| | | | |
|---|-----------|-----------|-----------|
| C | -0.452920 | 1.029841 | 0.484537 |
| H | -0.778137 | 1.096297 | 1.529758 |
| C | -1.688643 | 1.205983 | -0.404360 |
| C | -2.745075 | 0.132099 | -0.155493 |
| H | -3.128463 | 0.234135 | 0.864586 |
| H | -3.591145 | 0.272394 | -0.830318 |
| C | -0.932252 | -1.441895 | 0.575635 |
| C | -2.149206 | -1.263155 | -0.327991 |
| H | -1.845287 | -1.399215 | -1.371192 |
| H | -2.895044 | -2.029419 | -0.111030 |
| H | -2.109918 | 2.200061 | -0.239418 |
| H | -1.243263 | -1.369830 | 1.623368 |
| H | -0.493243 | -2.432918 | 0.437887 |
| H | -1.373234 | 1.167938 | -1.453216 |
| C | 0.545257 | 2.158393 | 0.228567 |
| C | 0.131962 | -0.383363 | 0.309172 |
| C | 0.910417 | -0.566655 | -1.035766 |
| C | 1.463950 | -0.599865 | 1.089358 |
| H | 0.758259 | 0.143728 | -1.846305 |
| H | 0.819054 | -1.585642 | -1.418601 |
| H | 1.724510 | 0.082295 | 1.896727 |
| H | 1.562175 | -1.632456 | 1.432106 |
| C | 2.188855 | -0.420320 | -0.231403 |
| O | 3.322856 | -0.154150 | -0.523685 |
| H | 1.427041 | 2.090822 | 0.866418 |
| H | 0.877849 | 2.167615 | -0.811334 |
| H | 0.071935 | 3.121010 | 0.426495 |

eq2

```
=====
```

| | | | |
|---|-----------|----------|----------|
| C | -0.866978 | 1.063412 | 0.375723 |
| H | -1.187739 | 1.087315 | 1.424363 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.071977 | 0.642664 | -0.473811 |
| C | -2.619387 | -0.725147 | -0.075116 |
| H | -3.460697 | -0.996989 | -0.714806 |
| H | -2.999072 | -0.675252 | 0.950186 |
| C | -0.318233 | -1.376321 | 0.685906 |
| C | -1.524148 | -1.785414 | -0.154799 |
| H | -1.217291 | -1.906694 | -1.198082 |
| H | -1.899916 | -2.753694 | 0.179577 |
| H | -2.851533 | 1.403388 | -0.394089 |
| H | -0.607546 | -1.337808 | 1.741208 |
| H | 0.476851 | -2.123388 | 0.602643 |
| H | -1.761723 | 0.617009 | -1.525147 |
| C | -0.425253 | 2.471459 | -0.014839 |
| C | 0.233440 | -0.003273 | 0.290497 |
| C | 1.039184 | -0.097141 | -1.047222 |
| C | 1.563345 | 0.269674 | 1.057271 |
| H | 1.034963 | 0.830496 | -1.621988 |
| H | 0.848270 | -0.939891 | -1.710010 |
| H | 1.752196 | 1.326355 | 1.249589 |
| H | 1.752824 | -0.308641 | 1.961006 |
| C | 2.291560 | -0.177545 | -0.195719 |
| O | 3.411508 | -0.554783 | -0.409613 |
| H | 0.442990 | 2.813444 | 0.547890 |
| H | -0.187724 | 2.532493 | -1.078369 |
| H | -1.236240 | 3.175903 | 0.175591 |



(3*R*,4*R*)-4-methyl-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -388.435635 | -388.216919 | -388.258903 |
| eq | -388.436734 | -388.218062 | -388.260007 |

ax

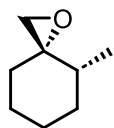
| | | | |
|---|-----------|-----------|-----------|
| C | 0.845360 | -0.130831 | 0.078842 |
| C | 0.047473 | 1.086167 | -0.345070 |
| H | 0.642444 | 1.609686 | -1.096772 |
| C | 2.307155 | -0.069605 | 0.095799 |
| C | -1.269525 | 0.628841 | -0.990884 |
| C | -2.048671 | -0.346163 | -0.104795 |
| H | -2.953332 | -0.668168 | -0.622669 |
| H | -2.371849 | 0.155210 | 0.811389 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.107882 | -1.125302 | 0.942349 |
| C | -1.190444 | -1.558856 | 0.257332 |
| H | -1.743523 | -2.241126 | 0.903964 |
| H | -0.943043 | -2.109043 | -0.655174 |
| H | 2.862368 | -0.728108 | 0.753990 |
| H | 2.803330 | 0.853459 | -0.183110 |
| H | -1.880099 | 1.502153 | -1.228993 |
| H | 0.757054 | -1.980208 | 1.134369 |
| H | -0.121101 | -0.660731 | 1.904988 |
| H | -1.038696 | 0.130557 | -1.936764 |
| O | 1.618067 | -0.727432 | -0.972207 |
| C | -0.176242 | 2.034162 | 0.833122 |
| H | 0.775801 | 2.339190 | 1.270798 |
| H | -0.698982 | 2.931914 | 0.500652 |
| H | -0.772842 | 1.574187 | 1.620829 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.535359 | -0.550062 | -0.134488 |
| C | -0.344762 | 0.930075 | -0.413642 |
| H | -0.159590 | 1.013070 | -1.491225 |
| C | -1.465961 | -1.024018 | 0.897006 |
| C | 0.915255 | 1.411415 | 0.318217 |
| C | 2.146865 | 0.578542 | -0.031637 |
| H | 3.012747 | 0.937178 | 0.526973 |
| H | 2.376323 | 0.703235 | -1.094258 |
| C | 0.663118 | -1.399912 | -0.481829 |
| C | 1.905052 | -0.901912 | 0.258530 |
| H | 2.773163 | -1.496924 | -0.027226 |
| H | 1.759370 | -1.039311 | 1.334310 |
| H | -2.066760 | -0.320792 | 1.459693 |
| H | -1.270137 | -1.973627 | 1.381873 |
| H | 1.084953 | 2.463973 | 0.082843 |
| H | 0.448928 | -2.442015 | -0.242495 |
| H | 0.832065 | -1.334431 | -1.561310 |
| H | 0.731380 | 1.351110 | 1.396562 |
| O | -1.795334 | -1.115760 | -0.493432 |
| C | -1.551081 | 1.790984 | -0.062027 |
| H | -1.411476 | 2.800888 | -0.448616 |
| H | -2.468623 | 1.387088 | -0.489603 |
| H | -1.678429 | 1.865967 | 1.019150 |



(3S,4R)-4-methyl-1-oxaspiro[2.5]octane

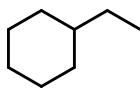
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -388.435686 | -388.216933 | -388.258913 |
| eq | -388.436085 | -388.217377 | -388.259288 |

ax

```
=====
C -0.823980 -0.168551 -0.014924
C -0.043182 1.069388 0.377255
H -0.628148 1.600025 1.131782
C -1.872172 -0.672009 0.878509
C 1.289622 0.631004 1.004661
C 2.068782 -0.336768 0.110499
H 2.981505 -0.649887 0.619561
H 2.378271 0.168947 -0.807694
C -0.093092 -1.138918 -0.909704
C 1.221869 -1.558783 -0.247223
H 1.775045 -2.228090 -0.906963
H 0.995996 -2.118861 0.665452
H -2.087830 -0.142707 1.799420
H -2.126117 -1.725659 0.861950
H 1.892198 1.513498 1.228370
H -0.731435 -2.001242 -1.104342
H 0.114934 -0.659055 -1.869927
H 1.080647 0.134268 1.956898
O -2.202576 0.044909 -0.317057
C 0.149737 2.006809 -0.814704
H -0.813094 2.275735 -1.251023
H 0.644554 2.924954 -0.495177
H 0.758583 1.555773 -1.598060
```

eq

```
=====
C -0.532661 -0.571451 -0.226479
C -0.390817 0.924683 -0.457897
H -0.170911 1.051908 -1.523189
C -1.834308 -1.243161 -0.177973
C 0.825893 1.423777 0.334193
C 2.097198 0.651392 -0.015503
H 2.935410 1.020288 0.577762
H 2.346056 0.828911 -1.066535
C 0.703304 -1.368252 -0.573985
C 1.909181 -0.847971 0.209807
H 2.807293 -1.395684 -0.078587
H 1.746085 -1.034359 1.275037
H -1.886732 -2.297256 -0.426184
H -2.748909 -0.680617 -0.315585
H 0.964349 2.489833 0.144660
H 0.522857 -2.422483 -0.360867
H 0.891577 -1.271193 -1.646960
H 0.612500 1.313367 1.402778
O -1.122244 -0.945272 1.026250
C -1.640984 1.723579 -0.113074
H -1.432807 2.791267 -0.190002
H -2.468145 1.497946 -0.785619
H -1.961515 1.514672 0.908756
```



ethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -314.445801 | -314.208652 | -314.250415 |
| ax2 | -314.439479 | -314.202189 | -314.244192 |
| eq | -314.448190 | -314.211445 | -314.253542 |
| eq2 | -314.446992 | -314.210038 | -314.252134 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.646962 | -1.368529 | 0.566911 |
| C | 0.558822 | -0.425782 | 0.696843 |
| H | 1.110887 | -0.705322 | 1.599849 |
| C | 0.061066 | 1.015490 | 0.879555 |
| C | -0.874733 | 1.452270 | -0.248819 |
| H | -1.221790 | 2.471538 | -0.069792 |
| H | -0.331355 | 1.467770 | -1.198269 |
| C | -1.607910 | -0.945141 | -0.547512 |
| C | -2.067488 | 0.501465 | -0.361518 |
| H | -2.717948 | 0.801122 | -1.185289 |
| H | -2.661274 | 0.570989 | 0.555925 |
| H | -0.487078 | 1.072093 | 1.825289 |
| H | -1.117647 | -1.044963 | -1.519414 |
| H | -2.470380 | -1.614106 | -0.563484 |
| H | 0.903348 | 1.703474 | 0.966587 |
| H | -0.300334 | -2.390887 | 0.397696 |
| H | -1.194169 | -1.370451 | 1.514760 |
| C | 1.527613 | -0.590697 | -0.481991 |
| H | 1.828497 | -1.641071 | -0.522076 |
| H | 1.017731 | -0.384317 | -1.425029 |
| C | 2.774053 | 0.284227 | -0.385696 |
| H | 3.495109 | 0.022375 | -1.160805 |
| H | 2.535123 | 1.341391 | -0.505044 |
| H | 3.264524 | 0.160545 | 0.582465 |

ax2

| | | | |
|---|-----------|-----------|-----------|
| C | -0.156435 | -1.101003 | 0.990228 |
| C | 0.609923 | 0.234903 | 0.978007 |
| H | 0.886766 | 0.438164 | 2.016319 |
| C | -0.305588 | 1.400327 | 0.556509 |
| C | -1.203931 | 1.124252 | -0.651671 |
| H | -1.877205 | 1.971192 | -0.798983 |
| H | -0.610098 | 1.033984 | -1.563312 |
| C | -1.060924 | -1.339590 | -0.223570 |
| C | -2.003599 | -0.160225 | -0.449613 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.648279 | -0.348623 | -1.309928 |
| H | -2.656475 | -0.044951 | 0.422196 |
| H | -0.962107 | 1.631269 | 1.401666 |
| H | -0.465530 | -1.488018 | -1.126009 |
| H | -1.632102 | -2.257253 | -0.068893 |
| H | 0.301617 | 2.292251 | 0.383149 |
| H | 0.552678 | -1.925733 | 1.101537 |
| H | -0.793800 | -1.117460 | 1.879872 |
| C | 1.958394 | 0.179538 | 0.238989 |
| H | 2.409703 | 1.173893 | 0.299535 |
| H | 2.613919 | -0.485489 | 0.808543 |
| C | 1.977172 | -0.282195 | -1.216924 |
| H | 2.994884 | -0.228936 | -1.607206 |
| H | 1.647318 | -1.316362 | -1.313653 |
| H | 1.348640 | 0.336039 | -1.856565 |

eq

```
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```

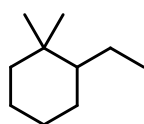
| | | | |
|---|-----------|-----------|-----------|
| C | 0.434073 | -1.355645 | -0.160408 |
| C | -0.559070 | -0.259921 | 0.237771 |
| H | -0.585793 | -0.212583 | 1.334309 |
| C | -0.074230 | 1.098854 | -0.276504 |
| C | 1.349775 | 1.412349 | 0.185155 |
| H | 1.672752 | 2.372363 | -0.221843 |
| H | 1.357101 | 1.511149 | 1.275494 |
| C | 1.856489 | -1.047791 | 0.305832 |
| C | 2.324200 | 0.308001 | -0.220617 |
| H | 3.327436 | 0.533053 | 0.145912 |
| H | 2.384199 | 0.266487 | -1.313026 |
| H | -0.105423 | 1.086447 | -1.372727 |
| H | 1.880387 | -1.034185 | 1.400243 |
| H | 2.537863 | -1.837123 | -0.017040 |
| H | -0.749102 | 1.891070 | 0.051438 |
| H | 0.102041 | -2.315580 | 0.242422 |
| H | 0.427331 | -1.450436 | -1.252565 |
| C | -1.965889 | -0.603271 | -0.255265 |
| H | -2.221438 | -1.605142 | 0.100319 |
| H | -1.950124 | -0.657921 | -1.348590 |
| C | -3.047205 | 0.376283 | 0.191891 |
| H | -2.910431 | 1.361709 | -0.253444 |
| H | -4.037580 | 0.021613 | -0.095503 |
| H | -3.038080 | 0.495922 | 1.277471 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.076278 | -1.253594 | 0.008033 |
| C | 0.527117 | 0.000302 | -0.631931 |
| H | 0.223346 | 0.000615 | -1.685863 |
| C | -0.076503 | 1.253765 | 0.008584 |
| C | -1.601370 | 1.260672 | -0.108870 |
| H | -2.013421 | 2.150846 | 0.370048 |
| H | -1.879323 | 1.309814 | -1.166508 |
| C | -1.601116 | -1.260871 | -0.109054 |
| C | -2.205856 | -0.000221 | 0.508951 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.290372 | -0.000337 | 0.385270 |
| H | -2.007127 | -0.000255 | 1.585610 |
| H | 0.195066 | 1.286338 | 1.068323 |
| H | -1.879272 | -1.310003 | -1.166632 |
| H | -2.012841 | -2.151210 | 0.369867 |
| H | 0.345587 | 2.148294 | -0.456878 |
| H | 0.345948 | -2.147838 | -0.457888 |
| H | 0.195566 | -1.286514 | 1.067668 |
| C | 2.060034 | 0.000423 | -0.613262 |
| H | 2.412305 | 0.876554 | -1.164605 |
| H | 2.412370 | -0.875001 | -1.165674 |
| C | 2.697644 | -0.000387 | 0.774907 |
| H | 2.413197 | -0.882916 | 1.348785 |
| H | 3.785197 | 0.000535 | 0.693809 |
| H | 2.411740 | 0.880541 | 1.350525 |



2-ethyl-1,1-dimethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -393.058742 | -392.762757 | -392.809406 |
| ax2 | -393.057008 | -392.761111 | -392.807669 |
| ax3 | -393.053268 | -392.757125 | -392.803615 |
| eq | -393.060516 | -392.764946 | -392.813089 |
| eq2 | -393.056926 | -392.761135 | -392.80823 |
| eq3 | -393.057216 | -392.761267 | -392.807979 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.941063 | -0.656381 | 0.053423 |
| C | 0.510888 | -0.417651 | 0.559488 |
| H | 0.648036 | -1.048680 | 1.445815 |
| C | 0.698268 | 1.044987 | 0.995037 |
| C | 0.374759 | 2.024158 | -0.133012 |
| H | 0.519784 | 3.050568 | 0.208783 |
| H | 1.064977 | 1.868336 | -0.968047 |
| C | -1.302298 | 0.373269 | -1.035237 |
| C | -1.061239 | 1.824573 | -0.617531 |
| H | -1.275865 | 2.487801 | -1.457617 |
| H | -1.750629 | 2.101720 | 0.184548 |
| H | 0.045266 | 1.258829 | 1.843681 |
| H | -0.708731 | 0.164418 | -1.929965 |
| H | -2.349130 | 0.229992 | -1.317598 |
| H | 1.716310 | 1.198376 | 1.353536 |
| C | 1.576144 | -0.858285 | -0.461336 |
| H | 1.501263 | -1.938209 | -0.591704 |
| H | 1.370070 | -0.418619 | -1.439970 |
| C | -1.924322 | -0.544410 | 1.226844 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.944378 | -0.723310 | 0.879974 |
| H | -1.693457 | -1.293674 | 1.987645 |
| H | -1.906493 | 0.432803 | 1.706033 |
| C | -1.097718 | -2.062537 | -0.533068 |
| H | -0.763927 | -2.823283 | 0.177310 |
| H | -2.148031 | -2.255823 | -0.761865 |
| H | -0.530624 | -2.186737 | -1.455642 |
| C | 3.009710 | -0.523702 | -0.055821 |
| H | 3.720461 | -1.018567 | -0.718622 |
| H | 3.209193 | 0.546987 | -0.102696 |
| H | 3.217127 | -0.857059 | 0.963680 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.130671 | 0.967725 | 0.058974 |
| C | -0.527895 | -0.336744 | 0.592889 |
| H | -1.090254 | -0.060574 | 1.491814 |
| C | 0.546058 | -1.356867 | 1.007486 |
| C | 1.491707 | -1.684173 | -0.148143 |
| H | 2.237614 | -2.414136 | 0.171220 |
| H | 0.926474 | -2.144998 | -0.964420 |
| C | 1.136522 | 0.634768 | -1.059653 |
| C | 2.172752 | -0.416828 | -0.662379 |
| H | 2.807586 | -0.647997 | -1.519823 |
| H | 2.830053 | -0.019879 | 0.115754 |
| H | 1.130476 | -0.971430 | 1.845866 |
| H | 0.586602 | 0.270801 | -1.932994 |
| H | 1.633211 | 1.558517 | -1.369188 |
| H | 0.053397 | -2.264864 | 1.361852 |
| C | -1.529970 | -0.982972 | -0.391180 |
| H | -1.288819 | -0.710959 | -1.420438 |
| H | -1.424252 | -2.069178 | -0.340161 |
| C | 0.846804 | 1.693332 | 1.206480 |
| H | 1.286479 | 2.625508 | 0.844778 |
| H | 0.137185 | 1.943438 | 1.998399 |
| H | 1.645836 | 1.102299 | 1.650340 |
| C | -0.918378 | 1.932895 | -0.498559 |
| H | -1.649785 | 2.202935 | 0.266438 |
| H | -0.433756 | 2.851784 | -0.836529 |
| H | -1.453920 | 1.509011 | -1.348815 |
| C | -2.988327 | -0.635604 | -0.098841 |
| H | -3.658514 | -1.115716 | -0.813657 |
| H | -3.268363 | -0.976116 | 0.899952 |
| H | -3.166913 | 0.438355 | -0.142830 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.727153 | 0.769431 | -0.003545 |
| C | -0.439592 | 0.277748 | 0.906671 |
| H | -0.277431 | 0.778658 | 1.867538 |
| C | -0.344748 | -1.235460 | 1.196247 |
| C | -0.070138 | -2.120354 | -0.023288 |
| H | 0.072027 | -3.151321 | 0.307325 |
| H | -0.926624 | -2.123185 | -0.699107 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.974280 | -0.174030 | -1.196527 |
| C | 1.155551 | -1.633909 | -0.790189 |
| H | 1.314904 | -2.248426 | -1.678171 |
| H | 2.047352 | -1.743640 | -0.167410 |
| H | 0.462402 | -1.405098 | 1.913758 |
| H | 0.134529 | -0.108933 | -1.892306 |
| H | 1.855813 | 0.182117 | -1.737196 |
| H | -1.264665 | -1.556702 | 1.691592 |
| C | -1.861471 | 0.720258 | 0.508375 |
| H | -2.515997 | 0.440796 | 1.338803 |
| H | -1.885160 | 1.810673 | 0.470272 |
| C | 2.003338 | 0.841599 | 0.850347 |
| H | 2.865693 | 1.093967 | 0.229059 |
| H | 1.902329 | 1.613952 | 1.615591 |
| H | 2.220171 | -0.098794 | 1.356352 |
| C | 0.459106 | 2.175878 | -0.543185 |
| H | 0.245819 | 2.876279 | 0.267639 |
| H | 1.338581 | 2.541695 | -1.078187 |
| H | -0.383251 | 2.191518 | -1.236350 |
| C | -2.478345 | 0.175665 | -0.778797 |
| H | -3.467451 | 0.613699 | -0.924298 |
| H | -1.882695 | 0.417063 | -1.658426 |
| H | -2.607151 | -0.905275 | -0.743134 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.458382 | 0.927852 | -0.034134 |
| C | 0.630739 | -0.158345 | -0.254182 |
| H | 0.721848 | -0.276214 | -1.342437 |
| C | 0.207154 | -1.520137 | 0.315464 |
| C | -1.142993 | -1.991814 | -0.218116 |
| H | -1.063048 | -2.161948 | -1.296716 |
| H | -1.414353 | -2.946815 | 0.235726 |
| C | -1.808134 | 0.396643 | -0.554551 |
| C | -2.222488 | -0.945754 | 0.041015 |
| H | -2.382267 | -0.845576 | 1.118146 |
| H | -3.173825 | -1.263420 | -0.389935 |
| H | 0.971317 | -2.262858 | 0.082310 |
| H | -1.734296 | 0.284929 | -1.642138 |
| H | -2.576821 | 1.151182 | -0.366923 |
| H | 0.161973 | -1.453510 | 1.407325 |
| C | 2.010975 | 0.243163 | 0.283770 |
| H | 2.222110 | 1.281347 | 0.023847 |
| H | 1.997341 | 0.194473 | 1.376141 |
| C | -0.129815 | 2.189276 | -0.839794 |
| H | -0.961092 | 2.895844 | -0.782227 |
| H | 0.758057 | 2.699768 | -0.467142 |
| H | 0.031931 | 1.947757 | -1.892853 |
| C | -0.580511 | 1.318116 | 1.443845 |
| H | 0.328411 | 1.808672 | 1.795100 |
| H | -1.406733 | 2.020563 | 1.575910 |
| H | -0.767940 | 0.460400 | 2.089821 |
| C | 3.150636 | -0.625520 | -0.245253 |
| H | 4.114762 | -0.258609 | 0.108853 |

| | | | |
|---|----------|-----------|-----------|
| H | 3.058565 | -1.662886 | 0.075782 |
| H | 3.170974 | -0.613978 | -1.336982 |

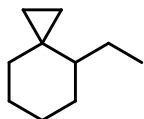
eq2

```
=====
C  0.035954    0.831093    0.014034
C  0.378521   -0.648196   -0.327719
H  0.415917   -0.707724   -1.423323
C -0.718707   -1.618650    0.146423
C -2.119197   -1.253563   -0.330097
H -2.161681   -1.318166   -1.422167
H -2.846928   -1.966844    0.061448
C -1.412139    1.133248   -0.430847
C -2.464270    0.166915    0.099362
H -2.508644    0.217671    1.191026
H -3.449942    0.454546   -0.271234
H -0.458637   -2.624029   -0.192065
H -1.442258    1.106157   -1.526096
H -1.651846    2.158475   -0.136798
H -0.713781   -1.651998    1.240972
C  1.711743   -1.189565    0.216356
H  1.666738   -1.205584    1.308953
H  1.760304   -2.237441   -0.090615
C  0.920709    1.816708   -0.762336
H  0.516266    2.826935   -0.660671
H  1.945509    1.840919   -0.402265
H  0.936783    1.571607   -1.826641
C  0.195516    1.109627    1.512246
H  1.240152    1.022650    1.816340
H -0.131448    2.126769    1.740231
H -0.390010    0.426098    2.128029
C  3.008839   -0.513027   -0.224591
H  3.856398   -1.170424   -0.024939
H  3.002564   -0.295685   -1.294399
H  3.192733    0.418531    0.307221
```

eq3

```
=====
C -0.237932    0.952542   -0.009904
C  0.478326   -0.257845   -0.671659
H  0.179463   -0.210502   -1.725937
C -0.034060   -1.601442   -0.136608
C -1.546266   -1.746163   -0.279667
H -1.812878   -1.741958   -1.341486
H -1.875048   -2.703474    0.129117
C -1.761309    0.743863   -0.132444
C -2.257351   -0.590223    0.417888
H -2.070361   -0.644931    1.494122
H -3.337721   -0.666948    0.281489
H  0.476460   -2.410693   -0.665806
H -2.028928    0.800525   -1.193446
H -2.268574    1.574668    0.365286
H  0.231144   -1.706804    0.918799
C  2.021287   -0.205648   -0.656565
```

| | | | |
|---|-----------|-----------|-----------|
| H | 2.378530 | -0.741649 | -1.539602 |
| H | 2.355439 | 0.825347 | -0.780721 |
| C | 0.098835 | 2.246667 | -0.758386 |
| H | -0.510040 | 3.068780 | -0.374786 |
| H | 1.143984 | 2.532780 | -0.640273 |
| H | -0.109000 | 2.145532 | -1.826089 |
| C | 0.148690 | 1.140310 | 1.461676 |
| H | 1.190233 | 1.450918 | 1.553101 |
| H | -0.468242 | 1.923763 | 1.908530 |
| H | 0.014382 | 0.233537 | 2.051563 |
| C | 2.719383 | -0.815598 | 0.561781 |
| H | 3.796010 | -0.653540 | 0.491705 |
| H | 2.381007 | -0.382070 | 1.501559 |
| H | 2.556522 | -1.892060 | 0.616200 |



4-ethylspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -391.829859 | -391.557356 | -391.602652 |
| ax2 | -391.830378 | -391.557812 | -391.603561 |
| ax3 | -391.824208 | -391.551416 | -391.596931 |
| ax5 | -391.824035 | -391.551211 | -391.597004 |
| eq1 | -391.829076 | -391.556406 | -391.602667 |
| eq2 | -391.827452 | -391.55481 | -391.600043 |
| eq3 | -391.825088 | -391.552264 | -391.597405 |
| eq4 | -391.824816 | -391.552032 | -391.598133 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.152943 | 0.828426 | 0.008318 |
| C | 0.405981 | -0.493124 | 0.720667 |
| H | 0.993478 | -0.278058 | 1.619605 |
| C | -0.009678 | 2.051135 | 0.868903 |
| C | 1.215697 | 1.883999 | 0.004297 |
| C | -0.948203 | -1.080458 | 1.151655 |
| C | -1.926360 | -1.214778 | -0.020436 |
| H | -1.557015 | -1.959783 | -0.729714 |
| H | -2.886748 | -1.582874 | 0.344975 |
| C | -0.778604 | 0.714225 | -1.181763 |
| C | -2.119580 | 0.118940 | -0.745281 |
| H | -2.612536 | 0.824538 | -0.069214 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.776421 | -0.010974 | -1.607170 |
| C | 1.203809 | -1.503708 | -0.115930 |
| H | 1.312257 | -2.413608 | 0.480554 |
| H | 0.634229 | -1.788780 | -1.002453 |
| H | 0.113930 | 1.937863 | 1.937555 |
| H | -0.743355 | 2.786210 | 0.567127 |
| H | 1.303506 | 2.510041 | -0.873538 |
| H | 2.148759 | 1.663519 | 0.503404 |
| H | -1.392320 | -0.421218 | 1.903317 |
| H | -0.925250 | 1.699527 | -1.628995 |
| H | -0.326368 | 0.078357 | -1.949579 |
| H | -0.795996 | -2.052071 | 1.627246 |
| C | 2.584710 | -1.020455 | -0.548173 |
| H | 3.170706 | -0.684688 | 0.309869 |
| H | 3.138129 | -1.823682 | -1.036337 |
| H | 2.516731 | -0.189529 | -1.250195 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.894804 | -0.570870 | -0.058654 |
| C | -0.533859 | -0.456919 | 0.455973 |
| H | -0.667704 | -1.210692 | 1.239275 |
| C | 1.937672 | -1.068890 | 0.900565 |
| C | 1.475605 | -1.937751 | -0.246765 |
| C | -0.722645 | 0.930493 | 1.088117 |
| C | -0.356799 | 2.058820 | 0.121171 |
| H | -1.037629 | 2.050773 | -0.735082 |
| H | -0.484902 | 3.024003 | 0.614180 |
| C | 1.307219 | 0.535469 | -1.010474 |
| C | 1.083118 | 1.908692 | -0.373758 |
| H | 1.763798 | 2.021609 | 0.476003 |
| H | 1.325907 | 2.698826 | -1.086344 |
| C | -1.553412 | -0.768847 | -0.647990 |
| H | -1.430406 | -0.076127 | -1.482866 |
| H | -1.326917 | -1.763656 | -1.039903 |
| H | 1.619287 | -1.346287 | 1.896305 |
| H | 2.929181 | -0.641442 | 0.837533 |
| H | 2.162090 | -2.090664 | -1.068377 |
| H | 0.850154 | -2.787377 | -0.007384 |
| H | -0.071022 | 0.998325 | 1.964668 |
| H | 2.356200 | 0.406647 | -1.285103 |
| H | 0.725771 | 0.465548 | -1.934689 |
| H | -1.745296 | 1.051233 | 1.448009 |
| C | -3.003563 | -0.733323 | -0.174339 |
| H | -3.322059 | 0.278733 | 0.076692 |
| H | -3.675233 | -1.105003 | -0.948858 |
| H | -3.140060 | -1.355690 | 0.712866 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.961556 | -0.282434 | -0.084762 |
| C | -0.245318 | -0.616941 | 0.789000 |
| H | 0.158889 | -1.136966 | 1.662355 |
| C | 2.300967 | -0.252675 | 0.602985 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.954577 | -1.371286 | -0.350525 |
| C | -0.898310 | 0.678477 | 1.305969 |
| C | -1.091425 | 1.767018 | 0.243042 |
| H | -1.851422 | 1.467865 | -0.479874 |
| H | -1.457929 | 2.674737 | 0.726520 |
| C | 0.753302 | 0.782452 | -1.144324 |
| C | 0.207516 | 2.059005 | -0.506427 |
| H | 0.951363 | 2.454227 | 0.192761 |
| H | 0.041656 | 2.824125 | -1.266719 |
| C | -1.235638 | -1.622998 | 0.171456 |
| H | -0.654326 | -2.449855 | -0.244569 |
| H | -1.816479 | -2.046703 | 0.995383 |
| H | 2.337185 | -0.488892 | 1.657534 |
| H | 3.020701 | 0.483699 | 0.272155 |
| H | 2.450223 | -1.384314 | -1.311670 |
| H | 1.759304 | -2.345822 | 0.076398 |
| H | -0.254095 | 1.090925 | 2.088506 |
| H | 1.702961 | 0.978479 | -1.646806 |
| H | 0.056136 | 0.431568 | -1.909124 |
| H | -1.854206 | 0.441678 | 1.780335 |
| C | -2.226309 | -1.131114 | -0.882427 |
| H | -1.734590 | -0.684377 | -1.745349 |
| H | -2.823210 | -1.970481 | -1.242963 |
| H | -2.917674 | -0.396921 | -0.468789 |

ax5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.933848 | -0.130291 | -0.030652 |
| C | -0.216292 | -0.539893 | 0.886471 |
| H | 0.241574 | -0.908994 | 1.808876 |
| C | 2.273793 | 0.095603 | 0.618553 |
| C | 2.039793 | -1.117294 | -0.250228 |
| C | -1.042052 | 0.697836 | 1.288101 |
| C | -1.390453 | 1.646781 | 0.138464 |
| H | -2.092083 | 1.174097 | -0.551600 |
| H | -1.893179 | 2.528121 | 0.541527 |
| C | 0.587772 | 0.823568 | -1.161230 |
| C | -0.135070 | 2.058764 | -0.627476 |
| H | 0.533512 | 2.608051 | 0.043203 |
| H | -0.391261 | 2.730424 | -1.448540 |
| C | -1.048281 | -1.731230 | 0.374396 |
| H | -0.421906 | -2.623721 | 0.450106 |
| H | -1.871875 | -1.881070 | 1.077863 |
| H | 2.355967 | -0.062393 | 1.684962 |
| H | 2.899022 | 0.883405 | 0.221069 |
| H | 2.515040 | -1.138970 | -1.221506 |
| H | 1.965255 | -2.076049 | 0.244693 |
| H | -0.454542 | 1.267182 | 2.015511 |
| H | 1.506461 | 1.108451 | -1.678615 |
| H | -0.052121 | 0.332032 | -1.896767 |
| H | -1.949617 | 0.375269 | 1.803372 |
| C | -1.607830 | -1.681105 | -1.045770 |
| H | -0.808348 | -1.662906 | -1.786449 |
| H | -2.206187 | -2.573553 | -1.236295 |

H -2.247090 -0.815809 -1.215184

eq1

```
=====
C -0.513354 0.831126 -0.178788
C 0.636309 -0.169001 -0.310760
H 0.707013 -0.424706 -1.376702
C -0.574185 1.766940 0.996270
C -0.318442 2.302752 -0.393562
C 0.269281 -1.452911 0.448037
C -1.068802 -2.038611 -0.001482
H -0.987751 -2.350214 -1.047853
H -1.299027 -2.933614 0.579311
C -1.842752 0.258980 -0.638251
C -2.193528 -1.014655 0.127194
H -2.340083 -0.769121 1.183659
H -3.133737 -1.430234 -0.239574
C 2.005310 0.362561 0.123188
H 2.000400 0.547809 1.200405
H 0.253065 1.784519 1.691028
H -1.543659 1.952330 1.438596
H -1.123505 2.836568 -0.879912
H 0.668699 2.684726 -0.605518
H 0.223691 -1.218799 1.517976
H -2.625029 1.010612 -0.513905
H -1.782191 0.030294 -1.708032
H 1.053888 -2.199063 0.318354
H 2.194849 1.321382 -0.360956
C 3.158980 -0.579113 -0.217352
H 4.117365 -0.108686 0.004404
H 3.111879 -1.507528 0.350741
H 3.151230 -0.834683 -1.278988
```

eq2

```
=====
C -0.088027 0.797000 -0.124250
C 0.456839 -0.630963 -0.123603
H 0.484283 -0.954082 -1.172453
C 0.047068 1.653049 1.103951
C 0.809402 1.998008 -0.152578
C -0.561731 -1.531131 0.588023
C -1.939961 -1.455245 -0.070737
H -1.866023 -1.864440 -1.083477
H -2.652609 -2.079123 0.471756
C -1.426821 0.892226 -0.831837
C -2.452293 -0.017197 -0.153175
H -2.640926 0.356863 0.857694
H -3.402446 0.015563 -0.689252
C 1.876361 -0.794529 0.437388
H 1.954910 -1.776269 0.909615
H 0.614566 1.278571 1.944226
H -0.798146 2.273790 1.368575
H 0.480757 2.855788 -0.723495
H 1.879111 1.849357 -0.130486
```

| | | | |
|---|-----------|-----------|-----------|
| H | -0.632546 | -1.224704 | 1.637550 |
| H | -1.774158 | 1.927456 | -0.830399 |
| H | -1.307054 | 0.590695 | -1.877839 |
| H | -0.203096 | -2.562766 | 0.579915 |
| H | 2.061051 | -0.066797 | 1.230442 |
| C | 2.960777 | -0.683935 | -0.632675 |
| H | 3.958660 | -0.733158 | -0.195033 |
| H | 2.870142 | -1.500787 | -1.350870 |
| H | 2.883839 | 0.250344 | -1.189500 |

eq3

```
=====
```

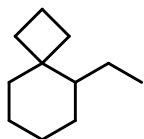
| | | | |
|---|-----------|-----------|-----------|
| C | -0.126524 | 0.839467 | -0.237148 |
| C | 0.367224 | -0.552851 | -0.622993 |
| H | 0.002705 | -0.712345 | -1.645903 |
| C | 0.374555 | 1.549881 | 0.990115 |
| C | 0.731929 | 2.057813 | -0.387979 |
| C | -0.357843 | -1.582632 | 0.253076 |
| C | -1.874937 | -1.477917 | 0.077046 |
| H | -2.128397 | -1.751335 | -0.952109 |
| H | -2.381640 | -2.191803 | 0.729026 |
| C | -1.620002 | 0.974059 | -0.475791 |
| C | -2.381200 | -0.061361 | 0.355165 |
| H | -2.240744 | 0.167884 | 1.415910 |
| H | -3.451916 | 0.002591 | 0.153227 |
| C | 1.880892 | -0.794956 | -0.708391 |
| H | 2.307046 | -0.124303 | -1.457636 |
| H | 1.151497 | 1.102926 | 1.588574 |
| H | -0.357314 | 2.115384 | 1.551494 |
| H | 0.263488 | 2.972146 | -0.726288 |
| H | 1.754938 | 1.923174 | -0.711056 |
| H | -0.100767 | -1.413608 | 1.303139 |
| H | -1.947119 | 1.983774 | -0.219011 |
| H | -1.836084 | 0.821353 | -1.538332 |
| H | -0.020431 | -2.590041 | -0.003316 |
| H | 1.999128 | -1.804188 | -1.111085 |
| C | 2.705255 | -0.696201 | 0.576223 |
| H | 3.677431 | -1.168083 | 0.428279 |
| H | 2.892610 | 0.336304 | 0.867052 |
| H | 2.219480 | -1.201635 | 1.412091 |

eq4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.021464 | 0.776260 | -0.114236 |
| C | 0.361052 | -0.695452 | -0.286896 |
| H | 0.357779 | -0.899498 | -1.365827 |
| C | 0.461312 | 1.554912 | 1.077710 |
| C | 0.945716 | 1.908146 | -0.309271 |
| C | -0.725847 | -1.576314 | 0.356517 |
| C | -2.136234 | -1.272111 | -0.138313 |
| H | -2.200798 | -1.494405 | -1.208270 |
| H | -2.856436 | -1.918894 | 0.365996 |
| C | -1.435657 | 1.081686 | -0.584868 |
| C | -2.478435 | 0.196235 | 0.088793 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.491171 | 0.403551 | 1.163464 |
| H | -3.473614 | 0.425899 | -0.295911 |
| C | 1.716636 | -1.159790 | 0.267174 |
| H | 1.729229 | -2.244180 | 0.136241 |
| H | 1.174564 | 1.086970 | 1.741677 |
| H | -0.234008 | 2.228980 | 1.559367 |
| H | 0.542961 | 2.805513 | -0.759408 |
| H | 1.973493 | 1.707399 | -0.556936 |
| H | -0.688371 | -1.426017 | 1.441597 |
| H | -1.651958 | 2.136467 | -0.403898 |
| H | -1.485265 | 0.926447 | -1.668612 |
| H | -0.483740 | -2.625405 | 0.174529 |
| H | 1.740325 | -0.995588 | 1.347426 |
| C | 2.990596 | -0.599602 | -0.368889 |
| H | 3.822550 | -1.284702 | -0.201311 |
| H | 2.876024 | -0.477209 | -1.447663 |
| H | 3.282396 | 0.360853 | 0.051215 |



5-ethylspiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -431.135117 | -430.832318 | -430.879986 |
| ax2 | -431.132947 | -430.829981 | -430.877051 |
| ax3 | -431.127837 | -430.8247 | -430.87208 |
| ax4 | -431.133337 | -430.830374 | -430.878403 |
| ax5 | -431.127446 | -430.824208 | -430.871151 |
| ax6 | -431.129193 | -430.826098 | -430.873679 |
| eq1 | -431.133618 | -430.830822 | -430.878953 |
| eq2 | -431.129627 | -430.826552 | -430.873814 |
| eq3 | -431.129563 | -430.826607 | -430.874188 |
| eq4 | -431.134399 | -430.831652 | -430.87911 |
| eq5 | -431.131295 | -430.828302 | -430.874929 |

eq6 | -431.131365 | -430.828427 | -430.875165

ax1

```
=====  
C 0.612299 -0.512578 0.490641  
H 0.491154 -1.238058 1.303584  
C 1.232017 0.762082 1.080258  
C 1.307123 1.889755 0.050015  
H 1.733441 2.784649 0.506831  
H 1.976566 1.604453 -0.766545  
C -0.750697 0.939314 -1.070368  
C -0.082460 2.196502 -0.509604  
H -0.022972 2.963795 -1.283590  
H -0.701643 2.606333 0.293946  
H 0.608569 1.095024 1.916548  
H -0.208514 0.604695 -1.959640  
H -1.769127 1.168909 -1.395067  
H 2.219276 0.551715 1.494074  
C -0.788243 -0.199037 -0.045912  
C -1.623616 -1.404282 -0.549005  
C -1.888968 0.043808 1.026766  
C -2.850638 -0.837483 0.198865  
H -1.278614 -2.336062 -0.097946  
H -1.702896 -1.538021 -1.628308  
H -1.625371 -0.428184 1.974340  
H -2.188646 1.074513 1.213899  
H -3.471531 -1.545431 0.743700  
H -3.486809 -0.241980 -0.453413  
C 1.493447 -1.182851 -0.572145  
H 1.619705 -0.525490 -1.434112  
H 0.968278 -2.068695 -0.938608  
C 2.868078 -1.597174 -0.054069  
H 2.778716 -2.196244 0.854887  
H 3.401559 -2.192989 -0.795447  
H 3.488813 -0.731261 0.178223
```

ax2

```
=====  
C -0.507622 0.603361 0.729859  
H -0.068765 1.037402 1.635709  
C -1.581982 -0.411190 1.155633  
C -2.164932 -1.167948 -0.040998  
H -2.893811 -1.903012 0.305344  
H -2.705443 -0.475182 -0.690359  
C 0.064851 -0.897675 -1.216791  
C -1.061600 -1.863733 -0.839354  
H -1.475875 -2.323202 -1.738629  
H -0.648978 -2.676081 -0.234680  
H -1.135298 -1.134666 1.844820  
H -0.302877 -0.168331 -1.945265  
H 0.874550 -1.444920 -1.706506  
H -2.376359 0.100404 1.703591  
C 0.613486 -0.152141 0.003456
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.934149 | 0.599601 | -0.321083 |
| C | 1.458497 | -1.099110 | 0.906652 |
| C | 2.730675 | -0.626169 | 0.171596 |
| H | 2.075800 | 1.452451 | 0.342713 |
| H | 2.082426 | 0.920898 | -1.352339 |
| H | 1.447110 | -0.756983 | 1.942778 |
| H | 1.227251 | -2.163270 | 0.882087 |
| H | 3.614832 | -0.435598 | 0.776264 |
| H | 3.000095 | -1.294165 | -0.644500 |
| C | -1.142436 | 1.758633 | -0.059345 |
| H | -1.983200 | 2.130486 | 0.533359 |
| H | -1.573254 | 1.390784 | -0.991781 |
| C | -0.213179 | 2.928974 | -0.373182 |
| H | 0.543460 | 2.662484 | -1.109688 |
| H | -0.782057 | 3.767937 | -0.776519 |
| H | 0.300953 | 3.276953 | 0.524950 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.435593 | 0.558499 | 0.850098 |
| H | 0.001245 | 0.960360 | 1.769887 |
| C | -1.285513 | -0.656570 | 1.260521 |
| C | -1.646812 | -1.598665 | 0.106251 |
| H | -2.149052 | -2.481120 | 0.508073 |
| H | -2.351324 | -1.120634 | -0.574159 |
| C | 0.370306 | -0.791467 | -1.164150 |
| C | -0.406081 | -2.015208 | -0.680293 |
| H | -0.688866 | -2.641186 | -1.528554 |
| H | 0.239335 | -2.624095 | -0.040621 |
| H | -0.716303 | -1.234421 | 1.996059 |
| H | -0.237419 | -0.229672 | -1.877967 |
| H | 1.270448 | -1.105119 | -1.699765 |
| H | -2.191565 | -0.315510 | 1.768553 |
| C | 0.767034 | 0.119475 | 0.000104 |
| C | 1.741939 | 1.238652 | -0.447617 |
| C | 1.954475 | -0.508476 | 0.793013 |
| C | 2.930286 | 0.332436 | -0.058903 |
| H | 1.677209 | 2.103838 | 0.213592 |
| H | 1.670673 | 1.574556 | -1.482891 |
| H | 1.949093 | -0.183602 | 1.834131 |
| H | 2.065504 | -1.591592 | 0.758629 |
| H | 3.764740 | 0.802692 | 0.456921 |
| H | 3.314193 | -0.227639 | -0.909471 |
| C | -1.247539 | 1.738420 | 0.274616 |
| H | -0.542868 | 2.473783 | -0.121725 |
| H | -1.738756 | 2.226389 | 1.120823 |
| C | -2.325637 | 1.474018 | -0.776646 |
| H | -3.129560 | 0.855327 | -0.378000 |
| H | -2.770037 | 2.422113 | -1.084480 |
| H | -1.937883 | 0.988853 | -1.670990 |

ax4

```
=====
```

| | | | |
|---|----------|----------|-----------|
| C | 0.575950 | 1.178375 | -1.127689 |
|---|----------|----------|-----------|

| | | | |
|---|-----------|-----------|-----------|
| H | 1.525909 | 1.554228 | -1.515506 |
| C | -0.170945 | 2.292661 | -0.392994 |
| C | -1.466434 | 1.773510 | 0.231441 |
| H | -1.954454 | 2.566637 | 0.800787 |
| H | -2.161961 | 1.482195 | -0.560796 |
| C | -0.453878 | -0.554607 | 0.401408 |
| C | -1.179904 | 0.579831 | 1.143656 |
| H | -2.102701 | 0.208656 | 1.590958 |
| H | -0.552851 | 0.921093 | 1.971341 |
| H | 0.471330 | 2.685804 | 0.402249 |
| H | -0.181391 | -1.320236 | 1.137906 |
| H | -0.377035 | 3.121666 | -1.072291 |
| C | 0.852828 | -0.009827 | -0.211387 |
| C | 1.778951 | -1.116964 | -0.786894 |
| C | 1.934861 | 0.240383 | 0.881883 |
| C | 2.569093 | -1.124287 | 0.538821 |
| H | 2.379901 | -0.729427 | -1.610611 |
| H | 1.319066 | -2.053335 | -1.097471 |
| H | 2.587776 | 1.069990 | 0.606885 |
| H | 1.590044 | 0.386106 | 1.904748 |
| H | 3.654195 | -1.166468 | 0.472248 |
| H | 2.228018 | -1.910529 | 1.210193 |
| C | -1.354898 | -1.237426 | -0.639161 |
| H | -1.643517 | -0.527303 | -1.415968 |
| H | -0.781913 | -2.018860 | -1.140445 |
| H | -0.009391 | 0.851234 | -1.992566 |
| C | -2.614417 | -1.861683 | -0.042545 |
| H | -3.313934 | -1.105256 | 0.313737 |
| H | -3.137082 | -2.465371 | -0.785280 |
| H | -2.367248 | -2.510625 | 0.800660 |

ax5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.129564 | -0.847407 | -1.302753 |
| H | -0.557895 | -1.368455 | -1.974106 |
| C | 1.160946 | -1.824115 | -0.741527 |
| C | 2.094465 | -1.112010 | 0.234053 |
| H | 2.811477 | -1.817999 | 0.657826 |
| H | 2.674487 | -0.357468 | -0.301970 |
| C | 0.179602 | 0.492629 | 0.884562 |
| C | 1.286748 | -0.466863 | 1.359898 |
| H | 1.946106 | 0.062018 | 2.051483 |
| H | 0.818215 | -1.273218 | 1.932841 |
| H | 0.644299 | -2.633591 | -0.214675 |
| H | -0.470871 | 0.642080 | 1.752715 |
| H | 1.727063 | -2.283402 | -1.553718 |
| C | -0.690951 | -0.185309 | -0.196679 |
| C | -1.878483 | 0.699756 | -0.664616 |
| C | -1.739749 | -1.126671 | 0.470559 |
| C | -2.779738 | 0.011760 | 0.383597 |
| H | -2.176207 | 0.435917 | -1.680488 |
| H | -1.763098 | 1.780434 | -0.600150 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.998311 | -1.956697 | -0.188304 |
| H | -1.502103 | -1.517576 | 1.459664 |
| H | -3.788738 | -0.256331 | 0.077390 |
| H | -2.834074 | 0.583347 | 1.308711 |
| C | 0.686651 | 1.911641 | 0.544730 |
| H | -0.142518 | 2.607058 | 0.692469 |
| H | 1.431592 | 2.179329 | 1.298887 |
| H | 0.642078 | -0.092932 | -1.901880 |
| C | 1.267014 | 2.187211 | -0.842039 |
| H | 0.518862 | 2.045532 | -1.622387 |
| H | 1.602062 | 3.224464 | -0.896523 |
| H | 2.121163 | 1.553763 | -1.076499 |

ax6

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.448780 | -0.738504 | 1.356113 |
| H | 0.016861 | -1.476324 | 2.013999 |
| C | -1.787525 | -1.270882 | 0.838702 |
| C | -2.437636 | -0.299790 | -0.148012 |
| H | -3.336999 | -0.747811 | -0.574793 |
| H | -2.761978 | 0.595311 | 0.387495 |
| C | -0.128202 | 0.619665 | -0.740171 |
| C | -1.470942 | 0.081685 | -1.274466 |
| H | -1.930081 | 0.831407 | -1.922675 |
| H | -1.293620 | -0.799928 | -1.893708 |
| H | -1.611339 | -2.226391 | 0.334139 |
| H | 0.551697 | 0.753120 | -1.590122 |
| H | -2.463503 | -1.474286 | 1.671105 |
| C | 0.494563 | -0.437375 | 0.195799 |
| C | 1.995546 | -0.211851 | 0.554904 |
| C | 0.950886 | -1.706095 | -0.592835 |
| C | 2.402027 | -1.189681 | -0.564779 |
| H | 2.215232 | -0.616220 | 1.544210 |
| H | 2.397617 | 0.792992 | 0.488240 |
| H | 0.829921 | -2.604560 | 0.014183 |
| H | 0.506636 | -1.881180 | -1.571078 |
| H | 3.184623 | -1.911467 | -0.339980 |
| H | 2.662791 | -0.664683 | -1.482560 |
| C | -0.372687 | 2.010452 | -0.124328 |
| H | -0.834342 | 2.616860 | -0.908535 |
| H | -1.118058 | 1.937140 | 0.668646 |
| H | -0.610265 | 0.163674 | 1.954959 |
| C | 0.832973 | 2.771808 | 0.419936 |
| H | 1.652729 | 2.796387 | -0.300509 |
| H | 0.551516 | 3.803400 | 0.637197 |
| H | 1.209224 | 2.335965 | 1.344610 |

eq1

```
=====
```

| | | | |
|---|----------|----------|-----------|
| C | 0.848589 | 0.042912 | -0.254388 |
| H | 1.083044 | 0.220507 | -1.313315 |
| C | 1.078854 | 1.355524 | 0.508434 |
| C | 0.216075 | 2.500678 | -0.013457 |
| H | 0.402822 | 3.408270 | 0.563558 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.491303 | 2.717677 | -1.050517 |
| C | -1.504456 | 0.815613 | -0.705562 |
| C | -1.260014 | 2.120211 | 0.047187 |
| H | -1.881833 | 2.914731 | -0.369338 |
| H | -1.556314 | 2.000997 | 1.093794 |
| H | 0.840022 | 1.180883 | 1.564339 |
| H | -1.280346 | 0.968878 | -1.767252 |
| H | -2.558782 | 0.532890 | -0.643858 |
| H | 2.134194 | 1.630146 | 0.467102 |
| C | -0.637939 | -0.343872 | -0.199399 |
| C | -1.085425 | -1.658469 | -0.894119 |
| C | -1.186172 | -0.916851 | 1.139370 |
| C | -1.970910 | -1.977031 | 0.333238 |
| H | -0.279130 | -2.379414 | -1.011798 |
| H | -1.590522 | -1.536465 | -1.852803 |
| H | -0.401393 | -1.372267 | 1.742323 |
| H | -1.763575 | -0.237246 | 1.765781 |
| H | -1.942218 | -2.998119 | 0.707674 |
| H | -3.009208 | -1.690621 | 0.177316 |
| C | 1.807712 | -1.038837 | 0.261626 |
| H | 1.452724 | -2.030879 | -0.020254 |
| H | 1.816930 | -1.015287 | 1.354580 |
| C | 3.233476 | -0.870494 | -0.259268 |
| H | 3.654584 | 0.096984 | 0.015885 |
| H | 3.891728 | -1.641554 | 0.142762 |
| H | 3.257228 | -0.946420 | -1.347949 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.038179 | 0.897293 | 0.593537 |
| H | 0.382596 | 0.975567 | 1.604950 |
| C | 0.964906 | 1.582896 | -0.341438 |
| C | 2.373146 | 1.029887 | -0.115901 |
| H | 3.083987 | 1.500683 | -0.797609 |
| H | 2.689038 | 1.284518 | 0.900632 |
| C | 1.331531 | -1.179139 | 0.552505 |
| C | 2.407422 | -0.488794 | -0.288668 |
| H | 3.393081 | -0.877427 | -0.026054 |
| H | 2.248132 | -0.728240 | -1.343488 |
| H | 0.669399 | 1.420378 | -1.383379 |
| H | 1.558648 | -1.051949 | 1.616251 |
| H | 1.334068 | -2.254188 | 0.351838 |
| H | 0.953917 | 2.662295 | -0.171906 |
| C | -0.065352 | -0.606715 | 0.277778 |
| C | -1.171397 | -1.475784 | 0.929131 |
| C | -0.558291 | -1.096481 | -1.120251 |
| C | -1.354585 | -2.218870 | -0.413365 |
| H | -2.055766 | -0.895241 | 1.187154 |
| H | -0.872222 | -2.068884 | 1.794162 |
| H | -1.197100 | -0.385620 | -1.634304 |
| H | 0.220460 | -1.420686 | -1.809534 |
| H | -2.378694 | -2.376066 | -0.745834 |
| H | -0.830106 | -3.172230 | -0.437066 |
| C | -1.381279 | 1.639203 | 0.675223 |

| | | | |
|---|-----------|----------|-----------|
| H | -1.143852 | 2.671898 | 0.945117 |
| H | -1.959164 | 1.241746 | 1.512037 |
| C | -2.270255 | 1.659234 | -0.567405 |
| H | -2.745029 | 0.694036 | -0.742743 |
| H | -3.066837 | 2.394077 | -0.442559 |
| H | -1.710558 | 1.928949 | -1.464542 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.011547 | 0.986697 | -0.333613 |
| H | -0.057067 | 1.185698 | -1.411827 |
| C | -1.259459 | 1.540286 | 0.336671 |
| C | -2.548749 | 0.864726 | -0.113080 |
| H | -3.401667 | 1.296449 | 0.413880 |
| H | -2.706270 | 1.043952 | -1.181402 |
| C | -1.239628 | -1.199135 | -0.582843 |
| C | -2.457229 | -0.635442 | 0.137480 |
| H | -3.361571 | -1.144660 | -0.200437 |
| H | -2.370737 | -0.817438 | 1.213367 |
| H | -1.156043 | 1.406081 | 1.419996 |
| H | -1.371289 | -1.053527 | -1.661191 |
| H | -1.161048 | -2.277726 | -0.420394 |
| H | -1.311481 | 2.617076 | 0.160996 |
| C | 0.088922 | -0.543652 | -0.177679 |
| C | 1.227996 | -1.322851 | -0.898665 |
| C | 0.606242 | -1.104005 | 1.178490 |
| C | 1.484830 | -2.115409 | 0.405960 |
| H | 2.070898 | -0.713916 | -1.203726 |
| H | 0.897569 | -1.908941 | -1.756824 |
| H | 1.208021 | -0.381659 | 1.728012 |
| H | -0.146992 | -1.515819 | 1.850262 |
| H | 2.521443 | -2.193925 | 0.727662 |
| H | 1.053569 | -3.114293 | 0.379741 |
| C | 1.185546 | 1.808696 | 0.229448 |
| H | 1.154796 | 1.752527 | 1.320939 |
| H | 0.969956 | 2.852268 | -0.014227 |
| C | 2.605917 | 1.499022 | -0.234823 |
| H | 2.674291 | 1.450253 | -1.322997 |
| H | 3.281521 | 2.286218 | 0.103458 |
| H | 2.976486 | 0.557785 | 0.170634 |

eq4

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.814441 | 0.317681 | -0.691923 |
| H | -1.780564 | 0.024381 | -1.747717 |
| C | -2.388566 | -0.829010 | 0.134689 |
| C | -1.476075 | -2.048512 | 0.053485 |
| H | -1.859277 | -2.858005 | 0.677571 |
| H | -1.464603 | -2.418026 | -0.976966 |
| C | 0.527382 | -0.522977 | -0.335940 |
| C | -0.050961 | -1.692534 | 0.471915 |
| H | 0.588677 | -2.569193 | 0.366353 |
| H | -0.041394 | -1.421742 | 1.534132 |
| H | -2.474483 | -0.511303 | 1.179215 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.537024 | -0.819533 | -1.394200 |
| H | -3.395323 | -1.077138 | -0.206003 |
| C | -0.406923 | 0.701015 | -0.242412 |
| C | 0.143897 | 1.983667 | -0.922158 |
| C | -0.347320 | 1.448914 | 1.123756 |
| C | 0.502432 | 2.561040 | 0.466464 |
| H | -0.655718 | 2.545686 | -1.405261 |
| H | 0.958379 | 1.855117 | -1.634590 |
| H | -1.332881 | 1.804885 | 1.425535 |
| H | 0.101941 | 0.918096 | 1.962198 |
| H | 0.193146 | 3.586201 | 0.659717 |
| H | 1.561355 | 2.465562 | 0.698050 |
| C | 1.979500 | -0.234323 | 0.066671 |
| H | 2.343388 | 0.630290 | -0.490154 |
| H | 2.017052 | 0.036819 | 1.125514 |
| H | -2.460354 | 1.196629 | -0.625675 |
| C | 2.933009 | -1.400803 | -0.187475 |
| H | 3.966658 | -1.095417 | -0.021358 |
| H | 2.733825 | -2.246514 | 0.469823 |
| H | 2.851553 | -1.751742 | -1.218619 |

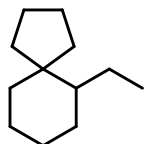
eq5

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```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.456447 | -1.282437 | -0.371642 |
| H | 1.736133 | -1.251186 | -1.431023 |
| C | 2.449441 | -0.453382 | 0.439490 |
| C | 2.386958 | 1.015399 | 0.027109 |
| H | 3.062070 | 1.614174 | 0.641358 |
| H | 2.725679 | 1.111792 | -1.009310 |
| C | -0.031189 | 0.702907 | -0.673814 |
| C | 0.958666 | 1.543225 | 0.141512 |
| H | 0.909105 | 2.584854 | -0.187051 |
| H | 0.660879 | 1.532114 | 1.194492 |
| H | 2.202652 | -0.538682 | 1.503106 |
| H | 0.338413 | 0.687937 | -1.707423 |
| H | 3.460677 | -0.845026 | 0.316022 |
| C | 0.023887 | -0.772163 | -0.224852 |
| C | -1.049426 | -1.677909 | -0.884148 |
| C | -0.633382 | -1.083085 | 1.152253 |
| C | -1.883149 | -1.616480 | 0.415642 |
| H | -0.654961 | -2.678539 | -1.063731 |
| H | -1.515124 | -1.314411 | -1.799878 |
| H | -0.097150 | -1.886251 | 1.659913 |
| H | -0.765053 | -0.260457 | 1.852249 |
| H | -2.303000 | -2.553487 | 0.775951 |
| H | -2.678656 | -0.875538 | 0.358565 |
| C | -1.414911 | 1.378615 | -0.748451 |
| H | -1.304097 | 2.235618 | -1.418347 |
| H | -2.125341 | 0.710569 | -1.238881 |
| H | 1.494135 | -2.329729 | -0.062164 |
| C | -2.025019 | 1.898754 | 0.554449 |
| H | -2.964106 | 2.411087 | 0.339720 |
| H | -2.243859 | 1.105986 | 1.267207 |
| H | -1.368333 | 2.618505 | 1.043935 |

eq6

| | | | |
|---|-----------|-----------|-----------|
| C | 1.381966 | -1.077805 | -0.791179 |
| H | 1.427923 | -0.764048 | -1.840752 |
| C | 2.561167 | -0.479068 | -0.032426 |
| C | 2.467356 | 1.042473 | -0.035577 |
| H | 3.280653 | 1.481240 | 0.545502 |
| H | 2.575596 | 1.405524 | -1.062679 |
| C | -0.081258 | 0.887450 | -0.221124 |
| C | 1.120991 | 1.499479 | 0.517432 |
| H | 1.049262 | 2.587939 | 0.469680 |
| H | 1.054850 | 1.228444 | 1.577454 |
| H | 2.545555 | -0.840462 | 1.001235 |
| H | -0.017593 | 1.197362 | -1.272991 |
| H | 3.503982 | -0.810108 | -0.471368 |
| C | 0.033911 | -0.652596 | -0.211088 |
| C | -1.166746 | -1.419088 | -0.828330 |
| C | -0.319224 | -1.304060 | 1.159212 |
| C | -1.697063 | -1.715920 | 0.592180 |
| H | -0.822113 | -2.329454 | -1.320345 |
| H | -1.811178 | -0.877127 | -1.516969 |
| H | 0.316346 | -2.167078 | 1.360292 |
| H | -0.318018 | -0.657851 | 2.036366 |
| H | -2.024610 | -2.734853 | 0.788568 |
| H | -2.486441 | -1.030551 | 0.895600 |
| C | -1.370671 | 1.496115 | 0.360838 |
| H | -1.588465 | 1.045000 | 1.332486 |
| H | -1.149747 | 2.545804 | 0.569335 |
| H | 1.438460 | -2.168959 | -0.782877 |
| C | -2.620114 | 1.467063 | -0.520930 |
| H | -3.373681 | 2.147949 | -0.122146 |
| H | -2.385169 | 1.794566 | -1.535801 |
| H | -3.077497 | 0.482390 | -0.584636 |



6-ethylspiro[4.5]decane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -470.467698 | -470.133517 | -470.182925 |
| ax2 | -470.465166 | -470.131181 | -470.180936 |
| ax3 | -470.460854 | -470.126647 | -470.176567 |
| ax4 | -470.466388 | -470.132237 | -470.181514 |
| ax5 | -470.459401 | -470.125075 | -470.174252 |
| ax6 | -470.464860 | -470.130731 | -470.179836 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| ax7 | | -470.461483 | | -470.127056 | | -470.176104 |
| ax8 | | -470.467279 | | -470.133298 | | -470.182968 |
| ax9 | | -470.460450 | | -470.126315 | | -470.1759 |
| eq1 | | -470.468417 | | -470.134634 | | -470.184266 |
| eq2 | | -470.464738 | | -470.13061 | | -470.179503 |
| eq3 | | -470.464783 | | -470.130843 | | -470.179875 |
| eq4 | | -470.466583 | | -470.132646 | | -470.182786 |
| eq5 | | -470.461892 | | -470.127723 | | -470.177649 |
| eq6 | | -470.462004 | | -470.127749 | | -470.177425 |
| eq7 | | -470.464227 | | -470.130148 | | -470.17901 |
| eq8 | | -470.464360 | | -470.130163 | | -470.178828 |
| eq9 | | -470.467898 | | -470.134127 | | -470.184066 |

ax1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.844020 | -0.498795 | 0.560503 |
| H | 0.700545 | -1.130668 | 1.445040 |
| C | 1.570652 | 0.778541 | 1.007851 |
| C | 1.704781 | 1.784278 | -0.135452 |
| H | 2.221769 | 2.680780 | 0.211547 |
| H | 2.317595 | 1.356300 | -0.934600 |
| C | -0.462900 | 0.904966 | -1.096165 |
| C | 0.327743 | 2.150925 | -0.688879 |
| H | 0.427302 | 2.818128 | -1.547200 |
| H | -0.224115 | 2.705609 | 0.074847 |
| H | 1.003809 | 1.242262 | 1.819862 |
| H | 0.018020 | 0.450098 | -1.966610 |
| H | -1.467170 | 1.193146 | -1.416410 |
| H | 2.550569 | 0.532266 | 1.418424 |
| C | 1.666732 | -1.327080 | -0.440870 |
| H | 1.143146 | -2.268617 | -0.615111 |
| H | 1.714564 | -0.821481 | -1.407472 |
| C | -0.561537 | -0.149988 | 0.024310 |
| C | -1.331758 | -1.383425 | -0.478953 |
| C | -1.503526 | 0.338587 | 1.145188 |
| C | -2.815704 | -0.977345 | -0.466254 |
| H | -1.164221 | -2.207810 | 0.220632 |
| H | -0.998062 | -1.715213 | -1.462649 |
| C | -2.929516 | 0.140696 | 0.600599 |
| H | -1.317482 | 1.367122 | 1.450652 |
| H | -1.348535 | -0.294297 | 2.023210 |
| H | -3.116836 | -0.601818 | -1.443974 |
| H | -3.459644 | -1.826320 | -0.241323 |
| H | -3.298522 | 1.061511 | 0.149203 |
| H | -3.625315 | -0.121649 | 1.396309 |
| C | 3.085521 | -1.637107 | 0.030184 |
| H | 3.559709 | -2.367428 | -0.626369 |
| H | 3.714796 | -0.746780 | 0.038250 |
| H | 3.081026 | -2.050662 | 1.041371 |

ax2

```
=====
```

| | | | |
|---|-----------|----------|----------|
| C | -0.963880 | 0.375664 | 0.620216 |
|---|-----------|----------|----------|

| | | | |
|---|-----------|-----------|-----------|
| H | -0.799285 | 0.970015 | 1.525748 |
| C | -1.688452 | -0.915880 | 1.030223 |
| C | -1.844467 | -1.872262 | -0.151984 |
| H | -2.368862 | -2.776897 | 0.160937 |
| H | -2.459493 | -1.401100 | -0.924955 |
| C | 0.306593 | -0.967905 | -1.113550 |
| C | -0.479258 | -2.226349 | -0.738482 |
| H | -0.596173 | -2.860849 | -1.619118 |
| H | 0.083274 | -2.810714 | -0.005428 |
| H | -1.125160 | -1.418594 | 1.821484 |
| H | -0.191165 | -0.480085 | -1.956645 |
| H | 1.302298 | -1.246679 | -1.465604 |
| H | -2.666215 | -0.664496 | 1.447094 |
| C | -1.845079 | 1.221050 | -0.327571 |
| H | -1.577169 | 1.032929 | -1.368907 |
| H | -2.883672 | 0.896378 | -0.224592 |
| C | 0.430745 | 0.041695 | 0.045700 |
| C | 1.208604 | 1.285434 | -0.416363 |
| C | 1.390916 | -0.500743 | 1.125832 |
| C | 2.678182 | 0.840071 | -0.489853 |
| H | 1.103270 | 2.062725 | 0.344787 |
| H | 0.837738 | 1.691771 | -1.358922 |
| C | 2.807817 | -0.298003 | 0.554604 |
| H | 1.199322 | -1.538038 | 1.395766 |
| H | 1.263774 | 0.099124 | 2.030939 |
| H | 2.917808 | 0.471645 | -1.487024 |
| H | 3.357440 | 1.666225 | -0.284872 |
| H | 3.166247 | -1.211845 | 0.081208 |
| H | 3.518873 | -0.049992 | 1.341361 |
| C | -1.790775 | 2.723359 | -0.056002 |
| H | -2.465821 | 3.264055 | -0.721275 |
| H | -2.092769 | 2.939090 | 0.970714 |
| H | -0.789949 | 3.128536 | -0.199313 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.780785 | 0.403599 | 0.961122 |
| H | -0.419442 | 0.642308 | 1.967228 |
| C | -1.673484 | -0.841892 | 1.119047 |
| C | -1.969845 | -1.593779 | -0.180821 |
| H | -2.528068 | -2.504013 | 0.048025 |
| H | -2.604737 | -0.994958 | -0.835001 |
| C | 0.161312 | -0.684476 | -1.158287 |
| C | -0.679023 | -1.938418 | -0.917552 |
| H | -0.903899 | -2.418954 | -1.871635 |
| H | -0.109075 | -2.662944 | -0.329931 |
| H | -1.169762 | -1.538328 | 1.796755 |
| H | -0.379658 | -0.027636 | -1.842268 |
| H | 1.091551 | -0.956083 | -1.662887 |
| H | -2.606952 | -0.554377 | 1.609408 |
| C | -1.554819 | 1.674493 | 0.553082 |
| H | -2.364277 | 1.791452 | 1.279416 |
| H | -0.894592 | 2.530725 | 0.707637 |
| C | 0.490232 | 0.085581 | 0.137681 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.321191 | 1.339360 | -0.184067 |
| C | 1.515439 | -0.718731 | 0.969963 |
| C | 2.734349 | 0.823844 | -0.506064 |
| H | 1.355285 | 1.972305 | 0.707067 |
| H | 0.892398 | 1.933135 | -0.992785 |
| C | 2.866634 | -0.517479 | 0.260251 |
| H | 1.255282 | -1.770549 | 1.081248 |
| H | 1.558456 | -0.286941 | 1.972777 |
| H | 2.848653 | 0.663014 | -1.577763 |
| H | 3.497667 | 1.542058 | -0.210279 |
| H | 3.064834 | -1.335011 | -0.432567 |
| H | 3.689465 | -0.501408 | 0.973536 |
| C | -2.153180 | 1.793073 | -0.848473 |
| H | -2.680396 | 2.744847 | -0.936448 |
| H | -1.388260 | 1.775437 | -1.623597 |
| H | -2.872597 | 1.004873 | -1.063240 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.134211 | -1.427779 | 1.142586 |
| H | 0.603363 | -2.118627 | 1.559497 |
| C | -1.192608 | -2.196847 | 0.353039 |
| C | -2.190287 | -1.235484 | -0.290340 |
| H | -2.925783 | -1.786292 | -0.879490 |
| H | -2.742380 | -0.706379 | 0.493108 |
| C | -0.406880 | 0.580190 | -0.393643 |
| C | -1.451924 | -0.233758 | -1.175488 |
| H | -2.155832 | 0.439890 | -1.664601 |
| H | -0.954157 | -0.783745 | -1.977253 |
| H | -0.708199 | -2.785857 | -0.432130 |
| H | 0.147622 | 1.175540 | -1.127269 |
| H | -1.705526 | -2.903035 | 1.008631 |
| C | 0.604484 | -0.373103 | 0.308917 |
| C | 1.629242 | 0.387289 | 1.168708 |
| C | 1.552233 | -0.995307 | -0.740065 |
| C | 2.554229 | 1.072006 | 0.157386 |
| H | 2.196648 | -0.353549 | 1.739800 |
| H | 1.181359 | 1.072911 | 1.886238 |
| C | 2.601927 | 0.096465 | -1.046347 |
| H | 1.042510 | -1.340719 | -1.637731 |
| H | 2.039857 | -1.864100 | -0.290745 |
| H | 2.132950 | 2.031263 | -0.146944 |
| H | 3.541788 | 1.271842 | 0.570555 |
| H | 2.365785 | 0.616785 | -1.974085 |
| H | 3.592205 | -0.339339 | -1.171793 |
| C | -1.053500 | 1.580509 | 0.580878 |
| H | -1.438636 | 1.058809 | 1.460127 |
| H | -0.277678 | 2.256263 | 0.943598 |
| H | -0.618533 | -0.938875 | 1.993677 |
| C | -2.170505 | 2.422711 | -0.031036 |
| H | -3.061774 | 1.830367 | -0.238884 |
| H | -2.460784 | 3.225609 | 0.647517 |
| H | -1.848012 | 2.879882 | -0.969398 |

ax5

```
=====
C  1.539466   -0.728064   1.294924
C  0.582701    0.428722    0.961649
C  0.159010   -0.719763   -1.283778
H -0.641413   -1.142768   -1.898644
H  0.650656    0.033644   -1.899683
C  2.218191   -1.324212    0.063109
C  1.169921   -1.814559   -0.933987
H  1.648911   -2.173078   -1.847235
H  0.650876   -2.672370   -0.498599
H  2.862686   -0.578935   -0.407126
H  2.864765   -2.152246    0.360600
H  2.286070   -0.383265    2.013468
H  0.971187   -1.521992    1.790419
C -0.488820   -0.042561   -0.056569
C -1.461014   -1.056265    0.622862
C -1.428805    1.115621   -0.516547
C -2.853809   -0.705462    0.097879
H -1.445837   -0.914175    1.706520
H -1.187704   -2.092750    0.429650
C -2.814151    0.819712    0.071335
H -1.491707    1.116257   -1.607611
H -1.061526    2.095903   -0.218936
H -2.983832   -1.088861   -0.917709
H -3.655164   -1.113111    0.714001
H -3.622518    1.271549   -0.503171
H -2.878592    1.200270    1.093991
C  1.329460    1.747541    0.639476
H  2.204569    1.786092    1.294133
H  0.694900    2.577492    0.956745
H  0.038730    0.648330    1.885965
C  1.780711    2.053924   -0.790219
H  0.933737    2.139216   -1.470686
H  2.304634    3.011454   -0.802230
H  2.459402    1.305542   -1.194658
```

ax6

```
=====
C -0.938749   -0.974728    1.261368
H -0.615541   -1.858114    1.818191
C -2.239163   -1.265186    0.512607
C -2.668630   -0.051503   -0.309332
H -3.582893   -0.269041   -0.864377
H -2.897652    0.777237    0.368190
C -0.242947    0.677480   -0.531654
C -1.555600    0.362859   -1.270548
H -1.856945    1.241583   -1.845060
H -1.397398   -0.441989   -1.992157
H -2.094143   -2.119727   -0.155453
H  0.527678    0.839735   -1.292223
H -3.022681   -1.544593    1.219394
C  0.200362   -0.537766    0.332938
C  1.487948   -0.245772    1.122848
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.690873 | -1.691059 | -0.568621 |
| C | 2.625624 | -0.321051 | 0.093084 |
| H | 1.612986 | -1.040176 | 1.864122 |
| H | 1.457521 | 0.698473 | 1.666259 |
| C | 2.120423 | -1.303775 | -0.993991 |
| H | 0.043657 | -1.886878 | -1.421659 |
| H | 0.718365 | -2.604033 | 0.032255 |
| H | 2.813187 | 0.659997 | -0.343176 |
| H | 3.558828 | -0.651971 | 0.546641 |
| H | 2.114707 | -0.821412 | -1.971219 |
| H | 2.758500 | -2.182302 | -1.079009 |
| C | -0.375239 | 1.992733 | 0.271733 |
| H | -1.283381 | 2.512519 | -0.042355 |
| H | -0.506425 | 1.781835 | 1.334726 |
| H | -1.126626 | -0.190429 | 2.001408 |
| C | 0.804690 | 2.944818 | 0.087690 |
| H | 0.926441 | 3.205370 | -0.965631 |
| H | 0.654021 | 3.871007 | 0.644615 |
| H | 1.740235 | 2.500605 | 0.427780 |

ax7

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| | | | |
|---|-----------|-----------|-----------|
| C | 0.535732 | -0.906978 | -1.334920 |
| H | -0.033109 | -1.487069 | -2.066680 |
| C | 1.583713 | -1.788218 | -0.659922 |
| C | 2.372620 | -0.975236 | 0.361285 |
| H | 3.097939 | -1.609404 | 0.875300 |
| H | 2.943741 | -0.207291 | -0.163000 |
| C | 0.260795 | 0.474650 | 0.814659 |
| C | 1.434289 | -0.345712 | 1.392951 |
| H | 2.000757 | 0.287517 | 2.080225 |
| H | 1.022383 | -1.158970 | 1.996897 |
| H | 1.091957 | -2.627048 | -0.157784 |
| H | -0.470159 | 0.542031 | 1.627205 |
| H | 2.254077 | -2.214654 | -1.408402 |
| C | -0.454780 | -0.288995 | -0.339764 |
| C | -1.498556 | 0.585820 | -1.053956 |
| C | -1.376352 | -1.366330 | 0.280490 |
| C | -2.645251 | 0.724783 | -0.047647 |
| H | -1.848889 | 0.038381 | -1.934099 |
| H | -1.106469 | 1.541711 | -1.399712 |
| C | -2.663338 | -0.625580 | 0.710707 |
| H | -0.908781 | -1.896911 | 1.109224 |
| H | -1.611441 | -2.107529 | -0.487255 |
| H | -2.439092 | 1.543980 | 0.642641 |
| H | -3.596263 | 0.943621 | -0.531159 |
| H | -2.686082 | -0.464523 | 1.787954 |
| H | -3.547135 | -1.211009 | 0.460480 |
| C | 0.627878 | 1.945720 | 0.538990 |
| H | -0.297068 | 2.506101 | 0.384924 |
| H | 1.058488 | 2.339154 | 1.464005 |
| H | 1.048547 | -0.117768 | -1.889988 |
| C | 1.581066 | 2.272863 | -0.609421 |
| H | 1.175083 | 1.975387 | -1.575629 |

| | | | |
|---|----------|----------|-----------|
| H | 1.753192 | 3.350028 | -0.646832 |
| H | 2.551429 | 1.793539 | -0.489024 |

ax8

```

=====
C  0.583723    2.213105   -0.600570
C -0.288933    1.079190   -1.141221
C  0.736263   -0.537983    0.512126
H  0.465561   -1.192537    1.349961
C  1.879652    1.672453    0.002688
C  1.565888    0.627273    1.072823
H  2.484259    0.253169    1.526684
H  1.002378    1.112572    1.874314
H  2.493467    1.227507   -0.786098
H  2.463676    2.486951    0.434972
H  0.799858    2.925006   -1.399400
H  0.038989    2.763532    0.172073
C -0.588242   -0.011326   -0.092242
C -1.536362    0.553430    1.016677
C -1.424660   -1.139565   -0.741197
C -2.855166   -0.235089    0.919014
H -1.725346    1.614331    0.846460
H -1.095443    0.467025    2.009655
C -2.880546   -0.730242   -0.526340
H -1.246756   -2.078981   -0.209012
H -1.163242   -1.299478   -1.788045
H -2.825283   -1.097601    1.588751
H -3.724041    0.363165    1.191706
H -3.583811   -1.546334   -0.691214
H -3.150283    0.086366   -1.200241
H -1.234007    1.479831   -1.517184
H  0.218387    0.623982   -1.996228
C  1.535930   -1.397866   -0.480760
H  0.922064   -2.252221   -0.769992
H  1.730382   -0.838562   -1.397976
C  2.859971   -1.915894    0.076287
H  3.297743   -2.656807   -0.593581
H  3.589933   -1.115743    0.200704
H  2.716401   -2.390086    1.049983

```

ax9

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=====
C -1.068563   -1.865435   -0.939056
C -0.139263   -0.707538   -1.299464
C -0.591551    0.413479    0.951230
H -0.056028    0.580235    1.893451
C -2.183009   -1.386996   -0.012346
C -1.597717   -0.719462    1.233585
H -2.399094   -0.335819    1.869223
H -1.089609   -1.495802    1.813090
H -2.829534   -0.693885   -0.552699
H -2.810485   -2.228138    0.289653
H -1.487827   -2.303660   -1.846637
H -0.501505   -2.656333   -0.439125

```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.493027 | -0.041890 | -0.061621 |
| C | 1.476614 | -1.052207 | 0.621605 |
| C | 1.417334 | 1.126210 | -0.496221 |
| C | 2.836387 | -0.346942 | 0.699581 |
| H | 1.576901 | -1.946264 | 0.003184 |
| H | 1.123187 | -1.379125 | 1.599242 |
| C | 2.829020 | 0.540593 | -0.542841 |
| H | 1.403000 | 1.912883 | 0.261218 |
| H | 1.099254 | 1.572120 | -1.439414 |
| H | 2.886936 | 0.283299 | 1.591284 |
| H | 3.671706 | -1.045814 | 0.738035 |
| H | 3.607179 | 1.303641 | -0.540716 |
| H | 2.961021 | -0.073185 | -1.437668 |
| H | 0.664542 | -1.056432 | -1.954010 |
| H | -0.708215 | 0.030717 | -1.866839 |
| C | -1.271659 | 1.772144 | 0.672229 |
| H | -2.033417 | 1.902820 | 1.445837 |
| H | -0.539126 | 2.561752 | 0.849358 |
| C | -1.915265 | 2.045171 | -0.688139 |
| H | -2.391729 | 3.027066 | -0.669675 |
| H | -1.177661 | 2.059792 | -1.489557 |
| H | -2.681611 | 1.317375 | -0.948492 |

eq1

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.928544 | -0.238369 | 0.592986 |
| C | 0.856193 | 0.512403 | -0.204417 |
| H | 1.204873 | 0.573637 | -1.244151 |
| C | -0.171654 | -1.699004 | -0.799313 |
| H | -1.096710 | -2.282778 | -0.788998 |
| H | 0.121779 | -1.597558 | -1.850081 |
| C | 2.211988 | -1.618427 | 0.005970 |
| C | 0.931441 | -2.446639 | -0.052149 |
| H | 1.118179 | -3.406559 | -0.537596 |
| H | 0.605879 | -2.670362 | 0.967297 |
| H | 2.613561 | -1.500506 | -1.005606 |
| H | 2.973388 | -2.134792 | 0.593559 |
| H | 2.846711 | 0.351160 | 0.627515 |
| H | 1.584913 | -0.346619 | 1.628122 |
| C | 0.700046 | 1.951043 | 0.308407 |
| H | -0.260474 | 2.361269 | -0.009932 |
| H | 0.687389 | 1.947828 | 1.401303 |
| C | -0.466369 | -0.289949 | -0.248866 |
| C | -1.169553 | -0.383730 | 1.133499 |
| C | -1.523192 | 0.398514 | -1.166661 |
| C | -2.665244 | -0.246925 | 0.835296 |
| H | -0.860480 | 0.444436 | 1.774243 |
| H | -0.928769 | -1.305788 | 1.661578 |
| C | -2.689350 | 0.816305 | -0.262171 |
| H | -1.882666 | -0.323641 | -1.903011 |
| H | -1.098708 | 1.235573 | -1.722254 |
| H | -3.057945 | -1.188707 | 0.442970 |
| H | -3.252791 | 0.019128 | 1.713870 |
| H | -3.638902 | 0.872155 | -0.794074 |

| | | | |
|---|-----------|----------|-----------|
| H | -2.496393 | 1.796183 | 0.181270 |
| C | 1.811645 | 2.878199 | -0.178461 |
| H | 1.692935 | 3.883452 | 0.227630 |
| H | 2.797086 | 2.517442 | 0.119016 |
| H | 1.800174 | 2.954518 | -1.267382 |

eq2

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.653819 | 1.219799 | 0.257559 |
| C | 0.462576 | 0.825529 | -0.622576 |
| H | 0.856616 | 0.732020 | -1.642811 |
| C | 1.142744 | -1.565499 | -0.451171 |
| H | 0.813907 | -2.575227 | -0.189832 |
| H | 1.418331 | -1.585514 | -1.511589 |
| C | 2.816434 | 0.245194 | 0.079981 |
| C | 2.369216 | -1.184253 | 0.376764 |
| H | 3.182247 | -1.886220 | 0.181665 |
| H | 2.130359 | -1.267790 | 1.441054 |
| H | 3.175686 | 0.304046 | -0.952350 |
| H | 3.651597 | 0.523236 | 0.725640 |
| H | 1.969036 | 2.235949 | 0.005902 |
| H | 1.356113 | 1.235872 | 1.310091 |
| C | -0.581510 | 1.953015 | -0.711727 |
| H | -0.071225 | 2.800377 | -1.178327 |
| H | -1.369804 | 1.663995 | -1.409829 |
| C | -0.043162 | -0.599789 | -0.270501 |
| C | -0.634231 | -0.724663 | 1.168405 |
| C | -1.207838 | -1.024415 | -1.197277 |
| C | -2.100523 | -1.176588 | 1.014086 |
| H | -0.572677 | 0.220715 | 1.702244 |
| H | -0.070082 | -1.446768 | 1.759247 |
| C | -2.493210 | -0.770859 | -0.409073 |
| H | -1.127213 | -2.095921 | -1.400871 |
| H | -1.175853 | -0.507858 | -2.158128 |
| H | -2.160909 | -2.263385 | 1.103119 |
| H | -2.753746 | -0.751464 | 1.776380 |
| H | -3.341310 | -1.339796 | -0.790384 |
| H | -2.762792 | 0.285207 | -0.441883 |
| C | -1.216969 | 2.455763 | 0.585892 |
| H | -1.787304 | 3.364569 | 0.387593 |
| H | -1.902802 | 1.733405 | 1.026108 |
| H | -0.462259 | 2.701145 | 1.334787 |

eq3

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```

| | | | |
|---|----------|-----------|-----------|
| C | 1.666416 | 1.168839 | 0.688423 |
| C | 0.351849 | 1.020877 | -0.091340 |
| H | 0.541322 | 1.402367 | -1.103294 |
| C | 1.177392 | -1.197110 | -0.930856 |
| H | 0.933814 | -2.259412 | -1.022702 |
| H | 1.281245 | -0.808693 | -1.950494 |
| C | 2.826781 | 0.450913 | 0.005537 |
| C | 2.504761 | -1.025750 | -0.196767 |
| H | 3.303199 | -1.519481 | -0.754030 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.452994 | -1.516760 | 0.778938 |
| H | 3.006410 | 0.917375 | -0.968532 |
| H | 3.742431 | 0.566481 | 0.588533 |
| H | 1.898562 | 2.230523 | 0.795468 |
| H | 1.532989 | 0.774192 | 1.702141 |
| C | -0.737057 | 1.916408 | 0.533780 |
| H | -1.263954 | 1.382284 | 1.327217 |
| H | -0.230772 | 2.749114 | 1.028195 |
| C | -0.009496 | -0.481257 | -0.258818 |
| C | -0.371077 | -1.166558 | 1.095177 |
| C | -1.275682 | -0.684754 | -1.133574 |
| C | -1.727529 | -1.857157 | 0.882918 |
| H | -0.456060 | -0.427612 | 1.892336 |
| H | 0.395958 | -1.874463 | 1.408062 |
| C | -2.419078 | -0.981393 | -0.162662 |
| H | -1.127897 | -1.564795 | -1.765650 |
| H | -1.459142 | 0.157294 | -1.799558 |
| H | -1.576735 | -2.857237 | 0.469055 |
| H | -2.295166 | -1.964362 | 1.807114 |
| H | -3.267762 | -1.470293 | -0.641146 |
| H | -2.780537 | -0.062876 | 0.304444 |
| C | -1.752721 | 2.518344 | -0.438357 |
| H | -2.365865 | 3.264616 | 0.069461 |
| H | -1.244541 | 3.016862 | -1.266226 |
| H | -2.427856 | 1.776463 | -0.860110 |

eq4

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.057833 | -0.246325 | -0.224122 |
| H | 1.342964 | -0.215744 | -1.284674 |
| C | 1.771646 | 0.918310 | 0.479682 |
| C | 1.397149 | 2.281069 | -0.093864 |
| H | 1.916009 | 3.074728 | 0.447065 |
| H | 1.724692 | 2.337010 | -1.137008 |
| C | -0.830536 | 1.336571 | -0.736801 |
| C | -0.113127 | 2.484096 | -0.031230 |
| H | -0.392958 | 3.433057 | -0.492740 |
| H | -0.427966 | 2.538102 | 1.014743 |
| H | 1.507879 | 0.893013 | 1.542626 |
| H | -0.554532 | 1.357259 | -1.796689 |
| H | -1.911492 | 1.487102 | -0.694655 |
| H | 2.851946 | 0.772351 | 0.422833 |
| C | 1.562463 | -1.578047 | 0.354255 |
| H | 0.855460 | -2.383007 | 0.152383 |
| H | 1.625053 | -1.492396 | 1.442304 |
| C | -0.477654 | -0.062240 | -0.187269 |
| C | -1.243974 | -1.103341 | -1.025343 |
| C | -1.103765 | -0.280321 | 1.203543 |
| C | -2.694955 | -1.056464 | -0.506525 |
| H | -0.831935 | -2.098445 | -0.859511 |
| H | -1.171238 | -0.893410 | -2.093857 |
| C | -2.604290 | -0.495852 | 0.936661 |
| H | -0.916778 | 0.540228 | 1.895852 |
| H | -0.678189 | -1.183393 | 1.645697 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.308409 | -0.406513 | -1.129629 |
| H | -3.155089 | -2.043142 | -0.530031 |
| H | -3.144556 | 0.447634 | 1.011808 |
| H | -3.045998 | -1.172069 | 1.667148 |
| C | 2.926554 | -1.983984 | -0.200003 |
| H | 3.681422 | -1.218090 | -0.018165 |
| H | 3.278684 | -2.908750 | 0.258605 |
| H | 2.870967 | -2.146358 | -1.278009 |

eq5

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| | | | |
|---|-----------|-----------|-----------|
| C | -1.026804 | 0.460537 | -0.581976 |
| H | -1.253861 | 0.126741 | -1.603194 |
| C | -2.083086 | -0.194823 | 0.317317 |
| C | -2.151140 | -1.701840 | 0.068094 |
| H | -2.882931 | -2.167711 | 0.730851 |
| H | -2.496982 | -1.869603 | -0.956851 |
| C | 0.296754 | -1.642903 | -0.567588 |
| C | -0.782968 | -2.358748 | 0.246755 |
| H | -0.829446 | -3.408787 | -0.048746 |
| H | -0.513728 | -2.347894 | 1.305845 |
| H | -1.850151 | -0.005731 | 1.369155 |
| H | 0.085586 | -1.775476 | -1.633842 |
| H | 1.265631 | -2.110115 | -0.379417 |
| H | -3.058842 | 0.257861 | 0.123543 |
| C | -1.188692 | 1.989866 | -0.641954 |
| H | -2.212217 | 2.162979 | -0.985411 |
| H | -0.545129 | 2.394607 | -1.425177 |
| C | 0.371724 | -0.126209 | -0.279032 |
| C | 1.493853 | 0.502163 | -1.120223 |
| C | 0.919354 | 0.094024 | 1.148464 |
| C | 2.801781 | 0.050689 | -0.448745 |
| H | 1.418268 | 1.589780 | -1.062961 |
| H | 1.431477 | 0.220451 | -2.173398 |
| C | 2.433052 | -0.184634 | 1.039227 |
| H | 0.439343 | -0.537051 | 1.894454 |
| H | 0.758990 | 1.125475 | 1.451406 |
| H | 3.169138 | -0.870218 | -0.900500 |
| H | 3.587800 | 0.795638 | -0.563037 |
| H | 2.657275 | -1.211021 | 1.328776 |
| H | 3.001489 | 0.462413 | 1.705748 |
| C | -0.979734 | 2.797665 | 0.639997 |
| H | 0.075141 | 2.937515 | 0.871172 |
| H | -1.417404 | 3.790741 | 0.528159 |
| H | -1.454015 | 2.324674 | 1.501407 |

eq6

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| | | | |
|---|-----------|-----------|-----------|
| C | -0.710424 | 0.996059 | -0.293022 |
| H | -0.879153 | 1.171305 | -1.364095 |
| C | -2.081404 | 0.720443 | 0.356186 |
| C | -2.780598 | -0.534992 | -0.149679 |
| H | -3.728719 | -0.671366 | 0.374035 |
| H | -3.014516 | -0.421568 | -1.213090 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.547505 | -1.496182 | -0.670184 |
| C | -1.874688 | -1.745152 | 0.035524 |
| H | -2.343673 | -2.646047 | -0.364694 |
| H | -1.711081 | -1.920117 | 1.102857 |
| H | -1.935884 | 0.628817 | 1.438366 |
| H | -0.750598 | -1.370030 | -1.739226 |
| H | 0.099200 | -2.371219 | -0.581213 |
| H | -2.721194 | 1.592304 | 0.203229 |
| C | -0.211833 | 2.317124 | 0.325772 |
| H | -0.151957 | 2.195699 | 1.410616 |
| H | -1.013453 | 3.041169 | 0.159010 |
| C | 0.218606 | -0.240989 | -0.191211 |
| C | 1.497725 | -0.165234 | -1.053036 |
| C | 0.813846 | -0.461851 | 1.211609 |
| C | 2.460895 | -1.211288 | -0.449854 |
| H | 1.947822 | 0.819437 | -0.991927 |
| H | 1.278848 | -0.357174 | -2.104859 |
| C | 1.972136 | -1.450990 | 1.002143 |
| H | 0.085245 | -0.815055 | 1.941787 |
| H | 1.211783 | 0.486370 | 1.579045 |
| H | 2.437510 | -2.139946 | -1.018868 |
| H | 3.489116 | -0.853196 | -0.473022 |
| H | 1.623584 | -2.476664 | 1.121436 |
| H | 2.765299 | -1.299518 | 1.732856 |
| C | 1.086507 | 2.946156 | -0.175824 |
| H | 1.135488 | 2.951920 | -1.266245 |
| H | 1.145640 | 3.981774 | 0.162963 |
| H | 1.971118 | 2.434467 | 0.200490 |

eq7

| | | | |
|---|-----------|-----------|-----------|
| C | 2.058694 | -1.523876 | -0.549591 |
| C | 0.801802 | -1.759497 | 0.281598 |
| H | 1.100704 | -1.928155 | 1.321663 |
| C | 0.559551 | 0.695819 | 0.717407 |
| H | 0.856349 | 0.470820 | 1.749789 |
| C | 2.787032 | -0.281350 | -0.045535 |
| C | 1.854380 | 0.925988 | -0.073831 |
| H | 2.362587 | 1.809417 | 0.322578 |
| H | 1.609802 | 1.151809 | -1.115474 |
| H | 3.125860 | -0.457532 | 0.980362 |
| H | 3.676329 | -0.083846 | -0.647082 |
| H | 2.710619 | -2.398098 | -0.501581 |
| H | 1.788366 | -1.385246 | -1.601287 |
| C | -0.187938 | -0.580331 | 0.241954 |
| C | -0.814523 | -0.442424 | -1.174762 |
| C | -1.399960 | -0.914293 | 1.163091 |
| C | -2.310453 | -0.213502 | -0.945654 |
| H | -0.687880 | -1.385952 | -1.713053 |
| H | -0.342767 | 0.329809 | -1.779040 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.603934 | -1.136258 | 0.237373 |
| H | -1.606356 | -0.088496 | 1.843808 |
| H | -1.191834 | -1.787659 | 1.782093 |
| H | -2.499795 | 0.823605 | -0.658508 |
| H | -2.914272 | -0.432566 | -1.826438 |
| H | -3.557085 | -0.931373 | 0.724423 |
| H | -2.624685 | -2.171825 | -0.111048 |
| H | 0.281437 | -2.662833 | -0.048792 |
| C | -0.268533 | 1.997732 | 0.794782 |
| H | 0.216402 | 2.638499 | 1.536209 |
| H | -1.261355 | 1.784998 | 1.193619 |
| C | -0.418917 | 2.823450 | -0.485137 |
| H | -0.925309 | 2.282959 | -1.282836 |
| H | -1.007439 | 3.717677 | -0.273727 |
| H | 0.547112 | 3.155231 | -0.865842 |

eq8

```
=====
```

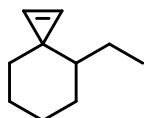
| | | | |
|---|-----------|-----------|-----------|
| C | -2.517260 | -1.048361 | 0.068765 |
| C | -1.247434 | -1.315292 | -0.728965 |
| H | -1.435892 | -1.061991 | -1.778130 |
| C | -0.379140 | 1.004948 | -0.277639 |
| H | -0.518667 | 1.262374 | -1.335976 |
| C | -2.873998 | 0.430128 | -0.026725 |
| C | -1.707725 | 1.290996 | 0.446156 |
| H | -1.951420 | 2.347977 | 0.318980 |
| H | -1.563795 | 1.135976 | 1.520876 |
| H | -3.105783 | 0.673066 | -1.068719 |
| H | -3.766617 | 0.655373 | 0.559970 |
| H | -3.334664 | -1.667866 | -0.304884 |
| H | -2.362607 | -1.321220 | 1.117533 |
| C | -0.027576 | -0.510672 | -0.243052 |
| C | 0.414743 | -0.978146 | 1.168564 |
| C | 1.183076 | -0.862073 | -1.160836 |
| C | 1.945274 | -0.987327 | 1.153358 |
| H | 0.055181 | -1.997392 | 1.334907 |
| H | 0.005576 | -0.360386 | 1.968297 |
| C | 2.282551 | -1.462569 | -0.263157 |
| H | 1.536494 | 0.019654 | -1.689688 |
| H | 0.879514 | -1.577653 | -1.925791 |
| H | 2.334027 | 0.017278 | 1.320784 |
| H | 2.366970 | -1.633239 | 1.923823 |
| H | 3.286542 | -1.177994 | -0.578987 |
| H | 2.228805 | -2.552637 | -0.295826 |
| H | -0.988476 | -2.377260 | -0.703060 |
| C | 0.670086 | 1.970427 | 0.304528 |
| H | 0.888560 | 1.681122 | 1.336185 |
| H | 0.182306 | 2.946208 | 0.373897 |
| C | 1.977315 | 2.176432 | -0.461272 |
| H | 1.783364 | 2.394348 | -1.513512 |
| H | 2.518370 | 3.027036 | -0.043401 |
| H | 2.642743 | 1.316273 | -0.415627 |

eq9

```

=====
C  -0.112736    -1.807333    -0.650123
H   0.199290    -1.811212    -1.699991
C   1.012971    -2.400807     0.188994
C   2.265160    -1.542960     0.043499
H   3.078941    -1.936536     0.655514
H   2.602077    -1.579352    -0.997522
C   0.799046     0.520718    -0.343723
C   1.975441    -0.094893     0.429424
H   2.870174     0.508518     0.272052
H   1.753336    -0.047901     1.501333
H   0.715510    -2.436528     1.241705
H   1.077596     0.547580    -1.406321
H   1.212066    -3.428505    -0.120402
C  -0.472977    -0.364668    -0.252893
C  -1.600929     0.139220    -1.199979
C  -1.118862    -0.333550     1.165468
C  -2.890337     0.122184    -0.371361
H  -1.670442    -0.482967    -2.092956
H  -1.399554     1.156282    -1.536884
C  -2.400875     0.494440     1.027758
H  -0.446817     0.053294     1.930767
H  -1.386437    -1.350612     1.462448
H  -3.655328     0.794162    -0.759940
H  -3.311279    -0.886417    -0.351150
H  -2.168754     1.561388     1.063303
H  -3.127245     0.283641     1.812733
H  -1.013987    -2.423462    -0.584965
C   0.569316     1.968851     0.112382
H  -0.330273     2.368258    -0.356499
H   0.384392     1.979364     1.190360
C   1.730868     2.908980    -0.207009
H   1.468609     3.940492     0.031035
H   2.628283     2.662446     0.359524
H   1.983318     2.866971    -1.268770

```



4-ethylspiro[2.5]oct-1-ene

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -390.560141 | -390.313124 | -390.358569 |
| ax2 | -390.559990 | -390.312881 | -390.358749 |
| ax3 | -390.554574 | -390.307289 | -390.353911 |
| eq1 | -390.561177 | -390.314249 | -390.359655 |
| eq2 | -390.559969 | -390.312873 | -390.357925 |

eq3 | -390.561793 | -390.314884 | -390.360496

ax1

```
=====
C 0.216376 0.862273 0.024098
C 0.381746 -0.482990 0.733901
H 0.971506 -0.303540 1.637861
C 1.291802 1.908283 0.089741
C -1.003105 -1.002548 1.154738
C -1.985739 -1.076023 -0.017588
H -2.964885 -1.395746 0.343736
H -1.655333 -1.832702 -0.733841
C -0.727317 0.784982 -1.168917
C -2.101921 0.272232 -0.729405
H -2.771010 0.191188 -1.588040
H -2.546320 1.001770 -0.044492
H 2.258751 2.219329 -0.267985
H -0.902819 -1.984051 1.624700
H -0.815619 1.770153 -1.629159
H -0.315652 0.109636 -1.926864
H -1.413672 -0.326769 1.911357
C 1.139548 -1.524278 -0.101972
H 1.239361 -2.429717 0.502777
H 0.553130 -1.807039 -0.978358
C 2.521404 -1.061733 -0.554198
H 3.072984 -1.878452 -1.021330
H 2.451878 -0.251384 -1.280194
H 3.110485 -0.700641 0.291914
C 0.262892 2.130246 0.837433
H -0.246907 2.755299 1.550941
```

ax2

```
=====
C 0.937019 -0.619628 -0.042491
C -0.497658 -0.473434 0.470749
H -0.640946 -1.214928 1.262556
C 1.551379 -1.984581 -0.166714
C -0.682364 0.921361 1.088860
C -0.305230 2.041102 0.118447
H -0.436475 3.010990 0.601486
H -0.974802 2.026987 -0.746744
C 1.358364 0.500941 -0.987555
C 1.139157 1.877460 -0.354643
H 1.401320 2.664308 -1.064271
H 1.808138 1.985066 0.505353
H 1.587968 -2.900304 -0.732204
H -1.706084 1.048817 1.444168
H 2.406625 0.367453 -1.258897
H 0.778354 0.440397 -1.914148
H -0.035102 0.992974 1.968684
C -1.515556 -0.793305 -0.633775
H -1.373552 -0.124187 -1.484778
```

| | | | |
|---|-----------|-----------|-----------|
| H | -1.303152 | -1.801955 | -0.998822 |
| C | -2.969186 | -0.722135 | -0.174906 |
| H | -3.640242 | -1.103617 | -0.945251 |
| H | -3.123351 | -1.317936 | 0.727521 |
| H | -3.273018 | 0.301405 | 0.046076 |
| C | 1.970526 | -1.279619 | 0.830994 |
| H | 2.605614 | -1.184444 | 1.695483 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.012435 | -0.109836 | -0.016324 |
| C | 0.046351 | 0.574945 | 0.864874 |
| H | -0.462122 | 0.814826 | 1.802579 |
| C | -2.313086 | 0.606817 | -0.249663 |
| C | 1.204173 | -0.373623 | 1.237722 |
| C | 1.696918 | -1.289361 | 0.115106 |
| H | 2.436039 | -1.983683 | 0.519596 |
| H | 2.198165 | -0.714390 | -0.666001 |
| C | -0.483797 | -1.066138 | -1.081278 |
| C | 0.531475 | -2.051451 | -0.506334 |
| H | 0.886346 | -2.725770 | -1.287716 |
| H | 0.049925 | -2.668665 | 0.259298 |
| H | -2.808399 | 1.409018 | -0.769963 |
| H | 2.033607 | 0.213629 | 1.640234 |
| H | -1.328174 | -1.595472 | -1.525802 |
| H | 0.000697 | -0.505354 | -1.886071 |
| H | 0.858466 | -1.019670 | 2.050428 |
| C | 0.499001 | 1.938724 | 0.317692 |
| H | -0.387990 | 2.575455 | 0.245834 |
| H | 1.144704 | 2.400806 | 1.069681 |
| C | 1.218793 | 1.958728 | -1.028000 |
| H | 1.470854 | 2.984564 | -1.301442 |
| H | 2.148586 | 1.391007 | -1.000432 |
| H | 0.595450 | 1.552617 | -1.824626 |
| C | -2.370002 | -0.378333 | 0.582132 |
| H | -2.940498 | -0.991744 | 1.258842 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.002915 | 0.812332 | -0.115453 |
| C | 0.377534 | -0.674258 | -0.206275 |
| H | 0.367601 | -0.950541 | -1.269102 |
| C | 1.022489 | 1.911759 | -0.051165 |
| C | -0.716565 | -1.496464 | 0.491179 |
| C | -2.105521 | -1.228680 | -0.086242 |
| H | -2.855824 | -1.811549 | 0.451347 |
| H | -2.127396 | -1.565244 | -1.127770 |
| C | -1.365464 | 1.085292 | -0.728431 |
| C | -2.450342 | 0.258130 | -0.037137 |
| H | -3.422041 | 0.439618 | -0.500258 |
| H | -2.528042 | 0.576611 | 1.007391 |
| H | 1.724946 | 2.513888 | -0.602113 |
| H | -0.478360 | -2.559608 | 0.412173 |
| H | -1.591474 | 2.150362 | -0.658075 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.343236 | 0.825270 | -1.792850 |
| H | -0.710268 | -1.247215 | 1.558694 |
| C | 1.755926 | -1.018369 | 0.356496 |
| H | 1.868264 | -0.557770 | 1.342603 |
| H | 1.799443 | -2.098173 | 0.517287 |
| C | 2.918034 | -0.613877 | -0.545350 |
| H | 3.873243 | -0.915912 | -0.113935 |
| H | 2.826763 | -1.092285 | -1.522389 |
| H | 2.955669 | 0.462945 | -0.708991 |
| C | 0.446147 | 1.631057 | 1.069730 |
| H | 0.329795 | 1.828065 | 2.121881 |

eq2

```
=====
```

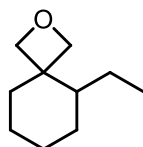
| | | | |
|---|-----------|-----------|-----------|
| C | -0.106589 | 0.925398 | -0.198880 |
| C | 0.367564 | -0.451634 | -0.679698 |
| H | 0.028181 | -0.534042 | -1.720399 |
| C | 0.766884 | 2.141189 | -0.329813 |
| C | -0.355699 | -1.552538 | 0.107613 |
| C | -1.874124 | -1.423279 | -0.005510 |
| H | -2.364114 | -2.207928 | 0.573972 |
| H | -2.170766 | -1.564575 | -1.049729 |
| C | -1.621279 | 1.062345 | -0.307196 |
| C | -2.339220 | -0.046241 | 0.465017 |
| H | -3.420349 | 0.051332 | 0.350144 |
| H | -2.119021 | 0.061490 | 1.531990 |
| H | 1.193109 | 2.871117 | -0.996968 |
| H | -0.029494 | -2.534608 | -0.245693 |
| H | -1.926496 | 2.044408 | 0.057347 |
| H | -1.911727 | 1.001629 | -1.362461 |
| H | -0.073719 | -1.483518 | 1.162763 |
| C | 1.888523 | -0.640923 | -0.698102 |
| H | 2.117109 | -1.475493 | -1.365407 |
| H | 2.346895 | 0.243073 | -1.149178 |
| C | 2.541124 | -0.917136 | 0.655449 |
| H | 3.626072 | -0.958860 | 0.551162 |
| H | 2.309317 | -0.146156 | 1.390532 |
| H | 2.214416 | -1.873056 | 1.065155 |
| C | 0.622494 | 1.690729 | 0.871853 |
| H | 0.842523 | 1.777732 | 1.922366 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.475183 | 0.907204 | -0.185600 |
| C | 0.596600 | -0.180394 | -0.332814 |
| H | 0.633559 | -0.455050 | -1.395963 |
| C | -0.128662 | 2.366348 | -0.261112 |
| C | 0.159888 | -1.428077 | 0.447781 |
| C | -1.224406 | -1.920110 | 0.024878 |
| H | -1.510727 | -2.789241 | 0.620078 |
| H | -1.180264 | -2.249996 | -1.018108 |
| C | -1.847059 | 0.421963 | -0.635330 |
| C | -2.272933 | -0.817646 | 0.152773 |
| H | -3.245115 | -1.174111 | -0.192790 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.386093 | -0.547427 | 1.207605 |
| H | 0.138832 | 3.192195 | -0.898458 |
| H | 0.887182 | -2.230185 | 0.313657 |
| H | -2.576628 | 1.224394 | -0.516115 |
| H | -1.809917 | 0.169285 | -1.701180 |
| H | 0.149252 | -1.180990 | 1.516057 |
| C | 1.988739 | 0.299147 | 0.072687 |
| H | 2.217397 | 1.215437 | -0.477752 |
| H | 1.978055 | 0.577889 | 1.131199 |
| C | 3.094166 | -0.722032 | -0.178603 |
| H | 4.075207 | -0.285301 | 0.010999 |
| H | 2.995266 | -1.595689 | 0.465218 |
| H | 3.077593 | -1.067253 | -1.214656 |
| C | -0.384732 | 1.921106 | 0.923821 |
| H | -0.482105 | 2.110985 | 1.979311 |



5-ethyl-2-oxaspiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -467.042000 | -466.762774 | -466.810698 |
| ax2 | -467.041067 | -466.761621 | -466.808373 |
| ax3 | -467.034823 | -466.755212 | -466.802624 |
| ax4 | -467.034952 | -466.755325 | -466.802987 |
| eq1 | -467.041523 | -466.762337 | -466.810453 |
| eq2 | -467.037987 | -466.758507 | -466.805661 |
| eq3 | -467.041524 | -466.762336 | -466.810444 |

ax1

| | | | |
|---|----------|-----------|----------|
| C | 0.594171 | -0.503805 | 0.473581 |
| H | 0.460570 | -1.242187 | 1.272131 |
| C | 1.196515 | 0.766212 | 1.091294 |
| C | 1.269562 | 1.915455 | 0.084553 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.678044 | 2.805055 | 0.566727 |
| H | 1.953212 | 1.656468 | -0.728666 |
| C | -0.755530 | 0.967603 | -1.092535 |
| C | -0.115734 | 2.218392 | -0.487927 |
| H | -0.057414 | 3.008789 | -1.237749 |
| H | -0.754907 | 2.592546 | 0.318189 |
| H | 0.562516 | 1.076943 | 1.928604 |
| H | -0.194482 | 0.656050 | -1.977870 |
| H | -1.774905 | 1.182500 | -1.423528 |
| H | 2.181843 | 0.556265 | 1.509148 |
| C | -0.791849 | -0.179912 | -0.084577 |
| C | -1.643839 | -1.371820 | -0.548956 |
| C | -1.915429 | -0.001009 | 0.955718 |
| H | -1.254936 | -2.345212 | -0.237776 |
| H | -1.916732 | -1.402750 | -1.605176 |
| H | -1.650852 | -0.338641 | 1.961483 |
| H | -2.392570 | 0.978596 | 1.008026 |
| C | 1.490183 | -1.152071 | -0.589908 |
| H | 1.655948 | -0.463233 | -1.419717 |
| H | 0.957085 | -2.010642 | -1.007993 |
| C | 2.838115 | -1.617493 | -0.046992 |
| H | 2.706263 | -2.262180 | 0.824557 |
| H | 3.387567 | -2.182415 | -0.800583 |
| H | 3.463447 | -0.775825 | 0.252066 |
| O | -2.750836 | -0.967430 | 0.284078 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.338659 | 0.677585 | 0.761643 |
| H | 0.207079 | 0.963979 | 1.667359 |
| C | -1.610446 | -0.079057 | 1.179301 |
| C | -2.365847 | -0.651596 | -0.023862 |
| H | -3.228640 | -1.223070 | 0.322601 |
| H | -2.758006 | 0.161686 | -0.638340 |
| C | -0.158038 | -0.834442 | -1.258138 |
| C | -1.459211 | -1.543735 | -0.873445 |
| H | -1.984297 | -1.874714 | -1.770773 |
| H | -1.216117 | -2.444224 | -0.301813 |
| H | -1.329923 | -0.904007 | 1.842455 |
| H | -0.368358 | -0.013344 | -1.949752 |
| H | 0.508537 | -1.526473 | -1.779044 |
| H | -2.260813 | 0.582930 | 1.754937 |
| C | 0.554434 | -0.286058 | -0.022950 |
| C | 2.020819 | 0.103439 | -0.288725 |
| C | 1.199768 | -1.416757 | 0.805658 |
| H | 2.377927 | 0.936567 | 0.320185 |
| H | 2.315615 | 0.248968 | -1.329401 |
| H | 1.195491 | -1.227902 | 1.883227 |
| H | 0.872140 | -2.437749 | 0.607708 |
| C | -0.693510 | 1.969931 | 0.013565 |
| H | -1.331343 | 2.563511 | 0.673981 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.297912 | 1.743439 | -0.865813 |
| C | 0.500213 | 2.816779 | -0.417695 |
| H | 1.090079 | 2.320574 | -1.189667 |
| H | 0.162946 | 3.768724 | -0.829404 |
| H | 1.159850 | 3.032904 | 0.424520 |
| O | 2.498575 | -1.151042 | 0.238114 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.388415 | 0.575529 | 0.829554 |
| H | 0.081492 | 0.988810 | 1.727126 |
| C | -1.238280 | -0.623136 | 1.284441 |
| C | -1.641109 | -1.581236 | 0.156647 |
| H | -2.131829 | -2.455028 | 0.589776 |
| H | -2.366912 | -1.111601 | -0.506501 |
| C | 0.336941 | -0.808981 | -1.197333 |
| C | -0.430818 | -2.018609 | -0.666466 |
| H | -0.745526 | -2.658383 | -1.492344 |
| H | 0.235351 | -2.618276 | -0.038384 |
| H | -0.652193 | -1.193548 | 2.012669 |
| H | -0.285858 | -0.247685 | -1.897854 |
| H | 1.224226 | -1.131062 | -1.748994 |
| H | -2.125598 | -0.264513 | 1.812096 |
| C | 0.771907 | 0.098635 | -0.049807 |
| C | 1.796452 | 1.164499 | -0.471454 |
| C | 1.978300 | -0.506526 | 0.702202 |
| H | 1.714904 | 2.103302 | 0.082614 |
| H | 1.885639 | 1.371385 | -1.539326 |
| H | 1.973891 | -0.317454 | 1.779155 |
| H | 2.210078 | -1.554881 | 0.511354 |
| C | -1.197349 | 1.752530 | 0.241638 |
| H | -0.497761 | 2.445912 | -0.232992 |
| H | -1.623317 | 2.296707 | 1.088325 |
| C | -2.343337 | 1.467964 | -0.729229 |
| H | -3.131960 | 0.884165 | -0.254550 |
| H | -2.786978 | 2.412334 | -1.048745 |
| H | -2.022234 | 0.937308 | -1.623952 |
| O | 2.897355 | 0.373562 | 0.022421 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.161107 | -0.784020 | 1.227424 |
| H | 1.010544 | -1.185288 | 1.786903 |
| C | -0.790760 | -1.908219 | 0.823220 |
| C | -1.935057 | -1.365317 | -0.029802 |
| H | -2.592648 | -2.179300 | -0.340416 |
| H | -2.542124 | -0.678532 | 0.564382 |
| C | -0.387624 | 0.475055 | -0.948647 |
| C | -1.380744 | -0.655622 | -1.264450 |
| H | -2.191320 | -0.262079 | -1.881102 |
| H | -0.859081 | -1.403955 | -1.871549 |
| H | -0.243256 | -2.659782 | 0.245035 |
| H | 0.120184 | 0.701533 | -1.891041 |
| H | -1.174301 | -2.409512 | 1.713141 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.699628 | -0.030070 | 0.008383 |
| C | 1.818633 | 0.963563 | 0.363712 |
| C | 1.847291 | -0.817123 | -0.661821 |
| H | 1.929010 | 1.216847 | 1.419608 |
| H | 1.820541 | 1.875851 | -0.238181 |
| H | 1.981024 | -1.853717 | -0.348874 |
| H | 1.859666 | -0.755419 | -1.752988 |
| C | -1.046608 | 1.810658 | -0.538765 |
| H | -0.364586 | 2.615130 | -0.823494 |
| H | -1.934995 | 1.940601 | -1.162134 |
| H | -0.359279 | -0.096609 | 1.894642 |
| C | -1.425722 | 2.042045 | 0.923790 |
| H | -0.545550 | 2.042624 | 1.568114 |
| H | -1.900461 | 3.019348 | 1.024385 |
| H | -2.121885 | 1.296987 | 1.305520 |
| O | 2.843456 | 0.048698 | -0.078778 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.548520 | 0.534349 | -0.283683 |
| H | 0.607031 | 0.832166 | -1.338972 |
| C | -0.066934 | 1.696449 | 0.507272 |
| C | -1.470516 | 2.057452 | 0.028104 |
| H | -1.876445 | 2.870618 | 0.632272 |
| H | -1.419431 | 2.418884 | -1.003766 |
| C | -1.790540 | -0.315571 | -0.714372 |
| C | -2.385815 | 0.838049 | 0.088060 |
| H | -3.381646 | 1.082127 | -0.284889 |
| H | -2.502057 | 0.527329 | 1.131941 |
| H | -0.114427 | 1.403902 | 1.562902 |
| H | -1.733217 | -0.031367 | -1.770733 |
| H | -2.433220 | -1.196794 | -0.654408 |
| H | 0.585150 | 2.569236 | 0.452849 |
| C | -0.391419 | -0.682247 | -0.234018 |
| C | 0.177480 | -1.970245 | -0.850981 |
| C | -0.329951 | -1.485452 | 1.081884 |
| H | 1.098092 | -1.885564 | -1.429913 |
| H | -0.557856 | -2.543962 | -1.420649 |
| H | 0.228039 | -1.050521 | 1.911309 |
| H | -1.304544 | -1.829543 | 1.437859 |
| C | 1.975845 | 0.245717 | 0.202785 |
| H | 2.298113 | -0.741657 | -0.130729 |
| H | 1.982198 | 0.218632 | 1.295585 |
| C | 2.990697 | 1.278419 | -0.282230 |
| H | 2.742054 | 2.284150 | 0.057450 |
| H | 3.990495 | 1.045387 | 0.085489 |
| H | 3.032166 | 1.295404 | -1.372915 |
| O | 0.401912 | -2.556244 | 0.447798 |

eq2

```
=====
```

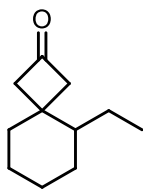
| | | | |
|---|-----------|----------|-----------|
| C | -0.040342 | 0.748398 | 0.669426 |
| H | 0.343334 | 0.778174 | 1.697089 |
| C | 0.929091 | 1.569026 | -0.189999 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.364832 | 1.062317 | -0.061454 |
| H | 3.029906 | 1.643341 | -0.702727 |
| H | 2.705581 | 1.206126 | 0.968588 |
| C | 1.469452 | -1.238492 | 0.426383 |
| C | 2.449462 | -0.421335 | -0.414257 |
| H | 3.466186 | -0.791986 | -0.275436 |
| H | 2.204432 | -0.552368 | -1.473797 |
| H | 0.624944 | 1.510685 | -1.239688 |
| H | 1.748689 | -1.172180 | 1.482954 |
| H | 1.514969 | -2.293020 | 0.145594 |
| H | 0.868810 | 2.621478 | 0.097695 |
| C | 0.041593 | -0.732091 | 0.256432 |
| C | -1.064087 | -1.637638 | 0.822563 |
| C | -0.611154 | -1.083931 | -1.095162 |
| H | -1.677923 | -1.252666 | 1.636022 |
| H | -0.709329 | -2.640626 | 1.074950 |
| H | -0.867816 | -0.271639 | -1.772809 |
| H | -0.066110 | -1.857261 | -1.644248 |
| C | -1.434591 | 1.396762 | 0.742087 |
| H | -1.289280 | 2.360585 | 1.237362 |
| H | -2.073900 | 0.815535 | 1.408933 |
| C | -2.187286 | 1.647876 | -0.565703 |
| H | -2.561326 | 0.724131 | -1.002627 |
| H | -3.048642 | 2.289044 | -0.372829 |
| H | -1.564817 | 2.154200 | -1.304658 |
| O | -1.768691 | -1.642112 | -0.437784 |

eq3

| | | | |
|---|-----------|-----------|-----------|
| C | 0.548349 | 0.534657 | -0.283556 |
| H | 0.606936 | 0.832404 | -1.338857 |
| C | -0.067640 | 1.696590 | 0.507233 |
| C | -1.471360 | 2.056961 | 0.027996 |
| H | -1.877645 | 2.869998 | 0.632099 |
| H | -1.420429 | 2.418331 | -1.003903 |
| C | -1.790361 | -0.316229 | -0.714377 |
| C | -2.386105 | 0.837152 | 0.088050 |
| H | -3.382071 | 1.080759 | -0.284850 |
| H | -2.502136 | 0.526410 | 1.131947 |
| H | -0.115060 | 1.404138 | 1.562892 |
| H | -1.733141 | -0.032002 | -1.770736 |
| H | -2.432679 | -1.197719 | -0.654423 |
| H | 0.584126 | 2.569616 | 0.452744 |
| C | -0.391085 | -0.682321 | -0.233986 |
| C | 0.178330 | -1.970037 | -0.851048 |
| C | -0.329365 | -1.485560 | 1.081858 |
| H | 1.099092 | -1.885016 | -1.429708 |
| H | -0.556676 | -2.543851 | -1.421042 |
| H | 0.228703 | -1.050539 | 1.911189 |
| H | -1.303843 | -1.829783 | 1.438016 |
| C | 1.975673 | 0.246572 | 0.203258 |
| H | 2.298080 | -0.741049 | -0.129416 |

| | | | |
|---|----------|-----------|-----------|
| H | 1.981910 | 0.220297 | 1.296077 |
| C | 2.990369 | 1.279071 | -0.282465 |
| H | 2.741068 | 2.285085 | 0.055908 |
| H | 3.990088 | 1.046929 | 0.086026 |
| H | 3.032347 | 1.294788 | -1.373146 |
| O | 0.402563 | -2.556241 | 0.447675 |



5-ethylspiro[3.5]nonan-2-one

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -505.163865 | -504.879934 | -504.92966 |
| ax2 | -505.161644 | -504.87772 | -504.927125 |
| ax3 | -505.156695 | -504.872499 | -504.922124 |
| ax4 | -505.156544 | -504.872386 | -504.921807 |
| ax5 | -505.155565 | -504.872502 | -504.920387 |
| eq1 | -505.162680 | -504.878904 | -504.929138 |
| eq2 | -505.160052 | -504.876099 | -504.925374 |
| eq3 | -505.160310 | -504.876411 | -504.925573 |
| eq4 | -505.163504 | -504.879786 | -504.929608 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.795861 | -0.553954 | 0.486447 |
| H | 0.555002 | -1.257196 | 1.291973 |
| C | 1.561918 | 0.628463 | 1.096589 |
| C | 1.809621 | 1.737883 | 0.073365 |
| H | 2.339583 | 2.566915 | 0.545116 |
| H | 2.454345 | 1.367717 | -0.728657 |
| C | -0.326467 | 1.075823 | -1.104111 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.487463 | 2.229758 | -0.517086 |
| H | 0.666765 | 2.984981 | -1.283921 |
| H | -0.092903 | 2.713884 | 0.274208 |
| H | 0.968492 | 1.038498 | 1.919966 |
| H | 0.183901 | 0.675799 | -1.984185 |
| H | -1.301404 | 1.436015 | -1.445983 |
| H | 2.502336 | 0.287656 | 1.531098 |
| C | -0.531770 | -0.049667 | -0.087576 |
| C | -1.501314 | -1.144692 | -0.625337 |
| C | -1.602401 | 0.350631 | 0.980630 |
| H | -1.279125 | -2.131332 | -0.211157 |
| H | -1.660345 | -1.220139 | -1.700397 |
| H | -1.412541 | -0.108407 | 1.953635 |
| H | -1.845921 | 1.404166 | 1.109943 |
| C | 1.609360 | -1.331720 | -0.556792 |
| H | 1.834225 | -0.697830 | -1.416195 |
| H | 0.988430 | -2.148238 | -0.933610 |
| C | 2.910511 | -1.909423 | -0.006809 |
| H | 2.728877 | -2.482693 | 0.904957 |
| H | 3.377358 | -2.575740 | -0.732724 |
| H | 3.630889 | -1.126028 | 0.229981 |
| C | -2.594005 | -0.476812 | 0.185921 |
| O | -3.793828 | -0.508221 | 0.140563 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.867103 | 0.493086 | 0.746838 |
| H | -0.503075 | 0.988005 | 1.654315 |
| C | -1.714525 | -0.721436 | 1.162209 |
| C | -2.148364 | -1.562168 | -0.042234 |
| H | -2.708249 | -2.434031 | 0.300343 |
| H | -2.827167 | -0.984356 | -0.673526 |
| C | -0.037917 | -0.834632 | -1.243121 |
| C | -0.940868 | -2.011638 | -0.866732 |
| H | -1.268772 | -2.531646 | -1.768203 |
| H | -0.362685 | -2.732389 | -0.281683 |
| H | -1.128063 | -1.351336 | 1.837918 |
| H | -0.551206 | -0.181938 | -1.955174 |
| H | 0.862113 | -1.199696 | -1.746854 |
| H | -2.589179 | -0.383664 | 1.721837 |
| C | 0.362783 | -0.016069 | -0.014371 |
| C | 1.496523 | 1.005536 | -0.345712 |
| C | 1.380703 | -0.812477 | 0.870433 |
| H | 1.472611 | 1.876423 | 0.312212 |
| H | 1.630736 | 1.322305 | -1.378986 |
| H | 1.307245 | -0.536099 | 1.925111 |
| H | 1.434187 | -1.895453 | 0.774555 |
| C | -1.731592 | 1.511660 | -0.011461 |
| H | -2.598722 | 1.723523 | 0.620013 |
| H | -2.128125 | 1.065622 | -0.924604 |
| C | -1.050623 | 2.831772 | -0.363592 |
| H | -0.301669 | 2.709533 | -1.144937 |
| H | -1.786290 | 3.550292 | -0.727243 |
| H | -0.559843 | 3.270279 | 0.507558 |

| | | | |
|---|----------|-----------|----------|
| C | 2.476666 | -0.013145 | 0.196721 |
| O | 3.656507 | -0.187289 | 0.051685 |

ax3

```
=====
C -0.698630    0.555031    0.858041
H -0.256265    0.924553    1.788489
C -1.600524   -0.633378    1.235615
C -1.976479   -1.545454    0.061846
H -2.522165   -2.410611    0.443376
H -2.646891   -1.030607   -0.625909
C  0.090778   -0.810472   -1.166786
C -0.740089   -2.006172   -0.706880
H -1.032107   -2.612335   -1.565826
H -0.129631   -2.644922   -0.061826
H -1.068007   -1.241758    1.973625
H -0.476271   -0.221052   -1.890408
H  0.994453   -1.151657   -1.681343
H -2.501891   -0.262702    1.730197
C  0.491536    0.073963    0.014701
C  1.512712    1.171120   -0.411053
C  1.626904   -0.629479    0.836940
H  1.464813    2.049304    0.237566
H  1.546516    1.480429   -1.454992
H  1.607598   -0.353640    1.893428
H  1.760832   -1.705125    0.736361
C -1.458337    1.772522    0.292050
H -0.723377    2.498662   -0.063421
H -1.958472    2.249284    1.139181
C -2.512432    1.565990   -0.795371
H -3.346434    0.964764   -0.434173
H -2.917044    2.534638   -1.093333
H -2.113481    1.089223   -1.689365
C  2.606156    0.243791    0.078094
O  3.783532    0.162347   -0.145600
```

ax4

```
=====
C -0.479348   -0.823662    1.325671
H  0.164900   -1.341687    2.040703
C -1.483878   -1.797285    0.713672
C -2.340474   -1.096138   -0.338553
H -3.033252   -1.805365   -0.795228
H -2.948403   -0.325122    0.139750
C -0.383713    0.487279   -0.885400
C -1.453437   -0.481032   -1.420704
H -2.059277    0.033865   -2.168817
H -0.945632   -1.300163   -1.939772
H -0.944921   -2.624969    0.240554
H  0.329139    0.629910   -1.705340
H -2.109632   -2.230076    1.495712
C  0.405196   -0.181362    0.258450
C  1.559812    0.715959    0.802921
C  1.473097   -1.170207   -0.324463
```

| | | | |
|---|-----------|-----------|-----------|
| H | 1.748084 | 0.546315 | 1.865664 |
| H | 1.535546 | 1.785478 | 0.601554 |
| H | 1.633304 | -2.040847 | 0.315410 |
| H | 1.376300 | -1.487942 | -1.361743 |
| C | -0.913298 | 1.908487 | -0.590121 |
| H | -0.082031 | 2.606359 | -0.710943 |
| H | -1.623346 | 2.158803 | -1.382383 |
| H | -1.017324 | -0.056763 | 1.883426 |
| C | -1.557402 | 2.203626 | 0.764048 |
| H | -0.845124 | 2.079250 | 1.580437 |
| H | -1.896899 | 3.240444 | 0.784596 |
| H | -2.419415 | 1.571401 | 0.970335 |
| C | 2.513461 | -0.104020 | -0.043346 |
| O | 3.637236 | 0.073906 | -0.428371 |

ax5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.227345 | -0.925794 | 1.284018 |
| H | 0.513183 | -1.398063 | 1.934795 |
| C | -1.091919 | -1.988198 | 0.607239 |
| C | -2.098656 | -1.349789 | -0.348043 |
| H | -2.648828 | -2.127125 | -0.881965 |
| H | -2.831508 | -0.794130 | 0.235798 |
| C | -0.458383 | 0.606476 | -0.752538 |
| C | -1.411194 | -0.434125 | -1.368648 |
| H | -2.159533 | 0.076637 | -1.979685 |
| H | -0.834449 | -1.066777 | -2.049582 |
| H | -0.442792 | -2.669831 | 0.048425 |
| H | 0.182918 | 0.967133 | -1.564444 |
| H | -1.610178 | -2.588376 | 1.356729 |
| C | 0.497244 | -0.081801 | 0.241221 |
| C | 1.602132 | 0.862604 | 0.810140 |
| C | 1.602389 | -0.900622 | -0.514031 |
| H | 1.802542 | 0.721710 | 1.874031 |
| H | 1.518207 | 1.927573 | 0.598264 |
| H | 1.811725 | -1.876661 | -0.071406 |
| H | 1.500794 | -1.007921 | -1.593998 |
| C | -1.174947 | 1.874584 | -0.239256 |
| H | -0.466293 | 2.470845 | 0.338199 |
| H | -1.411742 | 2.474071 | -1.122080 |
| H | -0.844551 | -0.285954 | 1.918973 |
| C | -2.467581 | 1.739374 | 0.566250 |
| H | -2.343621 | 1.159846 | 1.479564 |
| H | -2.815296 | 2.732996 | 0.853654 |
| H | -3.259898 | 1.277863 | -0.022776 |
| C | 2.607047 | 0.138497 | -0.062605 |
| O | 3.758325 | 0.344866 | -0.336872 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.982077 | -0.405182 | 0.249960 |
| H | -1.330542 | -0.393493 | 1.291118 |
| C | -1.900213 | 0.512387 | -0.569128 |
| C | -1.898100 | 1.953029 | -0.066253 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.553123 | 2.569038 | -0.684716 |
| H | -2.297422 | 1.982186 | 0.952392 |
| C | 0.446262 | 1.618924 | 0.750156 |
| C | -0.478945 | 2.513700 | -0.067628 |
| H | -0.463019 | 3.529445 | 0.330667 |
| H | -0.115962 | 2.570025 | -1.098552 |
| H | -1.555338 | 0.496551 | -1.609779 |
| H | 0.127050 | 1.630982 | 1.797571 |
| H | 1.470184 | 2.003806 | 0.727538 |
| H | -2.915916 | 0.113812 | -0.568327 |
| C | 0.443679 | 0.165081 | 0.268791 |
| C | 1.527928 | -0.639825 | 1.049569 |
| C | 1.279882 | 0.002286 | -1.043049 |
| H | 1.275657 | -1.684899 | 1.230624 |
| H | 1.908175 | -0.193778 | 1.968287 |
| H | 0.919710 | -0.799748 | -1.690136 |
| H | 1.482862 | 0.890605 | -1.640006 |
| C | -1.083030 | -1.847892 | -0.264979 |
| H | -0.215709 | -2.431244 | 0.048065 |
| H | -1.068408 | -1.838033 | -1.358036 |
| C | -2.344229 | -2.561439 | 0.216483 |
| H | -3.248412 | -2.032172 | -0.085842 |
| H | -2.402279 | -3.571662 | -0.189850 |
| H | -2.351050 | -2.638371 | 1.305181 |
| C | 2.417035 | -0.495923 | -0.171689 |
| O | 3.595549 | -0.636742 | -0.354949 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.428739 | 0.777680 | 0.676315 |
| H | 0.846195 | 0.705181 | 1.688327 |
| C | 1.547861 | 1.300496 | -0.231219 |
| C | 2.794754 | 0.421101 | -0.158320 |
| H | 3.565234 | 0.801418 | -0.831182 |
| H | 3.205247 | 0.461053 | 0.855420 |
| C | 1.330323 | -1.546270 | 0.389610 |
| C | 2.453604 | -1.026885 | -0.504244 |
| H | 3.335086 | -1.662833 | -0.408416 |
| H | 2.133140 | -1.081054 | -1.549922 |
| H | 1.194943 | 1.327931 | -1.266441 |
| H | 1.669955 | -1.561667 | 1.430543 |
| H | 1.069762 | -2.572610 | 0.120253 |
| H | 1.788702 | 2.329653 | 0.046924 |
| C | 0.080981 | -0.674695 | 0.295017 |
| C | -1.156473 | -1.243080 | 1.053420 |
| C | -0.701605 | -0.826757 | -1.051661 |
| H | -1.500524 | -0.753039 | 1.962051 |
| H | -1.053689 | -2.316563 | 1.227942 |
| H | -0.689218 | -0.024642 | -1.785260 |
| H | -0.454958 | -1.772607 | -1.540744 |
| C | -0.732682 | 1.784281 | 0.791078 |
| H | -0.331039 | 2.642705 | 1.335265 |
| H | -1.516979 | 1.373428 | 1.430303 |
| C | -1.364841 | 2.313622 | -0.498544 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.966013 | 1.567249 | -1.014181 |
| H | -2.026619 | 3.147648 | -0.261182 |
| H | -0.612668 | 2.683864 | -1.195683 |
| C | -1.954363 | -0.999938 | -0.213643 |
| O | -3.126793 | -0.871557 | -0.441358 |

eq3

```
=====
```

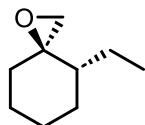
| | | | |
|---|-----------|-----------|-----------|
| C | 0.357898 | 0.982986 | 0.223810 |
| H | 0.562171 | 1.323483 | 1.246951 |
| C | 1.608139 | 1.266475 | -0.624240 |
| C | 2.852903 | 0.536210 | -0.129373 |
| H | 3.698661 | 0.751529 | -0.784643 |
| H | 3.115930 | 0.907538 | 0.866091 |
| C | 1.382587 | -1.249180 | 0.818463 |
| C | 2.601881 | -0.965865 | -0.051112 |
| H | 3.476474 | -1.484562 | 0.344639 |
| H | 2.425574 | -1.357254 | -1.058496 |
| H | 1.401937 | 0.969454 | -1.658988 |
| H | 1.580284 | -0.913788 | 1.842370 |
| H | 1.184270 | -2.322579 | 0.865476 |
| H | 1.787730 | 2.343152 | -0.638738 |
| C | 0.129925 | -0.541108 | 0.308901 |
| C | -1.164134 | -0.966553 | 1.068656 |
| C | -0.469763 | -1.147321 | -1.003300 |
| H | -1.635556 | -0.283449 | 1.769730 |
| H | -1.021286 | -1.939616 | 1.545533 |
| H | -0.417848 | -0.581465 | -1.931472 |
| H | -0.114238 | -2.166135 | -1.172381 |
| C | -0.804310 | 1.831717 | -0.324153 |
| H | -1.134036 | 1.433209 | -1.287632 |
| H | -0.380426 | 2.813401 | -0.546932 |
| C | -2.014938 | 2.055446 | 0.585173 |
| H | -1.700414 | 2.280162 | 1.606241 |
| H | -2.594620 | 2.906079 | 0.224432 |
| H | -2.689209 | 1.202449 | 0.619022 |
| C | -1.808403 | -1.169989 | -0.288741 |
| O | -2.947014 | -1.209814 | -0.669463 |

eq4

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```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.906809 | -1.705620 | 0.702826 |
| H | -1.221310 | -1.524696 | 1.736308 |
| C | -2.124067 | -1.648842 | -0.214609 |
| C | -2.741518 | -0.253836 | -0.191586 |
| H | -3.589254 | -0.198828 | -0.876674 |
| H | -3.127838 | -0.050431 | 0.812144 |
| C | -0.464078 | 0.753956 | 0.344993 |
| C | -1.705774 | 0.808537 | -0.553958 |
| H | -2.160211 | 1.797803 | -0.495972 |
| H | -1.388697 | 0.666757 | -1.593711 |
| H | -1.816019 | -1.891438 | -1.237039 |
| H | -0.787932 | 0.930723 | 1.379227 |
| H | -2.857172 | -2.399811 | 0.084126 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.140275 | -0.664083 | 0.322672 |
| C | 1.473748 | -0.790213 | 1.121925 |
| C | 0.921723 | -0.985499 | -0.995463 |
| H | 1.572160 | -1.779878 | 1.573560 |
| H | 1.734689 | -0.026351 | 1.852078 |
| H | 0.832794 | -2.038779 | -1.271196 |
| H | 0.769256 | -0.363632 | -1.875612 |
| C | 0.535452 | 1.860139 | -0.019545 |
| H | 1.445677 | 1.743207 | 0.571325 |
| H | 0.828185 | 1.757840 | -1.068113 |
| H | -0.449565 | -2.697561 | 0.674929 |
| C | -0.002794 | 3.270293 | 0.214501 |
| H | 0.781256 | 4.011497 | 0.057491 |
| H | -0.822378 | 3.513387 | -0.460756 |
| H | -0.366608 | 3.381396 | 1.238053 |
| C | 2.199223 | -0.753786 | -0.210100 |
| O | 3.333835 | -0.522185 | -0.528763 |



(3*R*,4*R*)-4-ethyl-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -427.741060 | -427.492321 | -427.537918 |
| ax2 | -427.735432 | -427.486553 | -427.531844 |
| ax3 | -427.741610 | -427.49292 | -427.537987 |
| eq1 | -427.741774 | -427.493055 | -427.538418 |
| eq2 | -427.739621 | -427.49096 | -427.536362 |
| eq3 | -427.738991 | -427.490151 | -427.534849 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.850437 | -0.630842 | -0.082383 |
| C | -0.560172 | -0.443937 | 0.440799 |
| H | -0.717205 | -1.198585 | 1.216794 |
| C | 1.443573 | -1.968212 | -0.113008 |
| C | -0.665797 | 0.948523 | 1.081574 |
| C | -0.230418 | 2.059016 | 0.123395 |
| H | -0.305078 | 3.026378 | 0.622325 |
| H | -0.902793 | 2.095487 | -0.738440 |
| C | 1.350417 | 0.450193 | -1.010858 |
| C | 1.203204 | 1.826506 | -0.356641 |
| H | 1.505946 | 2.605493 | -1.057448 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.879119 | 1.884997 | 0.501391 |
| H | 2.231039 | -2.187773 | -0.824859 |
| H | 0.859397 | -2.816005 | 0.227405 |
| H | -1.680399 | 1.122763 | 1.441007 |
| H | 2.390885 | 0.245757 | -1.265556 |
| H | 0.771512 | 0.419291 | -1.937368 |
| H | -0.012957 | 0.970121 | 1.958959 |
| O | 1.802016 | -1.035801 | 0.911811 |
| C | -1.587652 | -0.697540 | -0.670296 |
| H | -1.400637 | -1.693640 | -1.079879 |
| H | -1.438858 | 0.005214 | -1.492219 |
| C | -3.033002 | -0.612498 | -0.189775 |
| H | -3.304722 | 0.405007 | 0.091729 |
| H | -3.720739 | -0.930564 | -0.973669 |
| H | -3.194172 | -1.254790 | 0.678498 |

ax2

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.942217 | 0.338467 | -0.103108 |
| C | 0.266614 | 0.623871 | 0.773744 |
| H | -0.139224 | 1.159850 | 1.634917 |
| C | -1.966780 | 1.373605 | -0.250438 |
| C | 0.873994 | -0.691988 | 1.295691 |
| C | 1.002688 | -1.798445 | 0.242153 |
| H | 1.337429 | -2.715632 | 0.729939 |
| H | 1.760281 | -1.540410 | -0.498935 |
| C | -0.812586 | -0.751850 | -1.137973 |
| C | -0.323929 | -2.039940 | -0.475451 |
| H | -0.216723 | -2.828407 | -1.221307 |
| H | -1.074670 | -2.376650 | 0.245510 |
| H | -2.593986 | 1.382673 | -1.134632 |
| H | -1.831940 | 2.328425 | 0.245869 |
| H | 1.845719 | -0.485661 | 1.750688 |
| H | -1.781955 | -0.896215 | -1.616567 |
| H | -0.104953 | -0.443334 | -1.910210 |
| H | 0.227936 | -1.068558 | 2.093639 |
| O | -2.179684 | 0.266303 | 0.627892 |
| C | 1.282792 | 1.591932 | 0.138641 |
| H | 1.871953 | 2.012127 | 0.957421 |
| H | 0.726146 | 2.427042 | -0.294600 |
| C | 2.260066 | 1.047050 | -0.900665 |
| H | 1.757746 | 0.604932 | -1.760084 |
| H | 2.888797 | 1.858543 | -1.269952 |
| H | 2.921065 | 0.294645 | -0.470393 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.175922 | 0.812855 | -0.004610 |
| C | -0.417276 | -0.507769 | -0.708804 |
| H | -1.002441 | -0.288439 | -1.606409 |
| C | -1.138482 | 1.908049 | -0.129164 |
| C | 0.940675 | -1.091234 | -1.130998 |
| C | 1.925302 | -1.191209 | 0.038063 |
| H | 2.884608 | -1.564583 | -0.323735 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.563526 | -1.915292 | 0.772406 |
| C | 0.774093 | 0.752205 | 1.166537 |
| C | 2.115290 | 0.166545 | 0.716219 |
| H | 2.790188 | 0.077606 | 1.568389 |
| H | 2.579772 | 0.859004 | 0.008330 |
| H | -1.192356 | 2.661027 | 0.649245 |
| H | -2.041684 | 1.759564 | -0.709969 |
| H | 0.789810 | -2.071606 | -1.587603 |
| H | 0.901795 | 1.754239 | 1.577311 |
| H | 0.338490 | 0.125344 | 1.949447 |
| H | 1.374656 | -0.443083 | -1.897416 |
| O | 0.070189 | 1.914392 | -0.892559 |
| C | -1.223136 | -1.490867 | 0.149720 |
| H | -0.650758 | -1.772968 | 1.035201 |
| H | -1.356231 | -2.405223 | -0.433412 |
| C | -2.587354 | -0.960495 | 0.580669 |
| H | -3.172168 | -0.637075 | -0.282709 |
| H | -3.156055 | -1.732744 | 1.099425 |
| H | -2.491805 | -0.109391 | 1.256187 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.453725 | 0.843417 | -0.134501 |
| C | 0.612599 | -0.232357 | -0.255619 |
| H | 0.678503 | -0.476234 | -1.324087 |
| C | -0.358145 | 1.907703 | 0.871880 |
| C | 0.122330 | -1.485420 | 0.485236 |
| C | -1.249737 | -1.950837 | 0.000667 |
| H | -1.566956 | -2.829023 | 0.565204 |
| H | -1.177697 | -2.253042 | -1.048578 |
| C | -1.819926 | 0.416253 | -0.614627 |
| C | -2.284104 | -0.834776 | 0.131329 |
| H | -3.252492 | -1.159779 | -0.250813 |
| H | -2.419719 | -0.591141 | 1.189449 |
| H | 0.502876 | 1.966680 | 1.526046 |
| H | -1.269557 | 2.359070 | 1.247011 |
| H | 0.852088 | -2.287826 | 0.371326 |
| H | -2.521983 | 1.240372 | -0.483915 |
| H | -1.757017 | 0.199316 | -1.685644 |
| H | 0.067694 | -1.251372 | 1.554220 |
| O | -0.081325 | 2.169607 | -0.508032 |
| C | 1.998282 | 0.209813 | 0.217032 |
| H | 2.183232 | 1.228959 | -0.127015 |
| H | 2.014097 | 0.234576 | 1.309769 |
| C | 3.115715 | -0.698621 | -0.287786 |
| H | 4.088904 | -0.344654 | 0.053444 |
| H | 2.996501 | -1.723348 | 0.065170 |
| H | 3.132396 | -0.720460 | -1.378996 |

eq2

```
=====
```

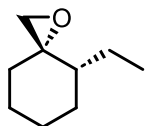
| | | | |
|---|-----------|-----------|-----------|
| C | -0.011629 | 0.753581 | -0.073756 |
| C | 0.336972 | -0.713724 | -0.266198 |
| H | 0.316162 | -0.896067 | -1.348345 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.603415 | 1.563678 | 0.985638 |
| C | -0.774801 | -1.560500 | 0.377466 |
| C | -2.171514 | -1.205093 | -0.125262 |
| H | -2.916893 | -1.822962 | 0.377931 |
| H | -2.238613 | -1.427492 | -1.194569 |
| C | -1.390582 | 1.132676 | -0.563460 |
| C | -2.466972 | 0.275280 | 0.098597 |
| H | -3.449345 | 0.538362 | -0.295281 |
| H | -2.482705 | 0.482749 | 1.172867 |
| H | 1.370135 | 1.140458 | 1.623364 |
| H | 0.045103 | 2.392872 | 1.405272 |
| H | -0.562997 | -2.615317 | 0.193826 |
| H | -1.554201 | 2.194116 | -0.374519 |
| H | -1.421666 | 0.980804 | -1.647213 |
| H | -0.734896 | -1.412003 | 1.462313 |
| O | 0.987490 | 1.726367 | -0.382279 |
| C | 1.697401 | -1.172330 | 0.267735 |
| H | 1.730607 | -1.019275 | 1.349559 |
| H | 1.735724 | -2.254489 | 0.120264 |
| C | 2.930949 | -0.553827 | -0.386086 |
| H | 3.829209 | -1.091992 | -0.080117 |
| H | 2.862432 | -0.612751 | -1.474192 |
| H | 3.052589 | 0.493601 | -0.120966 |

eq3

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```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.190444 | 0.886156 | -0.129997 |
| C | 0.422878 | -0.395773 | -0.673053 |
| H | 0.126011 | -0.420014 | -1.728381 |
| C | 0.512782 | 1.761243 | 0.818297 |
| C | -0.225798 | -1.609611 | 0.007550 |
| C | -1.749041 | -1.588302 | -0.092448 |
| H | -2.167999 | -2.461120 | 0.410700 |
| H | -2.048487 | -1.647268 | -1.143281 |
| C | -1.701345 | 0.916710 | -0.171864 |
| C | -2.306057 | -0.304465 | 0.518195 |
| H | -3.393198 | -0.276146 | 0.436102 |
| H | -2.061989 | -0.277113 | 1.584530 |
| H | 1.515406 | 1.524557 | 1.149047 |
| H | -0.070461 | 2.383374 | 1.487907 |
| H | 0.176829 | -2.523069 | -0.436034 |
| H | -2.054922 | 1.845433 | 0.277136 |
| H | -2.006203 | 0.922062 | -1.223341 |
| H | 0.053133 | -1.620378 | 1.064837 |
| O | 0.412508 | 2.106569 | -0.565042 |
| C | 1.958787 | -0.439573 | -0.626537 |
| H | 2.301560 | -1.073851 | -1.446505 |
| H | 2.341124 | 0.561071 | -0.837415 |
| C | 2.573056 | -0.969682 | 0.670078 |
| H | 3.654494 | -0.829415 | 0.657198 |
| H | 2.183367 | -0.464869 | 1.554300 |
| H | 2.382364 | -2.036034 | 0.792217 |



(3S,4R)-4-ethyl-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -427.741110 | -427.492322 | -427.537947 |
| ax2 | -427.735097 | -427.486073 | -427.531085 |
| ax3 | -427.740658 | -427.491924 | -427.537044 |
| eq1 | -427.740491 | -427.491688 | -427.536939 |
| eq2 | -427.740098 | -427.491317 | -427.536115 |
| eq3 | -427.738616 | -427.489819 | -427.534877 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.859979 | -0.607074 | -0.020570 |
| C | -0.559783 | -0.406166 | 0.470496 |
| H | -0.747051 | -1.148469 | 1.251823 |
| C | 1.818651 | -1.328294 | 0.822896 |
| C | -0.656584 | 0.997282 | 1.090396 |
| C | -0.192719 | 2.090278 | 0.125087 |
| H | -0.253130 | 3.063063 | 0.615290 |
| H | -0.859313 | 2.131512 | -0.740533 |
| C | 1.369076 | 0.441781 | -0.979339 |
| C | 1.238803 | 1.830507 | -0.347034 |
| H | 1.553118 | 2.594347 | -1.059109 |
| H | 1.913797 | 1.893176 | 0.512062 |
| H | 1.495229 | -1.725081 | 1.778299 |
| H | 2.877712 | -1.117872 | 0.726849 |
| H | -1.675357 | 1.189282 | 1.428299 |
| H | 2.405584 | 0.221498 | -1.236765 |
| H | 0.784741 | 0.400890 | -1.902402 |
| H | -0.019227 | 1.024081 | 1.979456 |
| O | 1.224095 | -1.954685 | -0.319805 |
| C | -1.571161 | -0.658889 | -0.655063 |
| H | -1.361125 | -1.644230 | -1.077621 |
| H | -1.429019 | 0.061192 | -1.462827 |
| C | -3.021257 | -0.610096 | -0.183931 |
| H | -3.310395 | 0.393513 | 0.128840 |
| H | -3.699215 | -0.912555 | -0.982465 |
| H | -3.179137 | -1.282839 | 0.661618 |

ax2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.977199 | -0.253411 | -0.053344 |
| C | -0.227253 | -0.616409 | 0.799382 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.174918 | -1.142137 | 1.668424 |
| C | 2.319490 | -0.390292 | 0.528419 |
| C | -0.901604 | 0.669111 | 1.313918 |
| C | -1.088660 | 1.761855 | 0.254587 |
| H | -1.462098 | 2.665369 | 0.739842 |
| H | -1.839706 | 1.464162 | -0.477600 |
| C | 0.776987 | 0.793857 | -1.120693 |
| C | 0.217532 | 2.063962 | -0.478094 |
| H | 0.060103 | 2.831306 | -1.236779 |
| H | 0.952598 | 2.456749 | 0.231476 |
| H | 2.428231 | -0.756372 | 1.542583 |
| H | 3.127029 | 0.229296 | 0.155189 |
| H | -1.861045 | 0.414601 | 1.770305 |
| H | 1.729992 | 0.986635 | -1.614775 |
| H | 0.082455 | 0.425289 | -1.878590 |
| H | -0.274942 | 1.081702 | 2.110001 |
| O | 1.818166 | -1.351572 | -0.406119 |
| C | -1.178270 | -1.628610 | 0.130565 |
| H | -1.720767 | -2.129774 | 0.935947 |
| H | -0.563051 | -2.397283 | -0.342922 |
| C | -2.213387 | -1.118833 | -0.870422 |
| H | -1.763639 | -0.613635 | -1.723758 |
| H | -2.791290 | -1.960637 | -1.254954 |
| H | -2.916318 | -0.430081 | -0.401350 |

ax3

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=====
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| | | | |
|---|-----------|-----------|-----------|
| C | 0.150227 | 0.820118 | 0.042048 |
| C | 0.389701 | -0.504317 | 0.738796 |
| H | 0.978302 | -0.299491 | 1.637493 |
| C | 0.175028 | 2.056373 | 0.831739 |
| C | -0.982968 | -1.061781 | 1.154354 |
| C | -1.956893 | -1.159091 | -0.024710 |
| H | -2.928160 | -1.504285 | 0.333055 |
| H | -1.603692 | -1.905803 | -0.739674 |
| C | -0.753824 | 0.751867 | -1.163335 |
| C | -2.112505 | 0.186913 | -0.735351 |
| H | -2.766881 | 0.086499 | -1.601985 |
| H | -2.587413 | 0.898915 | -0.053400 |
| H | 0.408908 | 2.009720 | 1.889277 |
| H | -0.419013 | 2.904688 | 0.511257 |
| H | -0.852502 | -2.040698 | 1.619858 |
| H | -0.860545 | 1.748275 | -1.593186 |
| H | -0.304329 | 0.108367 | -1.924758 |
| H | -1.414508 | -0.400163 | 1.911200 |
| O | 1.258683 | 1.717237 | -0.038731 |
| C | 1.173928 | -1.507344 | -0.116337 |
| H | 0.586922 | -1.796818 | -0.989603 |
| H | 1.303368 | -2.414831 | 0.478882 |
| C | 2.537889 | -1.001685 | -0.575764 |
| H | 3.138971 | -0.669010 | 0.272237 |
| H | 3.087611 | -1.790890 | -1.090014 |
| H | 2.439997 | -0.158683 | -1.259431 |

eq1

```
=====
C  -0.501602    0.845013   -0.228323
C   0.626839   -0.163503   -0.395350
H   0.641982   -0.437125   -1.457155
C  -0.278878    2.293553   -0.176968
C   0.262788   -1.424740    0.402546
C  -1.104567   -1.982953    0.006049
H  -1.334971   -2.863958    0.607252
H  -1.065190   -2.310179   -1.037827
C  -1.860718    0.324819   -0.635775
C  -2.203448   -0.934342    0.160169
H  -3.165023   -1.333678   -0.164972
H  -2.304538   -0.668757    1.216239
H  -1.087444    2.953131   -0.471725
H   0.717811    2.705228   -0.265194
H   1.024478   -2.189341    0.251667
H  -2.606164    1.104683   -0.476096
H  -1.842024    0.093002   -1.704420
H   0.264592   -1.175226    1.469371
O  -0.517646    1.550343    1.021036
C   2.002526    0.397460   -0.028858
H   2.238210    1.218797   -0.707332
H   1.958358    0.820467    0.977818
C   3.128875   -0.629983   -0.106445
H   4.097643   -0.143335    0.008950
H   3.046710   -1.385836    0.673877
H   3.125853   -1.142562   -1.071017
```

eq2

```
=====
C  -0.058155    0.785695   -0.155008
C   0.451524   -0.648725   -0.171209
H   0.471213   -0.957636   -1.222788
C   0.816015    1.950220    0.018265
C  -0.589319   -1.521062    0.545125
C  -1.975178   -1.390051   -0.086924
H  -2.694975   -2.005128    0.455543
H  -1.934831   -1.773363   -1.111440
C  -1.409824    0.957161   -0.808978
C  -2.440723    0.065175   -0.114381
H  -3.406257    0.149319   -0.614781
H  -2.577290    0.419336    0.911120
H   0.491822    2.908486   -0.372212
H   1.885287    1.825977    0.131270
H  -0.261081   -2.561674    0.521568
H  -1.705686    2.005647   -0.759452
H  -1.329356    0.680460   -1.863751
H  -0.632245   -1.221446    1.597538
O   0.041123    1.453265    1.111083
C   1.857962   -0.821416    0.407802
H   1.986438   -0.140269    1.252347
H   1.945319   -1.830600    0.815561
C   2.963325   -0.614479   -0.625217
```

```

H   3.950863   -0.652229   -0.164071
H   2.920662   -1.393672   -1.388220
H   2.867371    0.345557   -1.133749

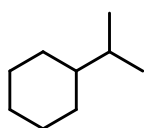
```

eq3

```

=====
C  -0.114791    0.847124   -0.277264
C   0.370025   -0.538308   -0.672317
H   0.014284   -0.680486   -1.699158
C   0.758351    2.023853   -0.253929
C  -0.364063   -1.566516    0.199989
C  -1.880905   -1.437479    0.053010
H  -2.384182   -2.166442    0.690238
H  -2.161177   -1.666580   -0.979888
C  -1.608356    1.023471   -0.433464
C  -2.349382   -0.024328    0.400493
H  -3.425495    0.070628    0.249662
H  -2.154441    0.167835    1.459316
H   0.322265    3.005981   -0.398378
H   1.806165    1.931523   -0.513768
H  -0.037717   -2.572719   -0.072460
H  -1.885640    2.032525   -0.126227
H  -1.869790    0.909980   -1.489026
H  -0.090194   -1.411026    1.247178
O   0.383702    1.371642    0.961740
C   1.887109   -0.756324   -0.709744
H   2.049579   -1.743849   -1.149292
H   2.333095   -0.042525   -1.405466
C   2.626728   -0.695646    0.625944
H   3.677588   -0.949369    0.480079
H   2.573360    0.293926    1.075064
H   2.214389   -1.407622    1.341902

```



isopropylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -353.751841 | -353.485079 | -353.530377 |
| ax2 | -353.746356 | -353.479609 | -353.524012 |
| ax3 | -353.745953 | -353.479126 | -353.523641 |
| eq1 | -353.753876 | -353.487483 | -353.532677 |
| eq2 | -353.753891 | -353.487539 | -353.533057 |

ax1

```

=====
C   0.580867    1.243608    0.780168

```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.323017 | -0.000151 | 0.791964 |
| H | -0.885846 | -0.000308 | 1.732498 |
| C | 0.580836 | -1.243932 | 0.779725 |
| C | 1.515048 | -1.265654 | -0.432212 |
| H | 2.155267 | -2.148934 | -0.391366 |
| H | 0.928552 | -1.346645 | -1.351826 |
| C | 1.514977 | 1.265757 | -0.431830 |
| C | 2.373143 | 0.000083 | -0.483750 |
| H | 2.997365 | 0.000230 | -1.379316 |
| H | 3.050391 | -0.000021 | 0.376689 |
| H | 1.192426 | -1.227142 | 1.687329 |
| H | 0.928393 | 1.346951 | -1.351374 |
| H | 2.155143 | 2.149066 | -0.390792 |
| H | -0.010929 | -2.158241 | 0.822923 |
| H | -0.010867 | 2.157912 | 0.823797 |
| H | 1.192533 | 1.226423 | 1.687713 |
| C | -1.375436 | 0.000003 | -0.338286 |
| H | -0.861997 | -0.000122 | -1.302890 |
| C | -2.256675 | 1.248783 | -0.280756 |
| H | -1.696897 | 2.160900 | -0.485028 |
| H | -3.059558 | 1.184297 | -1.016799 |
| H | -2.716264 | 1.348997 | 0.706669 |
| C | -2.257022 | -1.248523 | -0.280621 |
| H | -2.716979 | -1.348244 | 0.706681 |
| H | -3.059637 | -1.184091 | -1.016962 |
| H | -1.697426 | -2.160870 | -0.484367 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.242702 | -1.044122 | -0.937429 |
| C | -0.371987 | 0.360823 | -0.781544 |
| H | -0.806228 | 0.614624 | -1.753022 |
| C | 0.728089 | 1.411211 | -0.538560 |
| C | 1.770968 | 1.031406 | 0.513527 |
| H | 2.541894 | 1.803731 | 0.551922 |
| H | 1.320137 | 0.990504 | 1.507337 |
| C | 1.317034 | -1.401203 | 0.096854 |
| C | 2.394480 | -0.322593 | 0.183533 |
| H | 3.141832 | -0.593737 | 0.931427 |
| H | 2.914257 | -0.250873 | -0.777842 |
| H | 1.260484 | 1.559492 | -1.483920 |
| H | 0.872252 | -1.532319 | 1.084064 |
| H | 1.765419 | -2.359335 | -0.174216 |
| H | 0.264941 | 2.368942 | -0.289883 |
| H | -0.546236 | -1.799855 | -0.931982 |
| H | 0.709375 | -1.095866 | -1.925996 |
| C | -1.567327 | 0.445484 | 0.199496 |
| H | -1.739932 | 1.511156 | 0.380581 |
| C | -1.380403 | -0.231467 | 1.558480 |
| H | -0.503272 | 0.125873 | 2.094572 |
| H | -2.253620 | -0.040996 | 2.185436 |
| H | -1.291946 | -1.313733 | 1.443890 |
| C | -2.830974 | -0.115819 | -0.457071 |
| H | -2.710367 | -1.176056 | -0.691764 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.689796 | -0.023255 | 0.210039 |
| H | -3.064690 | 0.409374 | -1.384366 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.269078 | 1.394858 | -0.416262 |
| C | 0.353971 | 0.079470 | -0.920969 |
| H | 0.728533 | 0.301995 | -1.925040 |
| C | -0.733130 | -0.997609 | -1.096019 |
| C | -1.729867 | -1.114232 | 0.063575 |
| H | -2.516502 | -1.819109 | -0.213502 |
| H | -1.244415 | -1.520514 | 0.951695 |
| C | -1.237996 | 1.245151 | 0.757976 |
| C | -2.337103 | 0.240854 | 0.419379 |
| H | -3.032698 | 0.135976 | 1.253951 |
| H | -2.912865 | 0.616711 | -0.433077 |
| H | -1.306781 | -0.752142 | -1.995262 |
| H | -0.709742 | 0.914714 | 1.654966 |
| H | -1.674319 | 2.218558 | 0.991365 |
| H | -0.260563 | -1.965490 | -1.284756 |
| H | 0.511892 | 2.117484 | -0.177306 |
| H | -0.835550 | 1.824339 | -1.249199 |
| C | 1.613875 | -0.424182 | -0.174196 |
| H | 2.034560 | -1.193355 | -0.830700 |
| C | 1.395436 | -1.092943 | 1.183907 |
| H | 0.781425 | -1.988815 | 1.103893 |
| H | 2.359619 | -1.394761 | 1.598862 |
| H | 0.927572 | -0.418316 | 1.901556 |
| C | 2.665978 | 0.677253 | -0.041001 |
| H | 2.387687 | 1.399527 | 0.729024 |
| H | 3.629165 | 0.251153 | 0.243959 |
| H | 2.800463 | 1.220330 | -0.978774 |

eq1

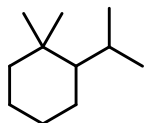
```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.597653 | -1.313286 | -0.200257 |
| C | 0.273380 | -0.074618 | -0.435177 |
| H | 0.142766 | 0.211808 | -1.486778 |
| C | -0.245692 | 1.088159 | 0.418042 |
| C | -1.716514 | 1.384993 | 0.119255 |
| H | -2.069284 | 2.205348 | 0.747126 |
| H | -1.811924 | 1.715453 | -0.919989 |
| C | -2.070851 | -1.030924 | -0.497770 |
| C | -2.584103 | 0.145219 | 0.332091 |
| H | -3.624303 | 0.361696 | 0.081845 |
| H | -2.560687 | -0.128442 | 1.391911 |
| H | -0.148383 | 0.828337 | 1.476940 |
| H | -2.182706 | -0.794779 | -1.560787 |
| H | -2.672145 | -1.921348 | -0.304904 |
| H | 0.355797 | 1.983977 | 0.252102 |
| H | -0.238382 | -2.138680 | -0.820032 |
| H | -0.503634 | -1.632011 | 0.842575 |
| C | 1.773954 | -0.369186 | -0.246310 |
| H | 1.982373 | -1.276364 | -0.823011 |

| | | | |
|---|----------|-----------|-----------|
| C | 2.165905 | -0.642580 | 1.206435 |
| H | 1.555241 | -1.424369 | 1.659199 |
| H | 3.207882 | -0.962069 | 1.261875 |
| H | 2.067392 | 0.258674 | 1.814512 |
| C | 2.647301 | 0.747623 | -0.817622 |
| H | 2.528651 | 1.672418 | -0.249883 |
| H | 3.702459 | 0.471842 | -0.775985 |
| H | 2.394520 | 0.956105 | -1.858840 |

eq2

```
=====
C -0.172861 -0.496947 1.254495
C 0.169417 0.317932 0.000000
H 1.253990 0.495752 0.000000
C -0.172861 -0.496947 -1.254495
C 0.471701 -1.883365 -1.251800
H 0.179221 -2.430193 -2.150223
H 1.560153 -1.770729 -1.288849
C 0.471701 -1.883365 1.251800
C 0.097281 -2.671310 -0.000000
H 0.589629 -3.645534 0.000000
H -0.981804 -2.856691 -0.000000
H -1.262718 -0.606297 -1.310392
H 1.560153 -1.770729 1.288849
H 0.179221 -2.430193 2.150223
H 0.138101 0.039275 -2.150918
H 0.138101 0.039275 2.150918
H -1.262718 -0.606297 1.310392
C -0.521248 1.695610 -0.000000
H -1.602945 1.517758 -0.000000
C -0.172861 2.512529 -1.245908
H -0.544925 2.057139 -2.162253
H -0.602833 3.512974 -1.178031
H 0.911348 2.622197 -1.338894
C -0.172861 2.512529 1.245908
H 0.911348 2.622197 1.338894
H -0.602833 3.512974 1.178031
H -0.544925 2.057139 2.162253
```



2-isopropyl-1,1-dimethylcyclohexane

Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| ax | | -432.358974 | | -432.033188 | | -432.082588 |
| ax2 | | -432.359441 | | -432.033622 | | -432.082266 |
| ax3 | | -432.355163 | | -432.029275 | | -432.078373 |
| ax4 | | -432.353716 | | -432.027669 | | -432.076694 |
| eq | | -432.364381 | | -432.039005 | | -432.088432 |
| eq2 | | -432.359349 | | -432.033926 | | -432.084257 |
| eq3 | | -432.359111 | | -432.033535 | | -432.083149 |

ax

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.894554 | -0.859192 | -0.034206 |
| C | -0.398931 | -0.227572 | -0.645962 |
| H | -0.559171 | -0.781561 | -1.577848 |
| C | -0.163527 | 1.241785 | -1.060128 |
| C | 0.543701 | 2.111100 | -0.016284 |
| H | 0.725794 | 3.100836 | -0.440293 |
| H | -0.091864 | 2.255705 | 0.858629 |
| C | 1.597028 | 0.072438 | 0.973076 |
| C | 1.855333 | 1.474849 | 0.430824 |
| H | 2.548850 | 1.430773 | -0.413282 |
| H | 2.332530 | 2.086859 | 1.198520 |
| H | 0.448422 | 1.252928 | -1.965746 |
| H | 2.537985 | -0.398489 | 1.271478 |
| H | 0.992012 | 0.154486 | 1.878870 |
| H | -1.113828 | 1.699612 | -1.338696 |
| C | -1.719649 | -0.456071 | 0.132372 |
| H | -1.757788 | -1.520774 | 0.368284 |
| C | 1.864113 | -1.158755 | -1.189931 |
| H | 2.818316 | -1.523271 | -0.802850 |
| H | 1.448633 | -1.930139 | -1.841534 |
| H | 2.066836 | -0.281118 | -1.803031 |
| C | 0.605334 | -2.188081 | 0.667550 |
| H | 0.076992 | -2.880270 | 0.007887 |
| H | 1.545530 | -2.659857 | 0.962228 |
| H | 0.006044 | -2.051290 | 1.568951 |
| C | -2.933157 | -0.175975 | -0.759630 |
| H | -3.849105 | -0.502846 | -0.264117 |
| H | -3.042537 | 0.888799 | -0.971741 |
| H | -2.859180 | -0.704528 | -1.711776 |
| C | -1.884815 | 0.307877 | 1.446477 |
| H | -2.802083 | -0.014071 | 1.944111 |
| H | -1.059355 | 0.142824 | 2.137111 |
| H | -1.972927 | 1.380969 | 1.269900 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.778777 | 0.920244 | 0.042673 |
| C | -0.387316 | 0.051199 | 0.621558 |
| H | -0.721098 | 0.546044 | 1.541557 |
| C | 0.161833 | -1.329779 | 1.032445 |
| C | 0.868059 | -2.060050 | -0.110647 |
| H | 1.228844 | -3.030749 | 0.235144 |
| H | 0.163056 | -2.254204 | -0.923800 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.515202 | 0.155836 | -1.075128 |
| C | 2.020456 | -1.222094 | -0.655895 |
| H | 2.794692 | -1.122086 | 0.109224 |
| H | 2.484428 | -1.720385 | -1.509244 |
| H | 0.873957 | -1.201111 | 1.849864 |
| H | 2.345660 | 0.774340 | -1.426389 |
| H | 0.835920 | 0.035495 | -1.925329 |
| H | -0.642596 | -1.944162 | 1.434783 |
| C | -1.639908 | -0.034787 | -0.303274 |
| H | -1.309961 | 0.031263 | -1.343999 |
| C | 1.763376 | 1.269886 | 1.169446 |
| H | 2.577795 | 1.882867 | 0.776638 |
| H | 1.257569 | 1.845899 | 1.947560 |
| H | 2.208279 | 0.395211 | 1.639420 |
| C | 0.306838 | 2.252395 | -0.547329 |
| H | -0.181824 | 2.873659 | 0.205168 |
| H | 1.172595 | 2.804762 | -0.919829 |
| H | -0.379830 | 2.114033 | -1.382713 |
| C | -2.616433 | 1.116469 | -0.028690 |
| H | -3.441294 | 1.098067 | -0.743596 |
| H | -3.043843 | 0.999932 | 0.970728 |
| H | -2.154982 | 2.098135 | -0.076371 |
| C | -2.446697 | -1.330500 | -0.159912 |
| H | -3.325340 | -1.283956 | -0.805744 |
| H | -1.885577 | -2.222649 | -0.430671 |
| H | -2.801572 | -1.453315 | 0.866122 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.401967 | 1.013324 | -0.044239 |
| C | -0.333588 | -0.071226 | 0.800946 |
| H | -0.662340 | 0.443503 | 1.710382 |
| C | 0.669935 | -1.148361 | 1.273014 |
| C | 1.524952 | -1.759631 | 0.161241 |
| H | 2.251654 | -2.446050 | 0.600850 |
| H | 0.905305 | -2.355615 | -0.510280 |
| C | 1.261331 | 0.374545 | -1.153446 |
| C | 2.245504 | -0.675599 | -0.637804 |
| H | 2.997082 | -0.199309 | -0.002941 |
| H | 2.783475 | -1.119378 | -1.477649 |
| H | 1.343788 | -0.704847 | 2.009418 |
| H | 1.804472 | 1.172570 | -1.667966 |
| H | 0.608224 | -0.086518 | -1.896895 |
| H | 0.124138 | -1.934555 | 1.798509 |
| C | -1.641073 | -0.716521 | 0.248108 |
| H | -1.782458 | -1.601269 | 0.876391 |
| C | 1.312652 | 1.827783 | 0.891749 |
| H | 1.866721 | 2.573570 | 0.317177 |
| H | 0.712944 | 2.356511 | 1.635749 |
| H | 2.038131 | 1.215948 | 1.424028 |
| C | -0.558004 | 2.021066 | -0.682619 |
| H | -1.194019 | 2.490049 | 0.070797 |
| H | 0.017770 | 2.811546 | -1.170250 |
| H | -1.198986 | 1.568547 | -1.436831 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.654663 | -1.218803 | -1.200286 |
| H | -2.592442 | -1.748769 | -1.381369 |
| H | -1.604937 | -0.400089 | -1.917668 |
| H | -0.843282 | -1.908169 | -1.421351 |
| C | -2.885441 | 0.150807 | 0.480194 |
| H | -3.785722 | -0.451735 | 0.343446 |
| H | -2.906424 | 0.555447 | 1.493458 |
| H | -2.944522 | 0.984301 | -0.218149 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.725022 | 0.886713 | 0.211605 |
| C | -0.396478 | -0.115379 | 0.627699 |
| H | -0.752308 | 0.234393 | 1.604132 |
| C | 0.225203 | -1.520409 | 0.821249 |
| C | 0.992832 | -2.006074 | -0.414894 |
| H | 1.462873 | -2.966491 | -0.194630 |
| H | 0.292181 | -2.188035 | -1.233717 |
| C | 1.428117 | 0.388120 | -1.060925 |
| C | 2.042469 | -1.000874 | -0.888693 |
| H | 2.863200 | -0.954729 | -0.169283 |
| H | 2.475943 | -1.335242 | -1.833145 |
| H | 0.893102 | -1.524234 | 1.682498 |
| H | 2.197356 | 1.109638 | -1.351122 |
| H | 0.697551 | 0.358789 | -1.876414 |
| H | -0.562943 | -2.238490 | 1.051034 |
| C | -1.668906 | -0.299221 | -0.258234 |
| H | -1.457748 | -1.098630 | -0.972153 |
| C | 1.739781 | 0.989026 | 1.367803 |
| H | 2.562368 | 1.645668 | 1.076626 |
| H | 1.259409 | 1.427739 | 2.245784 |
| H | 2.170594 | 0.037566 | 1.666403 |
| C | 0.232396 | 2.326051 | -0.003248 |
| H | -0.468783 | 2.623995 | 0.779613 |
| H | 1.085897 | 3.005986 | 0.043248 |
| H | -0.244230 | 2.478952 | -0.966228 |
| C | -2.184489 | 0.881032 | -1.082860 |
| H | -3.122123 | 0.588583 | -1.560547 |
| H | -2.391522 | 1.752876 | -0.461180 |
| H | -1.496139 | 1.173512 | -1.872839 |
| C | -2.819996 | -0.774927 | 0.637691 |
| H | -3.673647 | -1.093592 | 0.037389 |
| H | -2.534828 | -1.607066 | 1.280818 |
| H | -3.151912 | 0.044475 | 1.280565 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.663834 | 0.942710 | -0.037174 |
| C | 0.365405 | -0.166399 | -0.392583 |
| H | 0.307828 | -0.256032 | -1.484910 |
| C | -0.039755 | -1.535451 | 0.171757 |
| C | -1.436969 | -1.955779 | -0.275345 |
| H | -1.451751 | -2.071861 | -1.363876 |
| H | -1.694311 | -2.926014 | 0.153734 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.070973 | 0.459241 | -0.444333 |
| C | -2.461057 | -0.899828 | 0.129340 |
| H | -2.514484 | -0.846280 | 1.220438 |
| H | -3.457026 | -1.176257 | -0.221822 |
| H | 0.694748 | -2.283098 | -0.137434 |
| H | -2.104558 | 0.393839 | -1.537550 |
| H | -2.799263 | 1.220618 | -0.152256 |
| H | -0.015626 | -1.510112 | 1.264245 |
| C | 1.841042 | 0.181159 | -0.061107 |
| H | 1.946649 | 1.267237 | -0.082166 |
| C | -0.380161 | 2.213137 | -0.847043 |
| H | -1.185056 | 2.936926 | -0.698844 |
| H | 0.550470 | 2.697036 | -0.550743 |
| H | -0.323549 | 1.989267 | -1.914836 |
| C | -0.643105 | 1.308846 | 1.450840 |
| H | 0.304827 | 1.774917 | 1.724024 |
| H | -1.437675 | 2.027274 | 1.666215 |
| H | -0.791581 | 0.444105 | 2.097867 |
| C | 2.770907 | -0.387442 | -1.134763 |
| H | 3.816484 | -0.177270 | -0.901812 |
| H | 2.658502 | -1.472321 | -1.206204 |
| H | 2.549610 | 0.038091 | -2.114834 |
| C | 2.316478 | -0.295438 | 1.315282 |
| H | 3.308192 | 0.110451 | 1.522778 |
| H | 1.653345 | 0.014538 | 2.121699 |
| H | 2.396357 | -1.383596 | 1.347061 |

eq2

```
=====
```

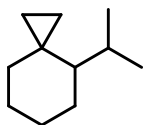
| | | | |
|---|-----------|-----------|-----------|
| C | 0.506236 | -0.942792 | -0.016751 |
| C | -0.350007 | 0.337930 | -0.288881 |
| H | -0.439407 | 0.417980 | -1.381109 |
| C | 0.367506 | 1.610561 | 0.210287 |
| C | 1.807198 | 1.765163 | -0.265857 |
| H | 1.819923 | 1.877188 | -1.354974 |
| H | 2.237335 | 2.676778 | 0.153454 |
| C | 1.966814 | -0.696522 | -0.463809 |
| C | 2.627557 | 0.544277 | 0.116878 |
| H | 2.689797 | 0.468774 | 1.206185 |
| H | 3.650480 | 0.628328 | -0.255059 |
| H | -0.194178 | 2.485921 | -0.108298 |
| H | 1.976255 | -0.610067 | -1.556435 |
| H | 2.546275 | -1.589521 | -0.216696 |
| H | 0.352980 | 1.614886 | 1.305877 |
| C | -1.792621 | 0.340452 | 0.288007 |
| H | -1.706180 | 0.375453 | 1.379092 |
| C | 0.051678 | -2.152355 | -0.852347 |
| H | 0.838116 | -2.910872 | -0.840614 |
| H | -0.851812 | -2.625141 | -0.482123 |
| H | -0.113454 | -1.866030 | -1.893383 |
| C | 0.481863 | -1.325211 | 1.467342 |
| H | -0.517306 | -1.630211 | 1.781095 |
| H | 1.156194 | -2.165777 | 1.647601 |
| H | 0.796590 | -0.502828 | 2.110881 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.649018 | -0.877832 | -0.069906 |
| H | -3.686465 | -0.689624 | 0.210922 |
| H | -2.627466 | -1.074747 | -1.144378 |
| H | -2.336368 | -1.779668 | 0.449159 |
| C | -2.562620 | 1.593170 | -0.155896 |
| H | -3.602642 | 1.525559 | 0.165034 |
| H | -2.158846 | 2.515096 | 0.255758 |
| H | -2.557346 | 1.677470 | -1.246397 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.336084 | 0.900902 | 0.020484 |
| C | 0.253235 | -0.485205 | -0.383659 |
| H | 0.140688 | -0.522452 | -1.475246 |
| C | -0.622255 | -1.625680 | 0.163857 |
| C | -2.068863 | -1.527741 | -0.320374 |
| H | -2.083910 | -1.685229 | -1.403706 |
| H | -2.671498 | -2.322096 | 0.124192 |
| C | -1.774130 | 0.954100 | -0.541841 |
| C | -2.674104 | -0.160530 | -0.014918 |
| H | -2.807182 | -0.049421 | 1.064355 |
| H | -3.666600 | -0.079361 | -0.462344 |
| H | -0.199907 | -2.579050 | -0.160415 |
| H | -1.723641 | 0.884845 | -1.633878 |
| H | -2.204410 | 1.930489 | -0.304512 |
| H | -0.596109 | -1.632524 | 1.257004 |
| C | 1.751493 | -0.795099 | -0.128829 |
| H | 1.823721 | -1.876813 | -0.278817 |
| C | 0.446864 | 2.053363 | -0.612480 |
| H | -0.095640 | 2.991409 | -0.469538 |
| H | 1.429575 | 2.170598 | -0.156536 |
| H | 0.581062 | 1.901804 | -1.685952 |
| C | -0.402291 | 1.153890 | 1.536917 |
| H | 0.571881 | 1.407664 | 1.947831 |
| H | -1.066169 | 2.001007 | 1.728082 |
| H | -0.789962 | 0.304521 | 2.096989 |
| C | 2.259635 | -0.521525 | 1.287347 |
| H | 3.222777 | -1.014048 | 1.434524 |
| H | 2.411789 | 0.545317 | 1.454663 |
| H | 1.574603 | -0.892509 | 2.050924 |
| C | 2.709185 | -0.178533 | -1.153456 |
| H | 3.692980 | -0.644472 | -1.065341 |
| H | 2.355734 | -0.339098 | -2.173607 |
| H | 2.844110 | 0.891768 | -1.006960 |



4-isopropylspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -431.135937 | -430.833834 | -430.882108 |
| ax2 | -431.129155 | -430.826758 | -430.875195 |
| ax3 | -431.130469 | -430.827931 | -430.876119 |
| ax4 | -431.128861 | -430.826376 | -430.874106 |
| ax5 | -431.131158 | -430.828815 | -430.876873 |
| eq1 | -431.132384 | -430.829987 | -430.877761 |
| eq2 | -431.132331 | -430.830065 | -430.877599 |
| eq3 | -431.128671 | -430.826249 | -430.873922 |
| eq4 | -431.126874 | -430.824316 | -430.872913 |
| eq5 | -431.130702 | -430.828323 | -430.87625 |

ax1

| ===== | | | |
|-------|-----------|-----------|-----------|
| C | 0.797437 | 0.749262 | 0.053222 |
| C | -0.415122 | 0.021484 | 0.623642 |
| H | -0.745313 | 0.567112 | 1.515687 |
| C | 0.891609 | 2.240686 | 0.146077 |
| C | 1.744904 | 1.375472 | 1.039696 |
| C | 0.057372 | -1.379184 | 1.053602 |
| C | 0.680041 | -2.154996 | -0.111040 |
| H | -0.078651 | -2.352921 | -0.873095 |
| H | 1.029852 | -3.127659 | 0.239575 |
| C | 1.430886 | 0.041736 | -1.128602 |
| C | 1.843003 | -1.380239 | -0.736581 |
| H | 2.231967 | -1.915158 | -1.604770 |
| H | 2.656861 | -1.317785 | -0.007545 |
| C | -1.619232 | -0.023546 | -0.343373 |
| H | 0.070065 | 2.770621 | 0.607004 |
| H | 1.378674 | 2.768009 | -0.663386 |
| H | 2.804082 | 1.319284 | 0.827957 |
| H | 1.484044 | 1.331793 | 2.088655 |
| H | -0.758312 | -1.949568 | 1.497246 |
| H | 0.724496 | 0.005659 | -1.963787 |
| H | 2.300107 | 0.607035 | -1.471349 |
| H | 0.813595 | -1.256450 | 1.834467 |
| H | -1.329879 | -0.578989 | -1.238687 |
| C | -2.050372 | 1.373741 | -0.789341 |
| H | -2.299941 | 1.995207 | 0.074940 |
| H | -1.271298 | 1.882854 | -1.354887 |
| H | -2.937882 | 1.310856 | -1.421236 |
| C | -2.810965 | -0.745968 | 0.287426 |
| H | -3.683489 | -0.682468 | -0.364596 |

| | | | |
|---|-----------|-----------|----------|
| H | -2.610964 | -1.801826 | 0.465570 |
| H | -3.075385 | -0.286282 | 1.243866 |

ax2

```
=====
C  0.383412    0.917129   -0.058974
C -0.383201   -0.112969    0.769412
H -0.788127    0.427385    1.629583
C -0.241857    2.253323   -0.333071
C  0.869433    2.136784    0.680744
C  0.620306   -1.133478    1.335847
C  1.532070   -1.746499    0.273137
H  0.940642   -2.321805   -0.443784
H  2.224663   -2.447337    0.742975
C  1.358459    0.367041   -1.088476
C  2.308908   -0.652672   -0.459297
H  2.953714   -1.085743   -1.225948
H  2.959990   -0.142549    0.257815
C -1.616341   -0.781798    0.092708
H -1.235334    2.440943    0.046669
H -0.015187    2.731026   -1.276719
H  1.839212    2.532869    0.412753
H  0.604431    2.237935    1.724166
H  0.080721   -1.914227    1.875553
H  0.823463   -0.103649   -1.913474
H  1.924820    1.197990   -1.514922
H  1.252627   -0.620503    2.067751
H -1.729117   -1.761380    0.567437
C -1.530590   -1.014754   -1.416930
H -1.428214   -0.067968   -1.951338
H -0.700823   -1.658316   -1.702537
H -2.450869   -1.489623   -1.762643
C -2.896854    0.005857    0.387336
H -3.772157   -0.533024    0.019947
H -3.027050    0.170922    1.457873
H -2.879881    0.979276   -0.105782
```

ax3

```
=====
C  0.937642   -0.672034   -0.024087
C -0.380423   -0.272064   -0.684956
H -0.461457   -0.871423   -1.597581
C  1.214587   -2.132652    0.166653
C  1.951979   -1.359420   -0.900164
C -0.292201    1.193337   -1.153568
C  0.249423    2.171004   -0.108562
H -0.443165    2.258534    0.731338
H  0.330981    3.164701   -0.553419
C  1.512292    0.303099    0.990612
C  1.612327    1.710228    0.404223
H  1.995844    2.404058    1.154230
H  2.324630    1.706617   -0.427124
C -1.642684   -0.669843    0.122865
H  0.461662   -2.836320   -0.161215
```


| | | | |
|---|-----------|-----------|-----------|
| H | 1.769857 | -2.432779 | 1.044928 |
| H | 2.996711 | -1.139372 | -0.728075 |
| H | 1.687185 | -1.553417 | -1.930336 |
| H | -1.258651 | 1.531320 | -1.527833 |
| H | 0.889112 | 0.339980 | 1.885639 |
| H | 2.496123 | -0.052600 | 1.304391 |
| H | 0.392276 | 1.216796 | -2.007842 |
| H | -1.650656 | -1.763937 | 0.104953 |
| C | -2.920381 | -0.202266 | -0.574999 |
| H | -3.068787 | 0.872357 | -0.451490 |
| H | -2.896519 | -0.417719 | -1.645260 |
| H | -3.790631 | -0.703734 | -0.148830 |
| C | -1.683481 | -0.269169 | 1.598010 |
| H | -2.625020 | -0.605850 | 2.037396 |
| H | -0.876244 | -0.729775 | 2.165984 |
| H | -1.627726 | 0.811238 | 1.733987 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.486853 | 0.898327 | -0.077109 |
| C | -0.377519 | 0.016235 | 0.821996 |
| H | -0.594036 | 0.624259 | 1.706642 |
| C | 0.162204 | 2.353497 | -0.238817 |
| C | 1.323898 | 1.939147 | 0.625688 |
| C | 0.471640 | -1.179439 | 1.300636 |
| C | 1.271016 | -1.892281 | 0.200115 |
| H | 0.606459 | -2.444957 | -0.463466 |
| H | 1.929094 | -2.629544 | 0.664656 |
| C | 1.206390 | 0.189900 | -1.209450 |
| C | 2.093889 | -0.916888 | -0.640630 |
| H | 2.603311 | -1.451708 | -1.444182 |
| H | 2.867924 | -0.459418 | -0.016832 |
| C | -1.782033 | -0.401152 | 0.308905 |
| H | -0.710754 | 2.742112 | 0.263428 |
| H | 0.380413 | 2.813123 | -1.193466 |
| H | 2.323368 | 2.114207 | 0.251564 |
| H | 1.210051 | 2.043561 | 1.696100 |
| H | -0.167708 | -1.897780 | 1.820494 |
| H | 0.491024 | -0.235026 | -1.917454 |
| H | 1.808513 | 0.914633 | -1.761866 |
| H | 1.187055 | -0.805587 | 2.039180 |
| H | -2.286409 | -0.787535 | 1.201288 |
| C | -1.845600 | -1.525346 | -0.727617 |
| H | -1.318982 | -1.271254 | -1.647655 |
| H | -1.437869 | -2.459119 | -0.344296 |
| H | -2.889346 | -1.711309 | -0.989288 |
| C | -2.602298 | 0.790014 | -0.184317 |
| H | -3.630617 | 0.480138 | -0.378057 |
| H | -2.627211 | 1.596015 | 0.550148 |
| H | -2.194922 | 1.193100 | -1.113322 |

ax5

```
=====
```

| | | | |
|---|----------|-----------|----------|
| C | 0.913400 | -0.733488 | 0.114155 |
|---|----------|-----------|----------|

| | | | |
|---|-----------|-----------|-----------|
| C | -0.398911 | -0.333524 | -0.556033 |
| H | -0.554934 | -1.068001 | -1.352011 |
| C | 1.104422 | -2.176004 | 0.467141 |
| C | 1.853053 | -1.581531 | -0.701821 |
| C | -0.235268 | 1.035794 | -1.244790 |
| C | 0.467827 | 2.104707 | -0.398013 |
| H | -0.171042 | 2.423052 | 0.426149 |
| H | 0.641817 | 2.987058 | -1.017224 |
| C | 1.576492 | 0.319364 | 0.979747 |
| C | 1.792071 | 1.598845 | 0.172693 |
| H | 2.254068 | 2.368606 | 0.793233 |
| H | 2.484954 | 1.387033 | -0.647892 |
| C | -1.652799 | -0.470062 | 0.344452 |
| H | 0.295819 | -2.859155 | 0.243708 |
| H | 1.668925 | -2.411993 | 1.358938 |
| H | 2.914757 | -1.412172 | -0.584020 |
| H | 1.542291 | -1.874715 | -1.695166 |
| H | -1.207813 | 1.404806 | -1.578563 |
| H | 0.961928 | 0.537291 | 1.856838 |
| H | 2.528876 | -0.067246 | 1.348891 |
| H | 0.363414 | 0.882598 | -2.147781 |
| H | -1.494689 | -1.362334 | 0.957374 |
| C | -2.889687 | -0.721992 | -0.521426 |
| H | -3.073900 | 0.120945 | -1.191912 |
| H | -2.770905 | -1.617722 | -1.132879 |
| H | -3.779101 | -0.849892 | 0.097889 |
| C | -1.945378 | 0.696644 | 1.289223 |
| H | -2.807266 | 0.452125 | 1.913037 |
| H | -1.113107 | 0.927856 | 1.951300 |
| H | -2.195432 | 1.599333 | 0.728112 |

eq1

| | | | |
|---|-----------|-----------|-----------|
| C | -0.692916 | 0.858967 | -0.194005 |
| C | 0.354848 | -0.234300 | -0.416886 |
| H | 0.304982 | -0.464654 | -1.488995 |
| C | -0.542873 | 1.879083 | 0.900860 |
| C | -0.417858 | 2.291425 | -0.546552 |
| C | -0.056032 | -1.515189 | 0.326289 |
| C | -1.462768 | -1.979802 | -0.041650 |
| H | -1.500347 | -2.228003 | -1.107208 |
| H | -1.711796 | -2.889445 | 0.507807 |
| C | -2.107673 | 0.393279 | -0.500386 |
| C | -2.478854 | -0.880090 | 0.253803 |
| H | -2.487700 | -0.677123 | 1.329410 |
| H | -3.485484 | -1.199311 | -0.021875 |
| C | 1.823044 | 0.160250 | -0.118290 |
| H | 0.364076 | 1.883854 | 1.486583 |
| H | -1.433353 | 2.177444 | 1.437498 |
| H | -1.235682 | 2.849422 | -0.981784 |
| H | 0.561394 | 2.574473 | -0.903569 |
| H | -0.024950 | -1.329950 | 1.403692 |
| H | -2.809746 | 1.197470 | -0.270941 |
| H | -2.184251 | 0.199521 | -1.576291 |

| | | | |
|---|----------|-----------|-----------|
| H | 0.669384 | -2.305282 | 0.118926 |
| H | 1.932372 | 1.232490 | -0.290197 |
| C | 2.764655 | -0.551529 | -1.091534 |
| H | 3.806886 | -0.310265 | -0.875108 |
| H | 2.651782 | -1.635655 | -1.012825 |
| H | 2.557109 | -0.265990 | -2.123740 |
| C | 2.280997 | -0.123694 | 1.316211 |
| H | 3.258675 | 0.330031 | 1.486617 |
| H | 1.595384 | 0.267280 | 2.067032 |
| H | 2.383842 | -1.196717 | 1.487814 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.587515 | 0.864311 | -0.057788 |
| C | 0.357933 | -0.321738 | -0.277185 |
| H | 0.372074 | -0.516143 | -1.358309 |
| C | -0.633064 | 1.541779 | 1.284171 |
| C | -0.114900 | 2.282453 | 0.076339 |
| C | -0.295889 | -1.553334 | 0.368319 |
| C | -1.680572 | -1.820512 | -0.227733 |
| H | -1.559681 | -2.074940 | -1.285745 |
| H | -2.133569 | -2.688037 | 0.255812 |
| C | -1.944365 | 0.637477 | -0.699245 |
| C | -2.604513 | -0.609649 | -0.111509 |
| H | -2.827601 | -0.426171 | 0.943826 |
| H | -3.554935 | -0.809002 | -0.609850 |
| C | 1.823200 | -0.051132 | 0.136294 |
| H | 0.088672 | 1.254240 | 2.036189 |
| H | -1.606038 | 1.814151 | 1.670130 |
| H | -0.740553 | 3.055753 | -0.348445 |
| H | 0.943726 | 2.491896 | 0.050818 |
| H | -0.380118 | -1.395093 | 1.448846 |
| H | -2.578101 | 1.513300 | -0.545321 |
| H | -1.819542 | 0.511875 | -1.779888 |
| H | 0.327454 | -2.435111 | 0.221309 |
| H | 1.826453 | 0.635496 | 0.987061 |
| C | 2.582178 | 0.606842 | -1.020146 |
| H | 3.557474 | 0.972852 | -0.694593 |
| H | 2.748191 | -0.125887 | -1.814020 |
| H | 2.032921 | 1.441226 | -1.454798 |
| C | 2.585706 | -1.303361 | 0.570060 |
| H | 3.623832 | -1.046709 | 0.788457 |
| H | 2.159788 | -1.759192 | 1.463479 |
| H | 2.590357 | -2.053311 | -0.224415 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.370481 | 0.824136 | -0.176779 |
| C | 0.235613 | -0.572701 | -0.341544 |
| H | 0.072423 | -0.834736 | -1.394998 |
| C | -0.208305 | 1.631879 | 1.083542 |
| C | 0.407147 | 2.106764 | -0.211072 |
| C | -0.630009 | -1.547280 | 0.473260 |
| C | -2.082076 | -1.536357 | -0.010140 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.110242 | -1.922280 | -1.034090 |
| H | -2.688662 | -2.209155 | 0.598970 |
| C | -1.783376 | 0.860969 | -0.739616 |
| C | -2.678566 | -0.128938 | 0.007561 |
| H | -2.781261 | 0.205255 | 1.044320 |
| H | -3.680352 | -0.137940 | -0.425808 |
| C | 1.744658 | -0.814454 | -0.114768 |
| H | 0.455203 | 1.283745 | 1.858788 |
| H | -1.086652 | 2.152547 | 1.441141 |
| H | -0.048762 | 2.953378 | -0.706836 |
| H | 1.482472 | 2.068728 | -0.281116 |
| H | -0.590980 | -1.270249 | 1.531589 |
| H | -2.186194 | 1.872583 | -0.656640 |
| H | -1.760155 | 0.606051 | -1.804124 |
| H | -0.223917 | -2.557853 | 0.389293 |
| H | 1.838284 | -1.904950 | -0.129115 |
| C | 2.316319 | -0.354577 | 1.227684 |
| H | 3.302327 | -0.798964 | 1.374681 |
| H | 2.442204 | 0.728003 | 1.267506 |
| H | 1.688195 | -0.658612 | 2.066054 |
| C | 2.609433 | -0.306669 | -1.270733 |
| H | 3.641894 | -0.637555 | -1.142004 |
| H | 2.251099 | -0.695114 | -2.225619 |
| H | 2.620937 | 0.780492 | -1.336362 |

eq4

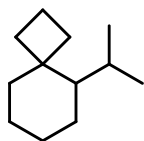
```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.551838 | 0.870480 | -0.120504 |
| C | 0.342103 | -0.369443 | -0.301885 |
| H | 0.425836 | -0.544229 | -1.383545 |
| C | -0.346793 | 1.810719 | 1.035461 |
| C | -0.113612 | 2.286508 | -0.379179 |
| C | -0.371832 | -1.592244 | 0.316490 |
| C | -1.816930 | -1.788767 | -0.129942 |
| H | -1.840391 | -1.992713 | -1.205374 |
| H | -2.236399 | -2.664330 | 0.369095 |
| C | -2.002224 | 0.646238 | -0.532957 |
| C | -2.645131 | -0.546627 | 0.158435 |
| H | -2.679735 | -0.371380 | 1.238383 |
| H | -3.674070 | -0.672923 | -0.183017 |
| C | 1.787648 | -0.308807 | 0.260906 |
| H | 0.528663 | 1.670205 | 1.654401 |
| H | -1.219605 | 2.176368 | 1.559499 |
| H | -0.868049 | 2.931983 | -0.808240 |
| H | 0.888320 | 2.512909 | -0.694602 |
| H | -0.348694 | -1.481132 | 1.407154 |
| H | -2.567112 | 1.558436 | -0.332232 |
| H | -2.034548 | 0.484493 | -1.616588 |
| H | 0.184435 | -2.495972 | 0.079407 |
| H | 1.711785 | -0.216626 | 1.348718 |
| C | 2.647023 | 0.853008 | -0.252658 |

| | | | |
|---|----------|-----------|-----------|
| H | 3.698455 | 0.649728 | -0.045963 |
| H | 2.541556 | 0.977102 | -1.333008 |
| H | 2.409912 | 1.798434 | 0.228146 |
| C | 2.543135 | -1.612159 | -0.039876 |
| H | 3.585864 | -1.514377 | 0.262937 |
| H | 2.136665 | -2.475097 | 0.481791 |
| H | 2.527812 | -1.824319 | -1.112713 |

eq5

```
=====
C -0.672158    0.814872   -0.304395
C  0.352870   -0.317513   -0.393265
H  0.211470   -0.744276   -1.394805
C -0.689930    1.802882    0.829513
C -0.323068    2.248194   -0.567474
C -0.070973   -1.411298    0.598026
C -1.474538   -1.927752    0.265129
H -1.440256   -2.423997   -0.709946
H -1.780573   -2.681409    0.993088
C -2.050746    0.327091   -0.716390
C -2.505738   -0.799612    0.213480
H -2.641170   -0.390537    1.219271
H -3.474154   -1.188894   -0.106056
C  1.850930    0.051374   -0.349669
H  0.083479    1.777118    1.579910
H -1.664883    2.089736    1.200727
H -1.037707    2.853351   -1.108828
H  0.713019    2.499676   -0.745685
H -0.061978   -1.005008    1.613998
H -2.761639    1.155437   -0.686551
H -2.017806   -0.038037   -1.748036
H  0.632872   -2.244348    0.577745
H  2.009552    0.794709   -1.135213
C  2.706285   -1.166399   -0.714575
H  3.732785   -0.858224   -0.917682
H  2.739203   -1.889447    0.102150
H  2.323587   -1.675049   -1.601377
C  2.361637    0.644263    0.966227
H  3.453223    0.658989    0.962998
H  2.028399    1.668371    1.121997
H  2.045148    0.045230    1.822650
```



5-isopropylspiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -470.434085 | -470.101355 | -470.15111 |
| ax2 | -470.438528 | -470.105912 | -470.155672 |
| ax3 | -470.432167 | -470.099403 | -470.149466 |
| ax4 | -470.431377 | -470.09849 | -470.148034 |
| ax5 | -470.434110 | -470.10137 | -470.15165 |
| ax6 | -470.433310 | -470.100437 | -470.149965 |
| eq1 | -470.433249 | -470.100587 | -470.150492 |
| eq2 | -470.435193 | -470.102497 | -470.152435 |
| eq3 | -470.432047 | -470.099302 | -470.149309 |
| eq4 | -470.437612 | -470.105006 | -470.15437 |
| eq5 | -470.432581 | -470.099794 | -470.148728 |
| eq6 | -470.433084 | -470.100299 | -470.149774 |

ax1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.477855 | -0.266448 | -0.717127 |
| H | -0.328421 | -0.815278 | -1.653922 |
| C | -0.894961 | 1.155187 | -1.132974 |
| C | -0.833933 | 2.183799 | -0.004326 |
| H | -1.104787 | 3.168403 | -0.390928 |
| H | -1.560356 | 1.940502 | 0.773933 |
| C | 0.999166 | 0.834891 | 1.071155 |
| C | 0.570152 | 2.222220 | 0.594311 |
| H | 0.617909 | 2.930649 | 1.423298 |
| H | 1.267968 | 2.580350 | -0.168671 |
| H | -0.200091 | 1.481826 | -1.914639 |
| H | 0.380160 | 0.547603 | 1.921585 |
| H | 2.029899 | 0.868407 | 1.434848 |
| H | -1.883610 | 1.143933 | -1.592095 |
| C | 0.900234 | -0.224538 | -0.036306 |
| C | 1.500815 | -1.582677 | 0.414025 |
| C | 2.112520 | -0.082510 | -1.007541 |
| C | 2.857353 | -1.163735 | -0.193764 |
| H | 1.061698 | -2.413016 | -0.140068 |
| H | 1.469966 | -1.808653 | 1.480426 |
| H | 1.862091 | -0.434577 | -2.008820 |
| H | 2.579997 | 0.899001 | -1.081569 |
| H | 3.404220 | -1.919085 | -0.754119 |
| H | 3.522860 | -0.728685 | 0.549426 |
| C | -1.547824 | -1.115545 | 0.021433 |
| H | -1.202432 | -2.148829 | -0.076613 |
| C | -2.901046 | -1.034269 | -0.686869 |
| H | -2.798186 | -1.154167 | -1.767279 |
| H | -3.567862 | -1.816969 | -0.321941 |
| H | -3.387772 | -0.074737 | -0.500078 |
| C | -1.742430 | -0.882136 | 1.521683 |
| H | -0.843297 | -1.114104 | 2.090516 |
| H | -2.037752 | 0.141936 | 1.749802 |
| H | -2.535355 | -1.539946 | 1.884707 |

ax2

```
=====
C  0.545871    -0.144611    0.622362
H  0.548838    -0.781001    1.516394
C  0.755748     1.314159    1.068186
C  0.702267     2.276602   -0.120223
H  0.838940     3.303191    0.224772
H  1.527366     2.065373   -0.805558
C -0.973911     0.700405   -1.207815
C -0.632558     2.153124   -0.859239
H -0.623510     2.760683   -1.766031
H -1.421249     2.558938   -0.219940
H -0.039918     1.580196    1.770277
H -0.304757     0.339553   -1.994632
H -1.987089     0.649166   -1.615118
H  1.693171     1.425831    1.611868
C -0.861996    -0.227362    0.006969
C -1.503107    -1.617828   -0.265183
C -2.024826     0.025738    1.013686
C -2.825368    -1.109102    0.342756
H -1.053649    -2.389090    0.359990
H -1.522218    -1.962079   -1.299338
H -1.723274    -0.245588    2.026763
H -2.472809     1.018451    1.031515
H -3.368082    -1.789861    0.995213
H -3.507276    -0.731846   -0.417186
C  1.694608    -0.650545   -0.280957
H  1.687775    -0.083690   -1.214338
C  1.551982    -2.130040   -0.643462
H  0.684431    -2.322791   -1.270807
H  2.434402    -2.467660   -1.189821
H  1.463686    -2.744028    0.256702
C  3.057328    -0.429733    0.380996
H  3.076095    -0.872788    1.380876
H  3.845656    -0.902048   -0.207017
H  3.307239     0.626245    0.476968
```

ax3

```
=====
C -0.556341    -0.038392    0.776799
H -0.575145     0.605412    1.661332
C -0.368626    -1.474889    1.291962
C -0.078758    -2.467047    0.167979
H  0.027615    -3.474294    0.575177
H -0.920365    -2.495445   -0.529537
C  1.107594    -0.626187   -1.092922
C  1.196504    -2.061034   -0.568986
H  1.400090    -2.743976   -1.395787
H  2.039145    -2.144926    0.123852
H  0.475128    -1.490775    1.990311
H  0.397244    -0.586727   -1.918029
H  2.074632    -0.325423   -1.505370
H -1.251999    -1.777483    1.857989
C  0.703466     0.378638   -0.004004
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.797191 | 1.841025 | -0.519298 |
| C | 1.936642 | 0.690051 | 0.899723 |
| C | 2.242591 | 1.920369 | 0.017882 |
| H | 0.136857 | 2.503300 | 0.039157 |
| H | 0.644894 | 2.000164 | -1.587165 |
| H | 1.627307 | 0.984186 | 1.903342 |
| H | 2.705852 | -0.078189 | 0.975251 |
| H | 2.532377 | 2.836457 | 0.528159 |
| H | 2.979984 | 1.699558 | -0.751518 |
| C | -1.946746 | 0.166161 | 0.098300 |
| H | -2.589180 | -0.633215 | 0.480725 |
| C | -2.005818 | 0.086218 | -1.429415 |
| H | -1.704070 | -0.885500 | -1.815212 |
| H | -3.031484 | 0.265467 | -1.758278 |
| H | -1.375292 | 0.847568 | -1.891697 |
| C | -2.584684 | 1.487757 | 0.540256 |
| H | -2.612592 | 1.571984 | 1.627572 |
| H | -2.030311 | 2.343129 | 0.150309 |
| H | -3.608786 | 1.562702 | 0.169764 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.366093 | 0.025184 | 1.174790 |
| H | 1.942736 | 0.790372 | 1.700896 |
| C | 2.311058 | -0.944537 | 0.466154 |
| C | 1.528321 | -1.945544 | -0.381352 |
| H | 2.211869 | -2.619451 | -0.901149 |
| H | 0.900217 | -2.566104 | 0.264586 |
| C | -0.346831 | -0.245477 | -0.724687 |
| C | 0.661233 | -1.198698 | -1.392106 |
| H | 0.122544 | -1.899046 | -2.033450 |
| H | 1.322371 | -0.620952 | -2.044709 |
| H | 2.983719 | -0.380763 | -0.189022 |
| H | -0.759126 | 0.371153 | -1.529477 |
| H | 2.937443 | -1.459030 | 1.196999 |
| C | 0.415470 | 0.728453 | 0.205919 |
| C | -0.466594 | 1.846303 | 0.831891 |
| C | 1.090770 | 1.846377 | -0.650538 |
| C | -0.107632 | 2.770841 | -0.348848 |
| H | -0.016295 | 2.199852 | 1.761038 |
| H | -1.517831 | 1.638850 | 1.011310 |
| H | 2.003495 | 2.205857 | -0.173495 |
| H | 1.300178 | 1.620787 | -1.695549 |
| H | 0.106981 | 3.813436 | -0.123666 |
| H | -0.858382 | 2.728407 | -1.136847 |
| C | -1.569851 | -1.020070 | -0.138862 |
| H | 0.800844 | -0.513854 | 1.935718 |
| C | -1.573942 | -1.300887 | 1.366696 |
| H | -2.498762 | -1.817212 | 1.632027 |
| H | -0.746154 | -1.938209 | 1.672480 |
| H | -1.529648 | -0.383288 | 1.954409 |
| C | -2.885231 | -0.340147 | -0.535362 |
| H | -2.977405 | 0.650472 | -0.087216 |
| H | -2.953488 | -0.222168 | -1.617987 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.741075 | -0.933036 | -0.207215 |
| H | -1.571408 | -1.996857 | -0.631848 |

ax5

```

=====
C   0.970962    0.716304   -1.306943
H   1.901591    0.537022   -1.851062
C   0.940731    2.152754   -0.779982
C  -0.319379    2.418093    0.043700
H  -0.266720    3.409139    0.498670
H  -1.185661    2.431420   -0.621522
C  -0.472820   -0.080460    0.597196
C  -0.512386    1.365646    1.141934
H  -1.451847    1.549334    1.663408
H   0.276611    1.493108    1.885136
H   1.820929    2.314523   -0.150020
H  -0.472924   -0.769969    1.450972
H   1.009299    2.863171   -1.605709
C   0.864513   -0.275056   -0.150554
C   1.259271   -1.755839   -0.447769
C   2.089687   -0.223918    0.819874
C   2.171913   -1.760933    0.792957
H   1.827422   -1.824396   -1.376800
H   0.472709   -2.501755   -0.462035
H   2.950493    0.235907    0.332256
H   1.948199    0.244724    1.791867
H   3.160012   -2.203619    0.684976
H   1.679589   -2.210315    1.654153
C  -1.767280   -0.355175   -0.216775
H   0.150491    0.564050   -2.015398
C  -1.737729   -1.546837   -1.174883
H  -2.682936   -1.589210   -1.719898
H  -0.934578   -1.479796   -1.907550
H  -1.630749   -2.489572   -0.635051
C  -2.956651   -0.538960    0.731278
H  -2.820737   -1.442079    1.331771
H  -3.086516    0.300003    1.413543
H  -3.883924   -0.652517    0.167124
H  -1.965740    0.527103   -0.829029

```

ax6

```

=====
C  -0.886410    1.080259    1.133831
H  -1.874040    1.218741    1.581302
C  -0.432750    2.369770    0.453161
C   0.913032    2.164034   -0.236955
H   1.217828    3.076428   -0.753572
H   1.680672    1.952807    0.511248
C   0.339403   -0.321200   -0.641448
C   0.811921    1.017377   -1.241476
H   1.756295    0.882405   -1.767931
H   0.082743    1.313334   -2.002124
H  -1.174109    2.665001   -0.297144
H   0.067818   -0.942616   -1.502484

```

| | | | |
|---|-----------|-----------|-----------|
| H | -0.377016 | 3.180426 | 1.181795 |
| C | -0.966740 | -0.094730 | 0.157896 |
| C | -1.584050 | -1.402441 | 0.728120 |
| C | -2.182722 | -0.029008 | -0.817497 |
| C | -2.454127 | -1.523481 | -0.540786 |
| H | -2.193455 | -1.180898 | 1.605562 |
| H | -0.915627 | -2.227998 | 0.964600 |
| H | -2.975452 | 0.602655 | -0.414370 |
| H | -1.982496 | 0.264101 | -1.847672 |
| H | -3.490368 | -1.828762 | -0.411182 |
| H | -1.990097 | -2.163972 | -1.289224 |
| C | 1.426437 | -1.164507 | 0.081206 |
| H | -0.201944 | 0.852493 | 1.952213 |
| C | 2.730540 | -1.203457 | -0.717233 |
| H | 3.385051 | -1.986577 | -0.331436 |
| H | 2.549782 | -1.405561 | -1.774897 |
| H | 3.270797 | -0.257505 | -0.642997 |
| C | 1.729954 | -0.822920 | 1.541193 |
| H | 2.096708 | 0.196927 | 1.659683 |
| H | 0.855896 | -0.947248 | 2.179469 |
| H | 2.505556 | -1.495850 | 1.913584 |
| H | 1.038531 | -2.186512 | 0.085511 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.400261 | -0.621925 | -0.273900 |
| H | -0.472601 | -0.899129 | -1.334989 |
| C | 0.260475 | -1.789205 | 0.489114 |
| C | 1.653760 | -2.150912 | -0.011035 |
| H | 2.051874 | -2.988425 | 0.564913 |
| H | 1.596850 | -2.476097 | -1.054728 |
| C | 1.950622 | 0.231166 | -0.661979 |
| C | 2.567257 | -0.937524 | 0.093593 |
| H | 3.561016 | -1.156595 | -0.301259 |
| H | 2.693428 | -0.672472 | 1.147901 |
| H | 0.335010 | -1.494862 | 1.542880 |
| H | 1.904465 | -0.019999 | -1.727933 |
| H | 2.584937 | 1.118157 | -0.577430 |
| H | -0.381619 | -2.668409 | 0.459621 |
| C | 0.531378 | 0.605872 | -0.205981 |
| C | 0.146775 | 1.919310 | -0.951222 |
| C | 0.558046 | 1.394512 | 1.135415 |
| C | 0.425164 | 2.719166 | 0.345876 |
| H | -0.877606 | 1.979478 | -1.297402 |
| H | 0.803415 | 2.151163 | -1.789986 |
| H | -0.303120 | 1.190150 | 1.770229 |
| H | 1.462762 | 1.278970 | 1.732144 |
| H | -0.371770 | 3.384665 | 0.672663 |
| H | 1.352454 | 3.287264 | 0.304617 |
| C | -1.848468 | -0.479380 | 0.274679 |
| H | -1.784671 | -0.607940 | 1.360225 |
| C | -2.731590 | -1.603956 | -0.280553 |
| H | -2.310665 | -2.595920 | -0.126838 |
| H | -3.715473 | -1.586009 | 0.190893 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.877042 | -1.464723 | -1.354787 |
| C | -2.588474 | 0.837411 | 0.030329 |
| H | -2.088383 | 1.700368 | 0.465726 |
| H | -2.731692 | 1.021550 | -1.036039 |
| H | -3.579675 | 0.771613 | 0.483560 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.561433 | 0.419846 | -0.389458 |
| H | 0.533535 | 0.872723 | -1.390072 |
| C | 0.437046 | 1.582202 | 0.605452 |
| C | -0.750962 | 2.473461 | 0.234000 |
| H | -0.852550 | 3.291009 | 0.950308 |
| H | -0.550344 | 2.927765 | -0.741387 |
| C | -1.906344 | 0.434803 | -0.720932 |
| C | -2.052536 | 1.676692 | 0.160242 |
| H | -2.861360 | 2.307008 | -0.214165 |
| H | -2.338120 | 1.371030 | 1.170185 |
| H | 0.300819 | 1.188916 | 1.618468 |
| H | -1.761447 | 0.737208 | -1.763378 |
| H | -2.825123 | -0.157303 | -0.685195 |
| H | 1.346972 | 2.182530 | 0.616878 |
| C | -0.716208 | -0.435792 | -0.293076 |
| C | -0.752007 | -1.814739 | -1.002645 |
| C | -1.069796 | -1.157461 | 1.045841 |
| C | -1.462908 | -2.413134 | 0.232326 |
| H | 0.238100 | -2.245247 | -1.138891 |
| H | -1.286227 | -1.850431 | -1.952878 |
| H | -0.218133 | -1.323196 | 1.697562 |
| H | -1.865388 | -0.699369 | 1.631867 |
| H | -1.083272 | -3.366897 | 0.593442 |
| H | -2.539560 | -2.496018 | 0.096534 |
| C | 1.917120 | -0.320993 | -0.354054 |
| H | 1.915660 | -1.003980 | -1.206873 |
| C | 2.196927 | -1.154390 | 0.897263 |
| H | 1.565512 | -2.040304 | 0.952947 |
| H | 3.234744 | -1.493731 | 0.889696 |
| H | 2.048428 | -0.569686 | 1.807973 |
| C | 3.075576 | 0.654641 | -0.583282 |
| H | 3.281107 | 1.249293 | 0.308311 |
| H | 3.987063 | 0.106244 | -0.825711 |
| H | 2.865538 | 1.341614 | -1.405684 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.271810 | -0.811871 | -0.265430 |
| H | -0.132780 | -1.171181 | -1.293575 |
| C | 0.589282 | -1.726975 | 0.619995 |
| C | 2.011383 | -1.840825 | 0.069223 |
| H | 2.621692 | -2.477334 | 0.712811 |
| H | 1.964340 | -2.328592 | -0.909476 |
| C | 1.758719 | 0.501962 | -0.846415 |
| C | 2.662446 | -0.467677 | -0.083507 |
| H | 3.624232 | -0.558490 | -0.591835 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.872134 | -0.061656 | 0.909349 |
| H | 0.616570 | -1.331302 | 1.641341 |
| H | 1.660767 | 0.172436 | -1.886075 |
| H | 2.217309 | 1.493902 | -0.869749 |
| H | 0.137329 | -2.719432 | 0.675581 |
| C | 0.351576 | 0.598440 | -0.232514 |
| C | -0.406148 | 1.814671 | -0.828778 |
| C | 0.444032 | 1.383722 | 1.114443 |
| C | 0.103777 | 2.680721 | 0.344147 |
| H | -1.484160 | 1.701376 | -0.775120 |
| H | -0.127779 | 2.111146 | -1.841156 |
| H | -0.330210 | 1.115366 | 1.825638 |
| H | 1.406661 | 1.356485 | 1.623183 |
| H | -0.620714 | 3.349136 | 0.804915 |
| H | 0.993141 | 3.252562 | 0.087333 |
| C | -1.783904 | -1.007681 | 0.012048 |
| H | -1.883779 | -2.080159 | 0.206605 |
| C | -2.662700 | -0.734329 | -1.212755 |
| H | -2.290415 | -1.269488 | -2.087993 |
| H | -3.682948 | -1.074518 | -1.023886 |
| H | -2.716143 | 0.323477 | -1.466474 |
| C | -2.349960 | -0.297087 | 1.241641 |
| H | -2.382238 | 0.785239 | 1.106358 |
| H | -3.372749 | -0.635072 | 1.419384 |
| H | -1.770409 | -0.512328 | 2.140247 |

eq4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -2.069531 | 0.163819 | -0.682038 |
| H | -2.042398 | -0.176570 | -1.723470 |
| C | -2.527146 | -0.982804 | 0.216353 |
| C | -1.522294 | -2.131449 | 0.179335 |
| H | -1.824217 | -2.924785 | 0.865744 |
| H | -1.509020 | -2.564937 | -0.825722 |
| C | 0.323603 | -0.489577 | -0.391285 |
| C | -0.120858 | -1.634120 | 0.529473 |
| H | 0.592998 | -2.458585 | 0.475572 |
| H | -0.117400 | -1.283821 | 1.566310 |
| H | -2.616330 | -0.617121 | 1.244797 |
| H | 0.216395 | -0.850282 | -1.422934 |
| H | -3.517823 | -1.328486 | -0.084277 |
| C | -0.684216 | 0.678680 | -0.292736 |
| C | -0.248018 | 1.970951 | -1.033532 |
| C | -0.660415 | 1.495967 | 1.032991 |
| C | 0.157140 | 2.596287 | 0.320713 |
| H | -1.111303 | 2.476860 | -1.467058 |
| H | 0.522503 | 1.875549 | -1.798211 |
| H | -1.664105 | 1.844354 | 1.281447 |
| H | -0.230486 | 1.030791 | 1.917373 |
| H | -0.144731 | 3.626611 | 0.498035 |
| H | 1.224795 | 2.505241 | 0.514302 |
| C | 1.828267 | -0.154232 | -0.232853 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.782606 | 0.990338 | -0.633828 |
| C | 2.330729 | -0.081292 | 1.211360 |
| H | 3.381948 | 0.212450 | 1.220108 |
| H | 1.783434 | 0.638592 | 1.816777 |
| H | 2.261182 | -1.055332 | 1.699384 |
| C | 2.674124 | -1.174093 | -1.001206 |
| H | 2.415808 | -1.183873 | -2.061177 |
| H | 3.736370 | -0.938902 | -0.914769 |
| H | 2.528034 | -2.183190 | -0.609675 |
| H | 2.008650 | 0.816271 | -0.698187 |

eq5

```
=====
```

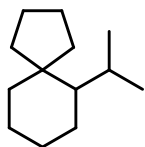
| | | | |
|---|-----------|-----------|-----------|
| C | -1.805036 | 0.972797 | -0.607816 |
| H | -1.890741 | 0.805778 | -1.687941 |
| C | -2.775013 | 0.052866 | 0.124752 |
| C | -2.392262 | -1.404836 | -0.102799 |
| H | -3.046355 | -2.068641 | 0.465767 |
| H | -2.523419 | -1.652457 | -1.160921 |
| C | 0.039092 | -0.714133 | -0.464148 |
| C | -0.936964 | -1.631763 | 0.294298 |
| H | -0.657334 | -2.673943 | 0.122925 |
| H | -0.839194 | -1.453025 | 1.369363 |
| H | -2.738310 | 0.270902 | 1.197318 |
| H | -0.150708 | -0.865977 | -1.535630 |
| H | -3.798405 | 0.243012 | -0.203710 |
| C | -0.343942 | 0.760990 | -0.196821 |
| C | 0.585819 | 1.858192 | -0.788716 |
| C | -0.008077 | 1.308703 | 1.223756 |
| C | 1.151401 | 2.135396 | 0.621533 |
| H | -0.006914 | 2.697654 | -1.153582 |
| H | 1.284494 | 1.567694 | -1.567973 |
| H | -0.811053 | 1.944673 | 1.598474 |
| H | 0.245412 | 0.583324 | 1.993802 |
| H | 1.213425 | 3.178926 | 0.923964 |
| H | 2.122574 | 1.671369 | 0.780218 |
| C | 1.486941 | -1.234735 | -0.250432 |
| H | -2.067282 | 2.017921 | -0.426813 |
| C | 2.553788 | -0.618385 | -1.158615 |
| H | 3.437186 | -1.260022 | -1.167431 |
| H | 2.201219 | -0.523198 | -2.186981 |
| H | 2.873860 | 0.364106 | -0.813736 |
| C | 1.996277 | -1.269133 | 1.193840 |
| H | 1.280964 | -1.728769 | 1.875591 |
| H | 2.914572 | -1.858339 | 1.236591 |
| H | 2.234645 | -0.274949 | 1.569151 |
| H | 1.409227 | -2.281791 | -0.561442 |

eq6

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.969595 | 0.571588 | -0.692774 |
| H | -1.929011 | 0.354150 | -1.766819 |
| C | -2.722254 | -0.542655 | 0.019483 |
| C | -1.958379 | -1.847923 | -0.138997 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.452973 | -2.658350 | 0.399941 |
| H | -1.946982 | -2.128821 | -1.197237 |
| C | 0.262957 | -0.566179 | -0.329112 |
| C | -0.521223 | -1.704774 | 0.353944 |
| H | -0.009967 | -2.651025 | 0.192006 |
| H | -0.525634 | -1.531641 | 1.436590 |
| H | -2.810549 | -0.298652 | 1.083424 |
| H | 0.294107 | -0.792977 | -1.404251 |
| H | -3.736575 | -0.631803 | -0.373623 |
| C | -0.540977 | 0.754149 | -0.176731 |
| C | 0.104748 | 2.053354 | -0.734885 |
| C | -0.449032 | 1.387572 | 1.245190 |
| C | 0.531117 | 2.449591 | 0.695428 |
| H | -0.676041 | 2.719133 | -1.104295 |
| H | 0.865109 | 1.964335 | -1.505580 |
| H | -1.402197 | 1.825376 | 1.543516 |
| H | -0.088588 | 0.752816 | 2.053831 |
| H | 0.353392 | 3.482077 | 0.989817 |
| H | 1.568672 | 2.198747 | 0.908903 |
| C | 1.740016 | -0.533709 | 0.165461 |
| H | -2.499768 | 1.520174 | -0.581488 |
| C | 2.318576 | -1.938883 | 0.383720 |
| H | 3.375765 | -1.862222 | 0.640069 |
| H | 1.825895 | -2.480601 | 1.188453 |
| H | 2.241627 | -2.538625 | -0.527474 |
| C | 2.693048 | 0.197327 | -0.790330 |
| H | 2.547318 | 1.272137 | -0.817579 |
| H | 3.726676 | 0.023035 | -0.487336 |
| H | 2.579721 | -0.186872 | -1.807447 |
| H | 1.765993 | -0.027127 | 1.134192 |



6-isopropylspiro[4.5]decane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -509.766053 | -509.402137 | -509.454113 |
| ax1 | -509.768258 | -509.404274 | -509.455993 |
| ax2 | -509.764274 | -509.400289 | -509.451951 |
| ax3 | -509.766719 | -509.402869 | -509.455725 |
| ax4 | -509.764916 | -509.400981 | -509.452809 |
| ax5 | -509.768258 | -509.404272 | -509.455982 |
| ax6 | -509.762876 | -509.398999 | -509.450669 |
| ax7 | -509.767126 | -509.403172 | -509.455326 |
| ax8 | -509.766934 | -509.402978 | -509.454485 |
| ax9 | -509.763737 | -509.399609 | -509.450804 |
| eq1 | -509.766230 | -509.402171 | -509.45309 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| eq2 | | -509.770183 | | -509.406493 | | -509.458434 |
| eq3 | | -509.765638 | | -509.401801 | | -509.452723 |
| eq4 | | -509.766965 | | -509.403061 | | -509.455692 |
| eq5 | | -509.764186 | | -509.400155 | | -509.452144 |
| eq6 | | -509.771026 | | -509.407417 | | -509.459022 |
| eq7 | | -509.764468 | | -509.400612 | | -509.452169 |

ax

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.110366 | 2.383717 | 0.615729 |
| C | 0.533386 | 1.105025 | 1.149124 |
| C | -0.603606 | -0.285070 | -0.678768 |
| H | -0.303452 | -0.807143 | -1.595926 |
| C | -1.450179 | 2.076054 | -0.047090 |
| C | -1.274280 | 1.023044 | -1.142234 |
| H | -2.230685 | 0.807960 | -1.618762 |
| H | -0.644043 | 1.464311 | -1.920136 |
| H | -2.159697 | 1.733018 | 0.707572 |
| H | -1.871913 | 2.984166 | -0.483048 |
| H | -0.239705 | 3.100876 | 1.428485 |
| H | 0.549022 | 2.855212 | -0.118753 |
| C | 0.726746 | 0.025868 | 0.063200 |
| C | 1.812534 | 0.519798 | -0.956260 |
| C | 1.372980 | -1.236724 | 0.686682 |
| C | 2.963339 | -0.496564 | -0.901878 |
| H | 2.185397 | 1.500508 | -0.657013 |
| H | 1.412674 | 0.626997 | -1.964301 |
| C | 2.880094 | -1.045541 | 0.520834 |
| H | 1.084069 | -2.122330 | 0.115778 |
| H | 1.061158 | -1.393551 | 1.720015 |
| H | 2.782956 | -1.310122 | -1.608854 |
| H | 3.927730 | -0.052321 | -1.146922 |
| H | 3.444979 | -1.966231 | 0.665828 |
| H | 3.255138 | -0.304772 | 1.231392 |
| H | 1.508077 | 1.331756 | 1.589891 |
| H | -0.089988 | 0.714755 | 1.954423 |
| C | -1.552990 | -1.306442 | 0.007420 |
| H | -0.996097 | -2.245620 | 0.036419 |
| C | -2.000923 | -1.036198 | 1.446459 |
| H | -2.665809 | -1.841461 | 1.767461 |
| H | -1.166227 | -1.010321 | 2.144154 |
| H | -2.555921 | -0.103126 | 1.539790 |
| C | -2.789590 | -1.567819 | -0.857561 |
| H | -2.525573 | -1.700303 | -1.908762 |
| H | -3.300399 | -2.471553 | -0.521517 |
| H | -3.504550 | -0.745606 | -0.791148 |

ax1

```
=====
```

| | | | |
|---|----------|-----------|-----------|
| C | 0.765974 | -0.164252 | 0.628946 |
| H | 0.704273 | -0.750509 | 1.554055 |
| C | 1.198689 | 1.263206 | 1.017078 |
| C | 1.188946 | 2.216165 | -0.179305 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.516083 | 3.210470 | 0.130969 |
| H | 1.900247 | 1.870037 | -0.934812 |
| C | -0.717854 | 0.887796 | -1.146682 |
| C | -0.202620 | 2.285812 | -0.804204 |
| H | -0.185132 | 2.902453 | -1.704945 |
| H | -0.887876 | 2.773105 | -0.105761 |
| H | 0.510047 | 1.646203 | 1.773693 |
| H | -0.114719 | 0.477488 | -1.961778 |
| H | -1.739730 | 0.954199 | -1.526380 |
| H | 2.181999 | 1.248925 | 1.484979 |
| C | 1.811088 | -0.884057 | -0.274507 |
| H | 1.615957 | -0.621824 | -1.318041 |
| C | -0.672038 | -0.092026 | 0.044065 |
| C | -1.276735 | -1.442154 | -0.383210 |
| C | -1.696910 | 0.329894 | 1.123145 |
| C | -2.797572 | -1.215243 | -0.437341 |
| H | -1.050665 | -2.186845 | 0.383120 |
| H | -0.876154 | -1.804193 | -1.330698 |
| C | -3.073903 | -0.066422 | 0.563342 |
| H | -1.650341 | 1.385399 | 1.382600 |
| H | -1.485063 | -0.237878 | 2.033301 |
| H | -3.109812 | -0.931845 | -1.442047 |
| H | -3.341671 | -2.123157 | -0.181133 |
| H | -3.537841 | 0.779313 | 0.055797 |
| H | -3.753559 | -0.369533 | 1.358483 |
| C | 3.256387 | -0.479597 | 0.041017 |
| H | 3.943862 | -1.065137 | -0.571206 |
| H | 3.460132 | 0.572456 | -0.148845 |
| H | 3.492093 | -0.684838 | 1.088663 |
| C | 1.744423 | -2.411138 | -0.143829 |
| H | 1.921621 | -2.703900 | 0.894506 |
| H | 0.795003 | -2.835418 | -0.453111 |
| H | 2.523976 | -2.872878 | -0.752490 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.783766 | 0.072985 | 0.820895 |
| H | -0.598119 | 0.593425 | 1.766199 |
| C | -1.171430 | -1.369065 | 1.203153 |
| C | -1.209313 | -2.332522 | 0.017176 |
| H | -1.439850 | -3.339789 | 0.370343 |
| H | -2.012074 | -2.054208 | -0.667671 |
| C | 0.573708 | -0.920985 | -1.106338 |
| C | 0.128142 | -2.334919 | -0.722226 |
| H | 0.064818 | -2.953918 | -1.619305 |
| H | 0.883997 | -2.796046 | -0.081105 |
| H | -0.442081 | -1.745979 | 1.925839 |
| H | -0.080334 | -0.539817 | -1.890741 |
| H | 1.575720 | -0.966942 | -1.539341 |
| H | -2.136906 | -1.359911 | 1.713346 |
| C | -1.981736 | 0.848375 | 0.190746 |
| H | -2.867129 | 0.429122 | 0.679349 |
| C | 0.578218 | 0.064300 | 0.081953 |
| C | 1.061108 | 1.454529 | -0.370334 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.725430 | -0.310503 | 1.052582 |
| C | 2.577459 | 1.312546 | -0.584713 |
| H | 0.875731 | 2.164160 | 0.439509 |
| H | 0.545623 | 1.822720 | -1.257050 |
| C | 3.017781 | 0.178348 | 0.373894 |
| H | 1.761869 | -1.371548 | 1.292557 |
| H | 1.572033 | 0.229304 | 1.990422 |
| H | 2.795419 | 1.045495 | -1.618518 |
| H | 3.097517 | 2.247766 | -0.382397 |
| H | 3.491745 | -0.630602 | -0.181751 |
| H | 3.743170 | 0.523703 | 1.109174 |
| C | -1.964789 | 2.338762 | 0.552909 |
| H | -2.924375 | 2.795533 | 0.302557 |
| H | -1.789144 | 2.491062 | 1.618973 |
| H | -1.194409 | 2.878155 | 0.001783 |
| C | -2.222435 | 0.729151 | -1.318270 |
| H | -2.319197 | -0.298040 | -1.661263 |
| H | -3.150320 | 1.247732 | -1.569435 |
| H | -1.423965 | 1.202618 | -1.890038 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.725182 | -0.225145 | -0.703822 |
| H | -0.573159 | -0.720886 | -1.669329 |
| C | -1.280080 | 1.173823 | -1.034691 |
| C | -1.213321 | 2.179502 | 0.116678 |
| H | -1.566345 | 3.152277 | -0.232156 |
| H | -1.876619 | 1.879195 | 0.929090 |
| C | 0.758250 | 0.927873 | 1.052222 |
| C | 0.211552 | 2.297031 | 0.648937 |
| H | 0.243449 | 2.971946 | 1.506431 |
| H | 0.847264 | 2.741118 | -0.121749 |
| H | -0.688029 | 1.579323 | -1.861106 |
| H | 0.195597 | 0.568007 | 1.915056 |
| H | 1.793988 | 1.030870 | 1.384083 |
| H | -2.301921 | 1.094022 | -1.407379 |
| C | -1.714577 | -1.180569 | 0.016039 |
| H | -1.219070 | -2.154637 | 0.024372 |
| C | 0.691018 | -0.117628 | -0.081581 |
| C | 1.240440 | -1.467727 | 0.411235 |
| C | 1.747075 | 0.231210 | -1.157500 |
| C | 2.765903 | -1.286419 | 0.487107 |
| H | 0.999804 | -2.233957 | -0.330915 |
| H | 0.803935 | -1.780715 | 1.360847 |
| C | 3.100753 | -0.191620 | -0.557879 |
| H | 1.733173 | 1.278841 | -1.454895 |
| H | 1.538227 | -0.362834 | -2.050376 |
| H | 3.064093 | -0.964783 | 1.484666 |
| H | 3.288966 | -2.220108 | 0.285634 |
| H | 3.594352 | 0.654553 | -0.080447 |
| H | 3.776922 | -0.557004 | -1.329499 |
| C | -2.093445 | -0.874147 | 1.466439 |
| H | -2.757768 | -1.659009 | 1.835420 |
| H | -1.230031 | -0.843413 | 2.127915 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.631025 | 0.069743 | 1.556599 |
| C | -2.996497 | -1.352794 | -0.804092 |
| H | -2.778541 | -1.521322 | -1.860602 |
| H | -3.568251 | -2.206852 | -0.437382 |
| H | -3.640351 | -0.474709 | -0.728830 |

ax4

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.216223 | 1.015069 | -1.185030 |
| C | 0.564847 | -0.297822 | -0.713943 |
| C | -0.474465 | 1.074171 | 1.189127 |
| H | -1.441757 | 1.358195 | 1.614839 |
| H | 0.090023 | 0.613141 | 1.999631 |
| C | 1.539396 | 1.979999 | -0.046250 |
| C | 0.266799 | 2.328442 | 0.722377 |
| H | 0.498055 | 2.956407 | 1.585059 |
| H | -0.379954 | 2.921951 | 0.070962 |
| H | 2.274603 | 1.535303 | 0.627322 |
| H | 1.992308 | 2.888669 | -0.448290 |
| H | 2.107674 | 0.806759 | -1.775453 |
| H | 0.514999 | 1.513875 | -1.861670 |
| C | -0.733521 | 0.031758 | 0.077536 |
| C | -1.814805 | 0.600306 | -0.894386 |
| C | -1.423105 | -1.228750 | 0.690502 |
| C | -3.142357 | -0.000618 | -0.431963 |
| H | -1.610228 | 0.261826 | -1.913370 |
| H | -1.830003 | 1.689131 | -0.913114 |
| C | -2.740748 | -1.426972 | -0.068956 |
| H | -1.640041 | -1.039232 | 1.744671 |
| H | -0.796318 | -2.116520 | 0.652275 |
| H | -3.504213 | 0.519118 | 0.459212 |
| H | -3.921732 | 0.056624 | -1.191724 |
| H | -3.489368 | -1.960269 | 0.516617 |
| H | -2.565735 | -1.996999 | -0.985065 |
| C | 1.542434 | -1.322487 | -0.062947 |
| H | 1.062078 | -2.295953 | -0.187025 |
| H | 0.235981 | -0.809455 | -1.625483 |
| C | 2.861558 | -1.403356 | -0.834550 |
| H | 3.485246 | -0.525873 | -0.651615 |
| H | 3.427292 | -2.281067 | -0.518151 |
| H | 2.695357 | -1.479840 | -1.910841 |
| C | 1.839832 | -1.195470 | 1.434028 |
| H | 2.316094 | -0.249086 | 1.688455 |
| H | 0.942348 | -1.298021 | 2.042141 |
| H | 2.524758 | -1.994313 | 1.727354 |

ax5

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| | | | |
|---|-----------|-----------|-----------|
| C | -1.198648 | -1.263332 | -1.016894 |
| C | -0.765879 | 0.164133 | -0.628899 |
| C | 0.717942 | -0.887743 | 1.146810 |
| H | 1.739902 | -0.954289 | 1.526268 |
| H | 0.115060 | -0.477224 | 1.961995 |
| C | -1.189245 | -2.215903 | 0.179798 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.202357 | -2.285716 | 0.804636 |
| H | 0.184842 | -2.902260 | 1.705441 |
| H | 0.887404 | -2.773267 | 0.106159 |
| H | -1.900419 | -1.869246 | 0.935180 |
| H | -1.516637 | -3.210258 | -0.130048 |
| H | -2.181784 | -1.249101 | -1.485153 |
| H | -0.509752 | -1.646592 | -1.773163 |
| C | 0.672064 | 0.091930 | -0.044044 |
| C | 1.696735 | -0.330117 | -1.123220 |
| C | 1.276763 | 1.442074 | 0.383182 |
| C | 3.073814 | 0.066313 | -0.563664 |
| H | 1.484788 | 0.237440 | -2.033486 |
| H | 1.650180 | -1.385675 | -1.382467 |
| C | 2.797651 | 1.215295 | 0.436830 |
| H | 0.876487 | 1.803765 | 1.330900 |
| H | 1.050233 | 2.186899 | -0.382899 |
| H | 3.537904 | -0.779345 | -0.056111 |
| H | 3.753329 | 0.369292 | -1.358978 |
| H | 3.110343 | 0.932171 | 1.441488 |
| H | 3.341596 | 2.123195 | 0.180246 |
| C | -1.811130 | 0.883793 | 0.274477 |
| H | -1.616754 | 0.620663 | 1.317906 |
| H | -0.704072 | 0.750419 | -1.553970 |
| C | -1.743981 | 2.410967 | 0.144980 |
| H | -1.920033 | 2.704492 | -0.893333 |
| H | -2.524221 | 2.872212 | 0.753181 |
| H | -0.794890 | 2.834930 | 0.455762 |
| C | -3.256387 | 0.480246 | -0.042458 |
| H | -3.944116 | 1.066023 | 0.569263 |
| H | -3.490860 | 0.685893 | -1.090307 |
| H | -3.460866 | -0.571769 | 0.146919 |

ax6

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.173904 | -1.154329 | 1.326180 |
| C | 0.646661 | 0.177644 | 0.764942 |
| C | -0.366971 | -1.172352 | -1.166114 |
| H | -1.327506 | -1.430743 | -1.622221 |
| H | 0.240718 | -0.747406 | -1.964423 |
| C | 1.537316 | -2.131502 | 0.209875 |
| C | 0.306432 | -2.443406 | -0.640327 |
| H | 0.574834 | -3.086636 | -1.480730 |
| H | -0.400602 | -3.010944 | -0.029830 |
| H | 2.324115 | -1.699749 | -0.414711 |
| H | 1.941969 | -3.053255 | 0.632136 |
| H | 2.038741 | -0.961836 | 1.964360 |
| H | 0.410053 | -1.613600 | 1.960478 |
| C | -0.624216 | -0.098984 | -0.086455 |
| C | -1.773667 | -0.599741 | 0.842623 |
| C | -1.226419 | 1.183282 | -0.744279 |
| C | -3.053373 | 0.015599 | 0.278310 |
| H | -1.618825 | -0.222456 | 1.856969 |
| H | -1.818660 | -1.686124 | 0.905039 |
| C | -2.594717 | 1.422866 | -0.091847 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.357595 | 1.010501 | -1.815280 |
| H | -0.578153 | 2.048613 | -0.641897 |
| H | -3.368779 | -0.520645 | -0.620563 |
| H | -3.881761 | -0.003090 | 0.986330 |
| H | -3.286100 | 1.954399 | -0.745337 |
| H | -2.477539 | 2.013957 | 0.820084 |
| C | 1.823333 | 1.009485 | 0.150404 |
| H | 2.737755 | 0.554117 | 0.542193 |
| H | 0.297748 | 0.765884 | 1.619021 |
| C | 1.990764 | 1.026343 | -1.373038 |
| H | 1.116713 | 1.429870 | -1.883849 |
| H | 2.841200 | 1.662503 | -1.627305 |
| H | 2.193325 | 0.037603 | -1.780186 |
| C | 1.817168 | 2.448867 | 0.678788 |
| H | 0.950646 | 3.010014 | 0.325075 |
| H | 1.798978 | 2.464334 | 1.769747 |
| H | 2.711430 | 2.982063 | 0.350537 |

ax7

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| | | | |
|---|-----------|-----------|-----------|
| C | -0.219733 | 1.547836 | 1.115779 |
| H | -1.070140 | 2.032025 | 1.603502 |
| C | 0.552288 | 2.559681 | 0.273813 |
| C | 1.721566 | 1.874900 | -0.425587 |
| H | 2.256091 | 2.585874 | -1.059123 |
| H | 2.432465 | 1.527869 | 0.326367 |
| C | 0.358368 | -0.335768 | -0.549854 |
| C | 1.225813 | 0.710004 | -1.284340 |
| H | 2.068082 | 0.215102 | -1.768490 |
| H | 0.627718 | 1.136897 | -2.093977 |
| H | -0.112242 | 2.999806 | -0.476161 |
| H | -0.171817 | -0.875066 | -1.342757 |
| H | 0.907419 | 3.377758 | 0.903239 |
| C | -0.752358 | 0.363734 | 0.297227 |
| C | -1.528050 | -0.621829 | 1.187642 |
| C | -1.884498 | 0.810999 | -0.659901 |
| C | -2.383043 | -1.440941 | 0.215533 |
| H | -2.181096 | -0.034785 | 1.840271 |
| H | -0.892707 | -1.231164 | 1.829253 |
| C | -2.744601 | -0.447106 | -0.916254 |
| H | -1.511187 | 1.250489 | -1.583998 |
| H | -2.482601 | 1.574768 | -0.156957 |
| H | -1.803107 | -2.274322 | -0.183667 |
| H | -3.264418 | -1.863802 | 0.695644 |
| H | -2.531955 | -0.879365 | -1.893429 |
| H | -3.805065 | -0.198541 | -0.905492 |
| C | 1.155877 | -1.459835 | 0.159889 |
| H | 0.411168 | -2.191143 | 0.483434 |
| H | 0.433847 | 1.188409 | 1.913543 |
| C | 2.071459 | -2.193726 | -0.824529 |
| H | 2.955299 | -1.602995 | -1.070789 |
| H | 2.419863 | -3.130975 | -0.387379 |
| H | 1.552491 | -2.428956 | -1.756044 |
| C | 1.963539 | -1.070884 | 1.398933 |

| | | | |
|---|----------|-----------|----------|
| H | 2.754507 | -0.360531 | 1.156515 |
| H | 1.344156 | -0.639254 | 2.183250 |
| H | 2.443457 | -1.960482 | 1.813139 |

ax8

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| | | | |
|---|-----------|-----------|-----------|
| C | 0.035492 | -1.468439 | 1.266588 |
| H | 0.831026 | -1.985853 | 1.808727 |
| C | -0.855549 | -2.475975 | 0.545437 |
| C | -1.940311 | -1.745140 | -0.239289 |
| H | -2.558796 | -2.453919 | -0.793515 |
| H | -2.598284 | -1.235715 | 0.469948 |
| C | -0.415010 | 0.304198 | -0.507065 |
| C | -1.318754 | -0.734434 | -1.203660 |
| H | -2.095363 | -0.227442 | -1.775042 |
| H | -0.724833 | -1.285388 | -1.935705 |
| H | -0.250637 | -3.077652 | -0.139560 |
| H | 0.096410 | 0.855308 | -1.304637 |
| H | -1.301682 | -3.165384 | 1.264687 |
| C | 0.680506 | -0.448697 | 0.318919 |
| C | 1.630080 | 0.478205 | 1.099132 |
| C | 1.701234 | -1.117353 | -0.631373 |
| C | 2.588593 | 1.070885 | 0.055317 |
| H | 2.200790 | -0.152549 | 1.786411 |
| H | 1.117976 | 1.221137 | 1.708081 |
| C | 2.659589 | 0.005893 | -1.068282 |
| H | 1.249656 | -1.627606 | -1.479396 |
| H | 2.251232 | -1.869363 | -0.058986 |
| H | 2.205123 | 2.010191 | -0.341506 |
| H | 3.566999 | 1.282389 | 0.484590 |
| H | 2.342047 | 0.433515 | -2.019136 |
| H | 3.671086 | -0.371094 | -1.213089 |
| C | -1.212213 | 1.366761 | 0.312639 |
| H | -1.240021 | 1.048610 | 1.358797 |
| H | -0.562541 | -0.940803 | 2.016848 |
| C | -0.547025 | 2.747785 | 0.247379 |
| H | -0.547082 | 3.107161 | -0.785110 |
| H | -1.107176 | 3.467958 | 0.846845 |
| H | 0.480116 | 2.754647 | 0.598928 |
| C | -2.661612 | 1.566274 | -0.147027 |
| H | -3.270963 | 0.668839 | -0.065213 |
| H | -3.131277 | 2.341238 | 0.461043 |
| H | -2.693932 | 1.901998 | -1.186307 |

ax9

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| | | | |
|---|----------|-----------|-----------|
| C | 0.744763 | -1.143760 | -1.275601 |
| H | 0.281107 | -1.866525 | -1.952572 |
| C | 1.893744 | -1.808540 | -0.516691 |
| C | 2.505063 | -0.851707 | 0.504497 |
| H | 3.276796 | -1.362773 | 1.083823 |
| H | 2.999690 | -0.027609 | -0.013737 |
| C | 0.243342 | 0.368765 | 0.731158 |
| C | 1.427898 | -0.317005 | 1.447251 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.864272 | 0.384530 | 2.160920 |
| H | 1.052179 | -1.156062 | 2.037296 |
| H | 1.519987 | -2.694853 | 0.005055 |
| H | -0.532639 | 0.483336 | 1.494775 |
| H | 2.653797 | -2.153959 | -1.220036 |
| C | -0.347410 | -0.589353 | -0.348764 |
| C | -1.509221 | 0.026635 | -1.151121 |
| C | -1.108120 | -1.741597 | 0.354931 |
| C | -2.712401 | 0.036971 | -0.197488 |
| H | -1.719012 | -0.644676 | -1.989158 |
| H | -1.288567 | 1.003719 | -1.573127 |
| C | -2.477990 | -1.161992 | 0.754648 |
| H | -0.575154 | -2.165681 | 1.203504 |
| H | -1.246417 | -2.545438 | -0.373003 |
| H | -2.744485 | 0.967994 | 0.367673 |
| H | -3.655094 | -0.041936 | -0.737322 |
| H | -2.471702 | -0.831251 | 1.793054 |
| H | -3.262705 | -1.912255 | 0.667209 |
| C | 0.603123 | 1.834083 | 0.329265 |
| H | 1.329733 | 2.153569 | 1.082453 |
| H | 1.145589 | -0.345082 | -1.901271 |
| C | 1.270758 | 2.075229 | -1.029565 |
| H | 0.606613 | 1.839987 | -1.861114 |
| H | 1.530244 | 3.132950 | -1.111699 |
| H | 2.187058 | 1.504069 | -1.160097 |
| C | -0.584396 | 2.793988 | 0.474159 |
| H | -1.330823 | 2.647686 | -0.306276 |
| H | -1.077166 | 2.672818 | 1.440229 |
| H | -0.238215 | 3.827133 | 0.403345 |

eq1

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| | | | |
|---|-----------|-----------|-----------|
| C | -2.644741 | -1.080799 | 0.118803 |
| C | -1.410207 | -1.493487 | -0.666538 |
| H | -1.585073 | -1.281286 | -1.727251 |
| C | -0.317336 | 0.770979 | -0.346090 |
| H | -0.424716 | 0.987806 | -1.418370 |
| C | -2.865192 | 0.411337 | -0.070707 |
| C | -1.628955 | 1.202870 | 0.343795 |
| H | -1.815702 | 2.253784 | 0.134096 |
| H | -1.499337 | 1.122149 | 1.429080 |
| H | -3.080805 | 0.605929 | -1.126411 |
| H | -3.729191 | 0.758661 | 0.499256 |
| H | -3.514774 | -1.649368 | -0.214984 |
| H | -2.504286 | -1.302368 | 1.181486 |
| C | -0.116611 | -0.776759 | -0.230123 |
| C | 0.283598 | -1.211223 | 1.204711 |
| C | 1.031439 | -1.328756 | -1.130232 |
| C | 1.804818 | -1.382092 | 1.195453 |
| H | -0.179316 | -2.177344 | 1.424103 |
| H | -0.056979 | -0.513202 | 1.969915 |
| C | 2.097943 | -1.945642 | -0.200286 |
| H | 1.442010 | -0.550166 | -1.766984 |
| H | 0.636242 | -2.091560 | -1.801520 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.298813 | -0.420586 | 1.332758 |
| H | 2.152765 | -2.041466 | 1.990938 |
| H | 3.116044 | -1.739515 | -0.531934 |
| H | 1.979999 | -3.030496 | -0.179670 |
| H | -1.239322 | -2.570105 | -0.585460 |
| C | 0.849397 | 1.655102 | 0.182061 |
| H | 1.047175 | 1.357151 | 1.216267 |
| C | 2.159258 | 1.545774 | -0.609231 |
| H | 1.987161 | 1.772133 | -1.664941 |
| H | 2.874475 | 2.277448 | -0.229642 |
| H | 2.635770 | 0.572460 | -0.547187 |
| C | 0.471950 | 3.144373 | 0.207464 |
| H | -0.290864 | 3.378112 | 0.946709 |
| H | 1.350893 | 3.743964 | 0.446750 |
| H | 0.106860 | 3.467806 | -0.771485 |

eq2

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| | | | |
|---|-----------|-----------|-----------|
| C | -1.848157 | -0.127435 | 0.596522 |
| C | -0.689397 | -0.432409 | -0.361676 |
| H | -1.107715 | -0.369506 | -1.374857 |
| C | -0.356488 | 2.013188 | -0.710220 |
| H | 0.363166 | 2.835854 | -0.673288 |
| H | -0.687036 | 1.926806 | -1.751355 |
| C | -2.550722 | 1.172582 | 0.206499 |
| C | -1.561267 | 2.334328 | 0.172834 |
| H | -2.051156 | 3.242788 | -0.183052 |
| H | -1.221444 | 2.539911 | 1.191953 |
| H | -2.998240 | 1.049356 | -0.784869 |
| H | -3.365560 | 1.389042 | 0.900049 |
| H | -2.566576 | -0.948559 | 0.594426 |
| H | -1.474738 | -0.040756 | 1.621084 |
| C | -0.169978 | -1.886886 | -0.254026 |
| H | 0.677431 | -1.976957 | -0.936891 |
| C | 0.366270 | 0.710613 | -0.315817 |
| C | 1.068874 | 0.883013 | 1.067304 |
| C | 1.531284 | 0.448865 | -1.302270 |
| C | 2.581649 | 0.713449 | 0.825734 |
| H | 0.707097 | 0.153763 | 1.787821 |
| H | 0.855634 | 1.863666 | 1.493188 |
| C | 2.684857 | -0.103959 | -0.464208 |
| H | 1.844367 | 1.400822 | -1.740011 |
| H | 1.235663 | -0.203478 | -2.125521 |
| H | 3.039878 | 1.691656 | 0.664261 |
| H | 3.092559 | 0.249901 | 1.669902 |
| H | 3.652233 | 0.002744 | -0.955343 |
| H | 2.536423 | -1.163607 | -0.252679 |
| C | 0.298201 | -2.332247 | 1.134241 |
| H | 0.520246 | -3.401291 | 1.120660 |
| H | 1.199361 | -1.818525 | 1.463987 |
| H | -0.479404 | -2.170287 | 1.884006 |
| C | -1.233145 | -2.870828 | -0.755784 |
| H | -1.624249 | -2.572748 | -1.730212 |
| H | -0.806853 | -3.870346 | -0.855293 |

H -2.072968 -2.943902 -0.062763

eq3

```
=====
C 1.416378 1.476025 0.510501
C 0.256990 0.938557 -0.345680
H 0.515376 1.170802 -1.387751
C 1.616252 -1.111776 -0.778761
H 1.629217 -2.203833 -0.718983
H 1.707306 -0.854236 -1.839942
C 2.769066 0.986032 0.000567
C 2.811557 -0.537974 -0.021643
H 3.739495 -0.889659 -0.476984
H 2.808767 -0.907975 1.007061
H 2.925454 1.369209 -1.012817
H 3.577055 1.380480 0.619799
H 1.393131 2.568116 0.508595
H 1.287105 1.160841 1.550804
C -1.021063 1.781575 -0.079379
H -0.647141 2.807908 -0.154133
C 0.240539 -0.617150 -0.277910
C -0.037530 -1.193125 1.145627
C -0.854814 -1.265768 -1.170689
C -1.105140 -2.282998 0.967018
H -0.404350 -0.419659 1.814893
H 0.867815 -1.593436 1.601217
C -1.932200 -1.789668 -0.220179
H -0.416957 -2.121807 -1.690929
H -1.227729 -0.588675 -1.935852
H -0.630397 -3.231762 0.704751
H -1.694113 -2.447634 1.869372
H -2.549848 -2.568282 -0.668202
H -2.593571 -0.983965 0.102038
C -2.113385 1.677428 -1.147896
H -2.810582 2.510276 -1.034611
H -1.694715 1.729426 -2.154458
H -2.693612 0.759624 -1.066801
C -1.649923 1.670511 1.312315
H -2.377276 2.474194 1.444109
H -2.180970 0.727863 1.447172
H -0.909824 1.762182 2.108290
```

eq4

```
=====
C 0.907686 0.173927 -0.363485
H 1.059093 0.548813 -1.384757
C 1.329995 1.319768 0.567955
C 0.651679 2.627566 0.152703
H 0.931474 3.434951 0.832251
H 1.020414 2.905542 -0.839837
C -1.294598 1.268371 -0.722182
C -0.868474 2.487600 0.098004
H -1.312583 3.389503 -0.328071
H -1.260038 2.403021 1.114524
```


| | | | |
|---|-----------|-----------|-----------|
| H | 1.069141 | 1.078122 | 1.602304 |
| H | -1.027364 | 1.431084 | -1.771401 |
| H | -2.381348 | 1.169194 | -0.687094 |
| H | 2.411292 | 1.456780 | 0.539376 |
| C | 1.830045 | -1.067063 | -0.293012 |
| H | 1.488566 | -1.756351 | -1.068051 |
| C | -0.623754 | -0.044273 | -0.253878 |
| C | -1.147765 | -1.215249 | -1.100683 |
| C | -1.179413 | -0.419129 | 1.139129 |
| C | -2.584954 | -1.454587 | -0.610222 |
| H | -0.550838 | -2.105325 | -0.894679 |
| H | -1.085701 | -1.014767 | -2.172419 |
| C | -2.591597 | -0.979727 | 0.866036 |
| H | -1.201901 | 0.421215 | 1.830276 |
| H | -0.561613 | -1.187967 | 1.594991 |
| H | -3.295746 | -0.876717 | -1.199998 |
| H | -2.870641 | -2.501090 | -0.705350 |
| H | -3.347414 | -0.208775 | 1.014424 |
| H | -2.830779 | -1.791529 | 1.551481 |
| C | 3.268746 | -0.685660 | -0.661655 |
| H | 3.768992 | -0.165119 | 0.156496 |
| H | 3.850583 | -1.582841 | -0.878130 |
| H | 3.301399 | -0.041118 | -1.542367 |
| C | 1.842882 | -1.830269 | 1.033852 |
| H | 0.936655 | -2.412808 | 1.188723 |
| H | 2.682086 | -2.528728 | 1.049802 |
| H | 1.963409 | -1.152733 | 1.882129 |

eq5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.811200 | -0.696669 | -0.272558 |
| H | -0.873163 | -1.020028 | -1.319922 |
| C | -0.556469 | -1.978639 | 0.539435 |
| C | 0.610198 | -2.779515 | -0.040441 |
| H | 0.800934 | -3.668734 | 0.563600 |
| H | 0.323999 | -3.128115 | -1.037890 |
| C | 1.601236 | -0.605096 | -0.857874 |
| C | 1.877195 | -1.935060 | -0.155401 |
| H | 2.646380 | -2.485803 | -0.700566 |
| H | 2.281549 | -1.748096 | 0.842200 |
| H | -0.355691 | -1.726791 | 1.585122 |
| H | 1.330771 | -0.799754 | -1.900846 |
| H | 2.515570 | -0.009784 | -0.878125 |
| H | -1.455680 | -2.598254 | 0.531944 |
| C | -2.222081 | -0.122638 | 0.026088 |
| H | -2.844068 | -1.016657 | 0.133804 |
| C | 0.452040 | 0.203466 | -0.208259 |
| C | 0.322332 | 1.556924 | -0.925999 |
| C | 0.901472 | 0.674166 | 1.194789 |
| C | 1.549817 | 2.368795 | -0.478152 |
| H | -0.574597 | 2.062236 | -0.571320 |
| H | 0.241921 | 1.453029 | -2.010224 |
| C | 1.909023 | 1.810890 | 0.923523 |
| H | 1.334555 | -0.120276 | 1.799372 |

| | | | |
|---|-----------|----------|-----------|
| H | 0.050320 | 1.066573 | 1.744596 |
| H | 2.380726 | 2.233599 | -1.169510 |
| H | 1.331126 | 3.435236 | -0.450156 |
| H | 2.930064 | 1.429965 | 0.932452 |
| H | 1.851859 | 2.579082 | 1.693318 |
| C | -2.386919 | 0.666244 | 1.325441 |
| H | -1.920223 | 1.650164 | 1.261540 |
| H | -3.448976 | 0.822761 | 1.524776 |
| H | -1.962532 | 0.140544 | 2.181802 |
| C | -2.838741 | 0.654149 | -1.142771 |
| H | -2.405312 | 1.645165 | -1.267055 |
| H | -2.717901 | 0.113131 | -2.083015 |
| H | -3.909052 | 0.788715 | -0.972832 |

eq6

```
=====
```

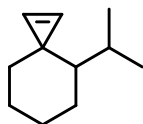
| | | | |
|---|-----------|-----------|-----------|
| C | -0.228531 | 2.768548 | 0.263706 |
| C | -1.014401 | 1.798620 | -0.612405 |
| H | -0.742534 | 1.975395 | -1.658553 |
| C | 0.784363 | 0.067212 | -0.412715 |
| H | 1.005749 | 0.300371 | -1.462520 |
| C | 1.267840 | 2.512076 | 0.110113 |
| C | 1.595635 | 1.057026 | 0.435547 |
| H | 2.662676 | 0.872715 | 0.290732 |
| H | 1.392695 | 0.882273 | 1.495658 |
| H | 1.563205 | 2.729786 | -0.921282 |
| H | 1.842262 | 3.179749 | 0.755133 |
| H | -0.471513 | 3.798593 | -0.003914 |
| H | -0.514288 | 2.635993 | 1.312055 |
| C | -0.744538 | 0.319888 | -0.278955 |
| C | -1.316991 | -0.033958 | 1.121592 |
| C | -1.559926 | -0.576756 | -1.259754 |
| C | -1.967195 | -1.410924 | 0.972154 |
| H | -2.096208 | 0.690188 | 1.376485 |
| H | -0.574059 | 0.012606 | 1.915327 |
| C | -2.604866 | -1.325496 | -0.415998 |
| H | -0.906472 | -1.285879 | -1.768269 |
| H | -2.029542 | 0.026668 | -2.037237 |
| H | -1.210230 | -2.197621 | 0.990757 |
| H | -2.688218 | -1.625620 | 1.761188 |
| H | -2.867903 | -2.297367 | -0.833134 |
| H | -3.522170 | -0.735618 | -0.350672 |
| H | -2.088790 | 1.984421 | -0.528640 |
| C | 1.260117 | -1.394736 | -0.195719 |
| H | 0.457745 | -2.065283 | -0.506564 |
| C | 2.462719 | -1.692469 | -1.094851 |
| H | 3.289943 | -1.012401 | -0.877616 |
| H | 2.823840 | -2.711079 | -0.941374 |
| H | 2.204294 | -1.580176 | -2.149026 |
| C | 1.617366 | -1.755323 | 1.249393 |
| H | 0.814812 | -1.538657 | 1.952557 |
| H | 1.836589 | -2.822576 | 1.316254 |
| H | 2.508562 | -1.218716 | 1.580015 |

eq7

```

=====
C  -2.737475    -0.644118    0.182564
C  -1.568990    -1.236042   -0.594422
H  -1.751261    -1.075535   -1.662185
C  -0.274186     0.910563   -0.481918
H  -0.494148     1.019897   -1.552980
C  -2.807818     0.855837   -0.075989
C  -1.475440     1.507283    0.277925
H  -1.520463     2.581198    0.081871
H  -1.316156     1.394045    1.353793
H  -3.031058     1.028988   -1.133581
H  -3.613540     1.313402    0.501355
H  -3.668307    -1.133696   -0.109984
H  -2.606432    -0.822234    1.254343
C  -0.192893    -0.625608   -0.241099
C   0.200206    -1.025280    1.215947
C   0.852687    -1.357767   -1.132893
C   1.568641    -1.708353    1.115140
H  -0.522318    -1.751432    1.596003
H   0.192159    -0.185882    1.907331
C   1.490065    -2.421652   -0.233532
H   1.623552    -0.679868   -1.481074
H   0.380229    -1.784935   -2.018516
H   2.367884    -0.963697    1.080811
H   1.771035    -2.376082    1.952620
H   2.456490    -2.765580   -0.601843
H   0.835036    -3.292562   -0.149337
H  -1.511570    -2.317476   -0.442548
C   0.953063     1.838891   -0.236946
H   0.562582     2.821223   -0.521875
C   1.425535     1.982587    1.213645
H   1.952286     1.092943    1.557679
H   2.126657     2.817168    1.279888
H   0.608585     2.186169    1.905148
C   2.177065     1.617531   -1.130760
H   1.898428     1.423531   -2.167747
H   2.799323     2.514704   -1.114852
H   2.798256     0.792477   -0.780286

```



4-isopropylspiro[2.5]oct-1-ene

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -429.860276 | -429.583441 | -429.631433 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| ax2 | | -429.866396 | | -429.589842 | | -429.63835 |
| ax3 | | -429.861286 | | -429.584565 | | -429.633271 |
| ax4 | | -429.860304 | | -429.583398 | | -429.631546 |
| eq1 | | -429.866018 | | -429.589467 | | -429.6374 |
| eq2 | | -429.863626 | | -429.58704 | | -429.635447 |
| eq3 | | -429.866883 | | -429.590348 | | -429.638249 |

ax1

```

=====
C  -0.352200    1.007598   -0.066016
C   0.345667   -0.027949    0.829292
H   0.639070    0.524427    1.726690
C   0.192380    2.402662   -0.191242
C  -0.669063   -1.096718    1.285131
C  -1.576436   -1.650583    0.179922
H  -2.326047   -2.304176    0.630839
H  -1.005840   -2.264084   -0.517894
C  -1.209261    0.422341   -1.181530
C  -2.255592   -0.530062   -0.602931
H  -2.876932   -0.946261   -1.398049
H  -2.918374    0.032988    0.062468
H   0.944049    3.028030   -0.641866
H  -0.139326   -1.914653    1.781165
H  -1.691233    1.236379   -1.725195
H  -0.587630   -0.120134   -1.899477
H  -1.315469   -0.641003    2.041516
C   1.680034   -0.625246    0.312136
H   2.133325   -1.086697    1.196107
C   2.635924    0.466254   -0.169090
H   3.637248    0.057110   -0.313679
H   2.306706    0.881728   -1.123313
H   2.705440    1.286318    0.548325
C  -0.831549    2.284979    0.584199
H  -1.551106    2.731308    1.249391
C   1.589162   -1.729310   -0.742488
H   1.052782   -2.602747   -0.374287
H   1.102405   -1.387248   -1.656329
H   2.596542   -2.055078   -1.010714

```

ax2

```

=====
C  -0.770498    0.834953    0.075095
C   0.393520    0.008539    0.630627
H   0.763396    0.521306    1.525279
C  -0.821744    2.324638    0.247961
C  -0.165979   -1.362047    1.053601
C  -0.858132   -2.086427   -0.103763
H  -1.268547   -3.035057    0.247269
H  -0.127367   -2.330726   -0.879577
C  -1.454321    0.159286   -1.106771
C  -1.970884   -1.226495   -0.706270
H  -2.416972   -1.729557   -1.566217
H  -2.764057   -1.101487    0.038033

```

| | | | |
|---|-----------|-----------|-----------|
| H | -0.438983 | 3.274963 | -0.084141 |
| H | 0.616717 | -1.989430 | 1.480726 |
| H | -2.276455 | 0.783876 | -1.459459 |
| H | -0.747315 | 0.057202 | -1.936961 |
| H | -0.899913 | -1.196254 | 1.848476 |
| C | 1.588174 | -0.097384 | -0.342204 |
| H | 1.278968 | -0.660931 | -1.225967 |
| C | 2.762197 | -0.839394 | 0.297835 |
| H | 3.624545 | -0.840044 | -0.370786 |
| H | 3.062207 | -0.349721 | 1.228460 |
| H | 2.523369 | -1.877663 | 0.525598 |
| C | -1.601657 | 1.654322 | 1.028742 |
| H | -2.335941 | 1.639460 | 1.816458 |
| C | 2.047650 | 1.283892 | -0.809866 |
| H | 1.286280 | 1.787407 | -1.404486 |
| H | 2.281384 | 1.922056 | 0.047184 |
| H | 2.948735 | 1.201296 | -1.419813 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.895688 | -0.833570 | 0.041537 |
| C | 0.384505 | -0.274054 | -0.605798 |
| H | 0.568378 | -0.914945 | -1.472635 |
| C | -0.952648 | -2.302659 | 0.354677 |
| C | 0.169554 | 1.150419 | -1.158007 |
| C | -0.638893 | 2.088129 | -0.256980 |
| H | -0.810429 | 3.028059 | -0.785424 |
| H | -0.080973 | 2.332109 | 0.648953 |
| C | -1.712689 | 0.141144 | 0.883362 |
| C | -1.966131 | 1.450707 | 0.139836 |
| H | -2.548587 | 2.132301 | 0.762332 |
| H | -2.557345 | 1.249693 | -0.759691 |
| H | -0.625284 | -3.086749 | 1.016176 |
| H | 1.133021 | 1.603498 | -1.400938 |
| H | -2.655124 | -0.337165 | 1.154898 |
| H | -1.191412 | 0.366664 | 1.818337 |
| H | -0.373840 | 1.062137 | -2.103585 |
| C | 1.646747 | -0.450441 | 0.270582 |
| H | 1.586886 | -1.464176 | 0.680644 |
| C | 1.776579 | 0.518904 | 1.445275 |
| H | 2.648429 | 0.256403 | 2.047689 |
| H | 1.920819 | 1.541500 | 1.091009 |
| H | 0.905309 | 0.504170 | 2.098409 |
| C | -1.626331 | -1.936412 | -0.683246 |
| H | -2.261762 | -2.187450 | -1.515658 |
| C | 2.916232 | -0.383929 | -0.580519 |
| H | 3.797430 | -0.601122 | 0.025777 |
| H | 2.883709 | -1.104470 | -1.399387 |
| H | 3.053355 | 0.610111 | -1.011211 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.246073 | 0.996157 | 0.047260 |
| C | -0.334902 | -0.152705 | -0.791401 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.763888 | 0.313987 | -1.682222 |
| C | -0.562222 | 2.243084 | 0.286581 |
| C | 0.796376 | -1.065280 | -1.304459 |
| C | 1.812197 | -1.491861 | -0.245243 |
| H | 2.599525 | -2.083733 | -0.716227 |
| H | 1.342118 | -2.134015 | 0.502940 |
| C | 1.308933 | 0.590057 | 1.067310 |
| C | 2.409676 | -0.264299 | 0.437434 |
| H | 3.135822 | -0.559939 | 1.196860 |
| H | 2.948005 | 0.330581 | -0.307812 |
| H | -1.366526 | 2.693691 | 0.842565 |
| H | 0.360502 | -1.940312 | -1.791840 |
| H | 1.735122 | 1.494960 | 1.503587 |
| H | 0.856199 | 0.025825 | 1.885593 |
| H | 1.342294 | -0.515836 | -2.078399 |
| C | -1.515820 | -0.921930 | -0.141711 |
| H | -1.607852 | -1.864156 | -0.691290 |
| C | -2.827705 | -0.155178 | -0.332926 |
| H | -3.671413 | -0.733139 | 0.048914 |
| H | -2.808420 | 0.793442 | 0.206672 |
| H | -3.014319 | 0.060265 | -1.386010 |
| C | 0.371201 | 2.356044 | -0.596483 |
| H | 0.907689 | 2.956758 | -1.311091 |
| C | -1.364741 | -1.265118 | 1.341209 |
| H | -0.468856 | -1.845051 | 1.554401 |
| H | -1.334645 | -0.357209 | 1.947291 |
| H | -2.225750 | -1.849941 | 1.670644 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.545379 | 0.926788 | -0.067928 |
| C | 0.324339 | -0.326714 | -0.285234 |
| H | 0.353650 | -0.522544 | -1.366479 |
| C | 0.011968 | 2.308758 | 0.115095 |
| C | -0.400435 | -1.516808 | 0.365769 |
| C | -1.819711 | -1.699509 | -0.174092 |
| H | -2.303220 | -2.539153 | 0.328937 |
| H | -1.759865 | -1.958484 | -1.236254 |
| C | -1.938751 | 0.755247 | -0.661438 |
| C | -2.656013 | -0.432635 | -0.021298 |
| H | -3.643472 | -0.570943 | -0.465716 |
| H | -2.808723 | -0.223932 | 1.042472 |
| H | 0.438465 | 3.173128 | -0.364895 |
| H | 0.159534 | -2.436510 | 0.198073 |
| H | -2.511109 | 1.673151 | -0.519463 |
| H | -1.856035 | 0.584115 | -1.740605 |
| H | -0.435699 | -1.357405 | 1.450032 |
| C | 1.781382 | -0.164765 | 0.185239 |
| H | 1.767351 | 0.324620 | 1.164133 |
| C | 2.571379 | 0.712605 | -0.787710 |
| H | 3.574190 | 0.911733 | -0.406330 |
| H | 2.675185 | 0.197733 | -1.746498 |
| H | 2.090287 | 1.670005 | -0.980244 |
| C | -0.399849 | 1.734745 | 1.195638 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.554649 | 1.774303 | 2.260452 |
| C | 2.516119 | -1.497168 | 0.343755 |
| H | 2.111700 | -2.102690 | 1.153631 |
| H | 2.461458 | -2.083226 | -0.577512 |
| H | 3.570664 | -1.317174 | 0.559485 |

eq2

```
=====
```

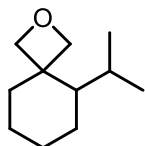
| | | | |
|---|-----------|-----------|-----------|
| C | -0.321458 | 0.900232 | -0.096393 |
| C | 0.177721 | -0.502119 | -0.464748 |
| H | 0.001179 | -0.610173 | -1.543719 |
| C | 0.568888 | 2.107805 | -0.014378 |
| C | -0.722112 | -1.539606 | 0.226271 |
| C | -2.189368 | -1.374425 | -0.166426 |
| H | -2.803571 | -2.116769 | 0.346787 |
| H | -2.296208 | -1.558342 | -1.240224 |
| C | -1.781416 | 1.083222 | -0.504273 |
| C | -2.682240 | 0.035619 | 0.151486 |
| H | -3.715356 | 0.163038 | -0.177287 |
| H | -2.669961 | 0.184658 | 1.236019 |
| H | 1.126174 | 2.846615 | -0.564387 |
| H | -0.376064 | -2.546556 | -0.021439 |
| H | -2.107849 | 2.089585 | -0.237543 |
| H | -1.864564 | 0.990918 | -1.593249 |
| H | -0.633376 | -1.428618 | 1.311248 |
| C | 1.670464 | -0.835197 | -0.265153 |
| H | 1.763912 | -1.861056 | -0.636352 |
| C | 2.158235 | -0.856636 | 1.186184 |
| H | 3.165124 | -1.277283 | 1.226350 |
| H | 2.207708 | 0.144297 | 1.613571 |
| H | 1.521913 | -1.469367 | 1.825032 |
| C | 0.180627 | 1.631625 | 1.120860 |
| H | 0.188239 | 1.684603 | 2.196210 |
| C | 2.599783 | 0.024115 | -1.124676 |
| H | 2.224875 | 0.116270 | -2.145956 |
| H | 2.720201 | 1.027417 | -0.716325 |
| H | 3.592875 | -0.427043 | -1.171252 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.650357 | 0.907133 | -0.273696 |
| C | 0.319028 | -0.274840 | -0.419560 |
| H | 0.212485 | -0.617271 | -1.457766 |
| C | -0.204569 | 2.324726 | -0.496753 |
| C | -0.154708 | -1.428668 | 0.476679 |
| C | -1.584889 | -1.850767 | 0.140493 |
| H | -1.901562 | -2.663446 | 0.796972 |
| H | -1.614399 | -2.237282 | -0.883268 |
| C | -2.079281 | 0.498016 | -0.614083 |
| C | -2.545899 | -0.669162 | 0.257666 |
| H | -3.557438 | -0.970311 | -0.021062 |
| H | -2.585154 | -0.341071 | 1.301374 |
| H | 0.086098 | 3.070649 | -1.216858 |
| H | 0.519234 | -2.283234 | 0.382720 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.742958 | 1.355763 | -0.494852 |
| H | -2.124707 | 0.193696 | -1.666104 |
| H | -0.119018 | -1.107162 | 1.522097 |
| C | 1.804730 | 0.080122 | -0.228217 |
| H | 1.963507 | 1.054224 | -0.700669 |
| C | 2.706114 | -0.925377 | -0.945293 |
| H | 3.757261 | -0.656160 | -0.826693 |
| H | 2.576574 | -1.930605 | -0.538459 |
| H | 2.485808 | -0.963487 | -2.013260 |
| C | -0.427488 | 2.001673 | 0.733697 |
| H | -0.455709 | 2.287347 | 1.771497 |
| C | 2.227606 | 0.195376 | 1.237037 |
| H | 3.245062 | 0.584044 | 1.305808 |
| H | 1.576966 | 0.857513 | 1.808682 |
| H | 2.216222 | -0.782606 | 1.722020 |



5-isopropyl-2-oxaspiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -506.341260 | -506.032061 | -506.08198 |
| ax2 | -506.347172 | -506.038153 | -506.087843 |
| ax3 | -506.338407 | -506.029044 | -506.078381 |
| ax4 | -506.339902 | -506.030668 | -506.080588 |
| eq1 | -506.341320 | -506.032165 | -506.081838 |
| eq2 | -506.343692 | -506.034659 | -506.085279 |
| eq3 | -506.341320 | -506.032165 | -506.081838 |
| eq4 | -506.340230 | -506.031038 | -506.080205 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | -0.453558 | -0.265509 | -0.721764 |
| H | -0.282042 | -0.813808 | -1.654347 |
| C | -0.860343 | 1.156897 | -1.144335 |
| C | -0.822548 | 2.182134 | -0.012105 |
| H | -1.097059 | 3.165308 | -0.398891 |
| H | -1.556005 | 1.928008 | 0.756615 |
| C | 0.994252 | 0.847365 | 1.098472 |
| C | 0.574568 | 2.229623 | 0.602534 |
| H | 0.614862 | 2.947135 | 1.423500 |
| H | 1.281815 | 2.575613 | -0.158172 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.147431 | 1.484001 | -1.909787 |
| H | 0.366044 | 0.566478 | 1.943379 |
| H | 2.023847 | 0.871067 | 1.465899 |
| H | -1.838083 | 1.145483 | -1.625048 |
| C | 0.903371 | -0.210858 | -0.006336 |
| C | 1.533810 | -1.551498 | 0.408620 |
| C | 2.133151 | -0.123071 | -0.937200 |
| H | 1.050048 | -2.430400 | -0.024731 |
| H | 1.697620 | -1.707264 | 1.476326 |
| H | 1.917812 | -0.345855 | -1.985582 |
| H | 2.743550 | 0.778478 | -0.868212 |
| C | -1.533273 | -1.114707 | 0.004096 |
| H | -1.214945 | -2.151975 | -0.134310 |
| C | -2.896036 | -0.978656 | -0.674922 |
| H | -2.817658 | -1.077459 | -1.759363 |
| H | -3.576578 | -1.750925 | -0.313599 |
| H | -3.351016 | -0.010135 | -0.457187 |
| O | 2.762024 | -1.245819 | -0.284999 |
| C | -1.688342 | -0.926342 | 1.514825 |
| H | -0.778771 | -1.190516 | 2.053978 |
| H | -1.960596 | 0.094853 | 1.782043 |
| H | -2.481917 | -1.583810 | 1.876164 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.542512 | -0.111932 | -0.626106 |
| H | -0.557869 | -0.749573 | -1.518409 |
| C | -0.688311 | 1.354834 | -1.071232 |
| C | -0.591224 | 2.319240 | 0.113725 |
| H | -0.668961 | 3.348585 | -0.240470 |
| H | -1.432000 | 2.159664 | 0.793068 |
| C | 0.987954 | 0.666375 | 1.231608 |
| C | 0.728520 | 2.131527 | 0.866045 |
| H | 0.745838 | 2.748586 | 1.765740 |
| H | 1.543737 | 2.485401 | 0.228432 |
| H | 0.118571 | 1.583936 | -1.775122 |
| H | 0.290239 | 0.342287 | 2.008880 |
| H | 1.994450 | 0.557672 | 1.643744 |
| H | -1.620622 | 1.505925 | -1.614186 |
| C | 0.844511 | -0.244719 | 0.012446 |
| C | 1.458400 | -1.641998 | 0.224992 |
| C | 2.033526 | -0.078845 | -0.958086 |
| H | 0.953994 | -2.438352 | -0.326103 |
| H | 1.636223 | -1.955643 | 1.255032 |
| H | 1.760534 | -0.210541 | -2.009285 |
| H | 2.658515 | 0.807678 | -0.846502 |
| C | -1.708568 | -0.574345 | 0.274289 |
| H | -1.743348 | 0.061901 | 1.160871 |
| C | -1.539588 | -2.015295 | 0.756202 |
| H | -0.670729 | -2.136030 | 1.403256 |
| H | -2.416094 | -2.323744 | 1.328205 |
| H | -1.435522 | -2.700567 | -0.088581 |
| O | 2.678776 | -1.258976 | -0.439852 |
| C | -3.049391 | -0.435796 | -0.448973 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.854178 | -0.849996 | 0.160045 |
| H | -3.300432 | 0.602347 | -0.663118 |
| H | -3.032456 | -0.981994 | -1.396142 |

ax3

```
=====
C  -0.455874    0.192541    0.850420
H  -0.157776    0.728724    1.757969
C  -0.765393   -1.257072    1.275054
C  -0.825755   -2.269843    0.122882
H  -0.922298   -3.274024    0.540658
H  -1.709409   -2.104205   -0.490048
C   0.691388   -0.768726   -1.230354
C   0.411549   -2.199901   -0.770236
H   0.288919   -2.855516   -1.633807
H   1.277285   -2.572261   -0.216208
H   0.022890   -1.580781    1.962896
H  -0.098163   -0.425179   -1.902211
H   1.627303   -0.732671   -1.794078
H  -1.699435   -1.279321    1.842080
C   0.800185    0.176364   -0.033266
C   1.512021    1.496663   -0.392183
C   2.121796   -0.093227    0.725453
H   1.232666    2.340602    0.238740
H   1.510130    1.795864   -1.441618
H   2.058642    0.123050    1.796204
H   2.615722   -1.051836    0.569550
C  -1.712915    0.966794    0.364991
H  -2.314539    1.078969    1.273133
C  -2.630640    0.283218   -0.652864
H  -3.066502   -0.633543   -0.260434
H  -3.456812    0.956876   -0.889143
H  -2.121836    0.050679   -1.588361
O   2.789584    0.972587    0.022306
C  -1.388441    2.378256   -0.123581
H  -0.808862    2.940059    0.608943
H  -0.829331    2.355835   -1.062052
H  -2.312793    2.927590   -0.308563
```

ax4

```
=====
C   1.235378   -0.485192    1.101000
H   2.153186   -0.038599    1.493325
C   1.522851   -1.878176    0.541554
C   0.295650   -2.447139   -0.168633
H   0.519674   -3.433459   -0.578212
H  -0.520143   -2.577233    0.549416
C  -0.529353   -0.114037   -0.748603
C  -0.143107   -1.501344   -1.284457
H  -0.981132   -1.920113   -1.844817
H   0.687922   -1.391230   -1.990052
H   2.346667   -1.820177   -0.176924
H  -0.643956    0.538369   -1.618607
H   1.849396   -2.539874    1.345282
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.661108 | 0.456364 | 0.038121 |
| C | 0.570889 | 1.911228 | 0.532792 |
| C | 1.791810 | 1.016515 | -0.854451 |
| H | 0.647806 | 2.063328 | 1.610952 |
| H | -0.278251 | 2.473866 | 0.139254 |
| H | 2.760458 | 0.518050 | -0.794186 |
| H | 1.510675 | 1.153780 | -1.901738 |
| C | -1.924389 | -0.124055 | -0.046990 |
| H | 0.546487 | -0.566313 | 1.940779 |
| C | -1.932877 | -0.052978 | 1.481290 |
| H | -2.963843 | 0.015069 | 1.833454 |
| H | -1.488417 | -0.933263 | 1.941712 |
| H | -1.403814 | 0.829137 | 1.848426 |
| C | -2.808750 | 0.995850 | -0.603858 |
| H | -2.406288 | 1.977493 | -0.344944 |
| H | -2.879506 | 0.939358 | -1.691106 |
| H | -3.818707 | 0.932065 | -0.195227 |
| H | -2.402287 | -1.069309 | -0.320120 |
| O | 1.791101 | 2.273355 | -0.146657 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.304048 | 0.649236 | -0.277849 |
| H | 0.339987 | 0.934422 | -1.337685 |
| C | -0.483044 | 1.731365 | 0.490183 |
| C | -1.909607 | 1.933682 | -0.005353 |
| H | -2.398085 | 2.718431 | 0.574931 |
| H | -1.893620 | 2.266172 | -1.047974 |
| C | -1.942969 | -0.465989 | -0.664249 |
| C | -2.680318 | 0.625003 | 0.098615 |
| H | -3.695193 | 0.731945 | -0.287598 |
| H | -2.765764 | 0.341115 | 1.152581 |
| H | -0.520258 | 1.427716 | 1.543433 |
| H | -1.930156 | -0.214164 | -1.730587 |
| H | -2.468117 | -1.419903 | -0.571828 |
| H | 0.056813 | 2.676469 | 0.459592 |
| C | -0.492335 | -0.669242 | -0.211394 |
| C | 0.068482 | -1.942298 | -0.878724 |
| C | -0.370481 | -1.485143 | 1.092093 |
| H | 1.044853 | -1.876159 | -1.350497 |
| H | -0.629267 | -2.420689 | -1.569044 |
| H | 0.366236 | -1.121315 | 1.811131 |
| H | -1.309445 | -1.694602 | 1.608394 |
| C | 1.760721 | 0.663345 | 0.265871 |
| H | 1.687094 | 0.784179 | 1.351462 |
| C | 2.512434 | 1.877615 | -0.292628 |
| H | 1.988409 | 2.818209 | -0.132400 |
| H | 3.495611 | 1.964092 | 0.172401 |
| H | 2.664242 | 1.757219 | -1.368179 |
| O | 0.115995 | -2.644753 | 0.382283 |
| C | 2.633884 | -0.568380 | 0.016442 |
| H | 2.221706 | -1.481870 | 0.441073 |
| H | 2.801562 | -0.725246 | -1.050904 |
| H | 3.610542 | -0.403153 | 0.475391 |

eq2

```
=====
C  -0.334123    -0.489646    -0.400265
H  -0.229644    -0.862692    -1.427050
C   0.107476    -1.623905     0.534598
C   1.507065    -2.128904     0.186607
H   1.805478    -2.918983     0.877938
H   1.492195    -2.567989    -0.815803
C   2.073262     0.159921    -0.688155
C   2.518784    -0.985767     0.218820
H   3.508032    -1.338549    -0.076808
H   2.606324    -0.613725     1.245356
H   0.109354    -1.259435     1.566715
H   2.052987    -0.183099    -1.727678
H   2.785146     0.986414    -0.634364
H  -0.609429    -2.445874     0.493947
C   0.686502     0.663332    -0.304686
C   0.247144     1.984634    -0.955103
C   0.629390     1.500259     0.987830
H  -0.583334     1.969790    -1.660049
H   1.083944     2.539302    -1.388871
H   0.115106     1.094617     1.856268
H   1.613240     1.871605     1.290913
C  -1.834103    -0.130583    -0.247351
H  -2.005669     0.821207    -0.752411
C  -2.337336     0.022005     1.189935
H  -1.860240     0.845686     1.716249
H  -3.410017     0.223944     1.178434
H  -2.185526    -0.892944     1.765526
O  -0.124605     2.538283     0.325608
C  -2.689741    -1.177867    -0.966943
H  -2.580280    -2.162548    -0.507422
H  -3.746257    -0.909504    -0.919359
H  -2.410496    -1.264361    -2.018123
```

eq3

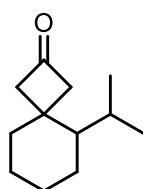
```
=====
C   0.304049     0.649235    -0.277849
H   0.339986     0.934424    -1.337684
C  -0.483044     1.731361     0.490188
C  -1.909606     1.933682    -0.005351
H  -2.398084     2.718430     0.574935
H  -1.893616     2.266176    -1.047971
C  -1.942968    -0.465988    -0.664252
C  -2.680318     0.625004     0.098612
H  -3.695192     0.731947    -0.287604
H  -2.765768     0.341114     1.152577
H  -0.520261     1.427706     1.543435
H  -1.930152    -0.214162    -1.730590
H  -2.468117    -1.419901    -0.571833
H   0.056815     2.676465     0.459604
C  -0.492335    -0.669243    -0.211395
C   0.068482    -1.942299    -0.878723
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.370482 | -1.485142 | 1.092093 |
| H | 1.044854 | -1.876161 | -1.350496 |
| H | -0.629266 | -2.420690 | -1.569043 |
| H | 0.366235 | -1.121313 | 1.811130 |
| H | -1.309446 | -1.694599 | 1.608394 |
| C | 1.760721 | 0.663345 | 0.265870 |
| H | 1.687095 | 0.784182 | 1.351461 |
| C | 2.512432 | 1.877615 | -0.292631 |
| H | 1.988403 | 2.818209 | -0.132409 |
| H | 3.495608 | 1.964097 | 0.172400 |
| H | 2.664243 | 1.757215 | -1.368181 |
| O | 0.115994 | -2.644753 | 0.382285 |
| C | 2.633884 | -0.568380 | 0.016442 |
| H | 2.221707 | -1.481870 | 0.441074 |
| H | 2.801563 | -0.725247 | -1.050903 |
| H | 3.610543 | -0.403152 | 0.475392 |

eq4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.814627 | 0.976112 | -0.617404 |
| H | -1.905116 | 0.807936 | -1.695841 |
| C | -2.773395 | 0.048985 | 0.123022 |
| C | -2.383093 | -1.407715 | -0.102230 |
| H | -3.033859 | -2.071526 | 0.469712 |
| H | -2.516763 | -1.657911 | -1.159285 |
| C | 0.044084 | -0.713628 | -0.471787 |
| C | -0.925736 | -1.633391 | 0.290517 |
| H | -0.644781 | -2.674395 | 0.116688 |
| H | -0.822658 | -1.454517 | 1.365404 |
| H | -2.730516 | 0.271151 | 1.194722 |
| H | -0.139611 | -0.874422 | -1.542183 |
| H | -3.799599 | 0.230967 | -0.199876 |
| C | -0.361044 | 0.752349 | -0.206726 |
| C | 0.603607 | 1.848140 | -0.691114 |
| C | 0.021100 | 1.301349 | 1.182737 |
| H | 0.071037 | 2.755724 | -0.990586 |
| H | 1.351979 | 1.606396 | -1.439519 |
| H | -0.716692 | 2.008408 | 1.573832 |
| H | 0.301668 | 0.598931 | 1.964370 |
| C | 1.501810 | -1.197932 | -0.243449 |
| H | -2.077188 | 2.019886 | -0.432521 |
| C | 2.554137 | -0.580251 | -1.167820 |
| H | 3.437852 | -1.220747 | -1.191783 |
| H | 2.189335 | -0.476942 | -2.191242 |
| H | 2.875802 | 0.398462 | -0.812303 |
| C | 2.022211 | -1.157907 | 1.196370 |
| H | 1.318071 | -1.585388 | 1.910265 |
| H | 2.945315 | -1.737527 | 1.259612 |
| H | 2.256095 | -0.138240 | 1.501640 |
| H | 1.445663 | -2.256043 | -0.518762 |
| O | 1.157455 | 2.004140 | 0.633120 |



5-isopropylspiro[3.5]nonan-2-one

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -544.463130 | -544.149308 | -544.201279 |
| ax3 | -544.461282 | -544.147521 | -544.199606 |
| ax4 | -544.460328 | -544.146693 | -544.199265 |
| ax5 | -544.462488 | -544.148677 | -544.200669 |
| ax6 | -544.467090 | -544.153371 | -544.205297 |
| eq1 | -544.462730 | -544.149116 | -544.201222 |
| eq2 | -544.466117 | -544.152554 | -544.204955 |
| eq3 | -544.462427 | -544.148634 | -544.199797 |
| eq4 | -544.462160 | -544.148351 | -544.200374 |

ax1

```

=====
C  -0.660109   -0.298804   -0.716212
H  -0.391107   -0.810097   -1.647112
C  -1.317448    1.025750   -1.142966
C  -1.465575    2.047499   -0.016048
H  -1.902980    2.966015   -0.411895
H  -2.150889    1.676619    0.748855
C   0.557929    1.058186    1.103225
C  -0.104830    2.343135    0.610465
H  -0.203909    3.048380    1.437126
H   0.532899    2.820649   -0.139736
H  -0.678629    1.472759   -1.912437
H  -0.012837    0.662030    1.942623
H   1.561297    1.274223    1.483710
H  -2.278594    0.835408   -1.619725
C   0.668157    0.000810   -0.002892

```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.489474 | -1.236728 | 0.472796 |
| C | 1.842375 | 0.381222 | -0.970114 |
| H | 1.204174 | -2.151964 | -0.050955 |
| H | 1.569651 | -1.429827 | 1.541949 |
| H | 1.674495 | 0.037001 | -1.992744 |
| H | 2.197219 | 1.410734 | -0.979577 |
| C | -1.573582 | -1.327189 | 0.004783 |
| H | -1.052763 | -2.284030 | -0.093442 |
| C | -2.910534 | -1.479333 | -0.722230 |
| H | -2.774184 | -1.572121 | -1.801505 |
| H | -3.432796 | -2.369837 | -0.369675 |
| H | -3.560683 | -0.621746 | -0.537369 |
| C | 2.693089 | -0.614221 | -0.205752 |
| O | 3.878466 | -0.774374 | -0.096665 |
| C | -1.824102 | -1.140158 | 1.502948 |
| H | -0.905051 | -1.209346 | 2.083457 |
| H | -2.303346 | -0.188050 | 1.730541 |
| H | -2.488768 | -1.932826 | 1.853221 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.750610 | 0.192059 | 0.776085 |
| H | -0.447070 | 0.753104 | 1.664858 |
| C | -1.308657 | -1.150688 | 1.275907 |
| C | -1.542070 | -2.146380 | 0.141604 |
| H | -1.956582 | -3.074410 | 0.539098 |
| H | -2.278698 | -1.745773 | -0.560123 |
| C | 0.412181 | -1.140383 | -1.101629 |
| C | -0.228699 | -2.429451 | -0.586359 |
| H | -0.386576 | -3.119313 | -1.416862 |
| H | 0.455956 | -2.923452 | 0.109729 |
| H | -0.593128 | -1.590899 | 1.978488 |
| H | -0.174386 | -0.746442 | -1.930183 |
| H | 1.406910 | -1.356078 | -1.504733 |
| H | -2.230811 | -0.974493 | 1.832704 |
| C | 0.547852 | -0.076651 | -0.004592 |
| C | 1.349897 | 1.159664 | -0.518603 |
| C | 1.759943 | -0.445067 | 0.920217 |
| H | 1.093482 | 2.075898 | 0.015893 |
| H | 1.384544 | 1.349999 | -1.590513 |
| H | 1.633207 | -0.079454 | 1.941559 |
| H | 2.109758 | -1.476189 | 0.936576 |
| C | -1.848848 | 1.066818 | 0.094422 |
| H | -2.805986 | 0.680214 | 0.456888 |
| C | -1.917897 | 1.048413 | -1.434541 |
| H | -2.136103 | 0.060791 | -1.835908 |
| H | -2.713622 | 1.719167 | -1.764225 |
| H | -0.986772 | 1.401374 | -1.881414 |
| C | 2.580972 | 0.537152 | 0.108699 |
| O | 3.760927 | 0.690461 | -0.054968 |
| C | -1.760562 | 2.522915 | 0.563642 |
| H | -1.758606 | 2.589989 | 1.652469 |
| H | -0.853170 | 3.004521 | 0.194696 |
| H | -2.610769 | 3.097345 | 0.191633 |

ax4

```
=====  
C -0.363521 -1.363931 1.194734  
H 0.335616 -1.987703 1.757770  
C -1.348839 -2.241870 0.424068  
C -2.238589 -1.397964 -0.487117  
H -2.922168 -2.039322 -1.045960  
H -2.855117 -0.726011 0.117371  
C -0.417052 0.365297 -0.717815  
C -1.376256 -0.587144 -1.451792  
H -1.998761 -0.010727 -2.138391  
H -0.796002 -1.285280 -2.062501  
H -0.791926 -2.955728 -0.191861  
H 0.278573 0.749802 -1.471444  
H -1.950256 -2.826176 1.122242  
C 0.444061 -0.457067 0.266256  
C 1.567125 0.368269 0.972518  
C 1.551926 -1.237288 -0.527731  
H 1.785108 -0.013318 1.973033  
H 1.491814 1.451811 1.007053  
H 1.768401 -2.216895 -0.096037  
H 1.453150 -1.325781 -1.608666  
C -1.168495 1.621554 -0.169399  
H -0.905057 -0.765896 1.926785  
C -1.494162 1.657042 1.326460  
H -1.971318 2.609678 1.564341  
H -2.182659 0.866749 1.619928  
H -0.599505 1.575973 1.945307  
C -0.435046 2.908043 -0.563327  
H 0.539206 2.981419 -0.076795  
H -0.271981 2.951259 -1.641277  
H -1.015767 3.785964 -0.274941  
H -2.129551 1.646162 -0.690901  
C 2.541710 -0.201538 -0.036538  
O 3.645129 0.116702 -0.389619
```

ax5

```
=====  
C -0.150618 1.405091 1.154963  
H -1.001785 1.875968 1.653501  
C 0.644498 2.445546 0.369450  
C 1.778946 1.782915 -0.408731  
H 2.316278 2.527982 -0.998484  
H 2.500694 1.351293 0.288644  
C 0.401969 -0.384769 -0.616286  
C 1.219334 0.704389 -1.335174  
H 2.015071 0.251197 -1.924710  
H 0.554832 1.197678 -2.051574  
H -0.020684 2.952790 -0.337321  
H -0.133228 -0.922404 -1.408561  
H 1.031282 3.208439 1.046915  
C -0.681683 0.290727 0.252543  
C -1.634740 -0.728608 0.953240
```


| | | | |
|---|-----------|-----------|-----------|
| C | -1.878567 | 0.757328 | -0.647728 |
| H | -2.008307 | -0.349081 | 1.907203 |
| H | -1.315647 | -1.762069 | 1.072116 |
| H | -2.344112 | 1.675878 | -0.283662 |
| H | -1.726227 | 0.822713 | -1.724080 |
| C | 1.221283 | -1.501830 | 0.090111 |
| H | 0.482184 | 0.989553 | 1.938938 |
| C | 2.391393 | -1.969485 | -0.776311 |
| H | 2.799833 | -2.901696 | -0.383535 |
| H | 2.083951 | -2.144305 | -1.809145 |
| H | 3.198099 | -1.233674 | -0.784588 |
| C | 1.713313 | -1.228138 | 1.512635 |
| H | 2.386583 | -0.372172 | 1.561945 |
| H | 0.889017 | -1.054987 | 2.203930 |
| H | 2.263312 | -2.099997 | 1.873103 |
| H | 0.537901 | -2.351291 | 0.168075 |
| C | -2.636024 | -0.457472 | -0.151060 |
| O | -3.605460 | -1.044499 | -0.549328 |

ax6

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.540525 | 0.921597 | 1.248999 |
| H | -1.537473 | 1.057972 | 1.678808 |
| C | 0.051793 | 2.283202 | 0.873974 |
| C | 1.366205 | 2.153363 | 0.100138 |
| H | 1.680101 | 3.135381 | -0.257815 |
| H | 2.155762 | 1.797223 | 0.766612 |
| C | 0.744309 | -0.199993 | -0.622485 |
| C | 1.212272 | 1.193467 | -1.082076 |
| H | 2.142441 | 1.124018 | -1.644015 |
| H | 0.467277 | 1.601851 | -1.770905 |
| H | -0.666811 | 2.822094 | 0.250330 |
| H | 0.597498 | -0.827501 | -1.510370 |
| H | 0.196656 | 2.883994 | 1.773237 |
| C | -0.630523 | -0.012686 | 0.039515 |
| C | -1.499963 | -1.273363 | 0.349975 |
| C | -1.750021 | 0.472219 | -0.944843 |
| H | -1.624379 | -1.581999 | 1.386800 |
| H | -1.218483 | -2.130726 | -0.264258 |
| H | -2.072914 | 1.511213 | -0.913151 |
| H | -1.537147 | 0.180958 | -1.976403 |
| C | 1.804226 | -0.908610 | 0.253394 |
| H | 0.068499 | 0.445657 | 2.022403 |
| C | 1.389880 | -2.322009 | 0.666910 |
| H | 2.218223 | -2.818355 | 1.174905 |
| H | 0.541783 | -2.325147 | 1.348393 |
| H | 1.127544 | -2.923923 | -0.207105 |
| C | 3.153246 | -0.976100 | -0.467634 |
| H | 3.040785 | -1.439703 | -1.451792 |
| H | 3.600578 | 0.007013 | -0.607767 |
| H | 3.858285 | -1.579160 | 0.105949 |
| H | 1.949588 | -0.331438 | 1.168833 |
| C | -2.660164 | -0.547291 | -0.295330 |
| O | -3.854027 | -0.664025 | -0.224487 |

eq1

```
=====
C  0.884310    0.376918    0.266097
H  1.223818    0.444564    1.308208
C  1.984466   -0.320723   -0.560339
C  2.332232   -1.723963   -0.078383
H  3.120605   -2.147393   -0.703148
H  2.721787   -1.676009    0.943312
C -0.011755   -1.953185    0.719288
C  1.088949   -2.601807   -0.106455
H  1.302279   -3.601513    0.275428
H  0.752804   -2.718518   -1.141665
H  1.629383   -0.385572   -1.595689
H  0.303017   -1.911085    1.767652
H -0.920638   -2.560497    0.689047
H  2.882628    0.294254   -0.579322
C -0.367113   -0.526081    0.277652
C -1.621936   -0.079773    1.099349
C -1.219371   -0.525869   -1.033414
H -1.621473    0.917076    1.528640
H -1.927342   -0.791531    1.867839
H -0.989485    0.278272   -1.734600
H -1.282181   -1.468373   -1.578025
C  0.744980    1.825641   -0.278874
H  0.792759    1.756614   -1.370700
C  1.931827    2.675645    0.192711
H  2.897628    2.226504   -0.030090
H  1.907713    3.658539   -0.279867
H  1.873250    2.826190    1.273559
C -2.433263   -0.203851   -0.178466
O -3.606473   -0.113736   -0.419124
C -0.527190    2.604493    0.061165
H -1.434229    2.153374   -0.337531
H -0.645193    2.726542    1.139438
H -0.452166    3.603776   -0.371484
```

eq2

```
=====
C  0.281434    0.711173    0.393594
H  0.637865    0.954169    1.402471
C  1.324647    1.251711   -0.592312
C  2.723029    0.716248   -0.288738
H  3.438822    1.098696   -1.018466
H  3.041875    1.078355    0.693622
C  1.681020   -1.353695    0.679874
C  2.729768   -0.810596   -0.287010
H  3.717930   -1.190601   -0.022850
H  2.507826   -1.172602   -1.296353
H  1.045057    0.958160   -1.608942
H  1.937164   -1.054908    1.701756
H  1.668001   -2.445977    0.657128
H  1.327554    2.343301   -0.570905
C  0.284086   -0.832584    0.352672
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.856838 | -1.484855 | 1.192605 |
| C | -0.344674 | -1.458925 | -0.936272 |
| H | -1.351128 | -0.909667 | 1.972878 |
| H | -0.541231 | -2.452973 | 1.587900 |
| H | -0.425140 | -0.880781 | -1.852408 |
| H | 0.119452 | -2.423936 | -1.155997 |
| C | -1.092326 | 1.418935 | 0.257749 |
| H | -1.848164 | 0.800368 | 0.745983 |
| C | -1.562745 | 1.674530 | -1.176859 |
| H | -1.652898 | 0.765511 | -1.768261 |
| H | -2.545887 | 2.147681 | -1.156744 |
| H | -0.884692 | 2.352772 | -1.697779 |
| C | -1.599819 | -1.684261 | -0.115881 |
| O | -2.758402 | -1.829064 | -0.397754 |
| C | -1.061289 | 2.750332 | 1.013640 |
| H | -0.300772 | 3.416974 | 0.601046 |
| H | -2.022880 | 3.260415 | 0.938665 |
| H | -0.839290 | 2.599479 | 2.070914 |

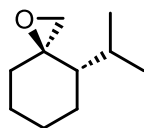
eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.379980 | 0.841879 | 0.436217 |
| H | 0.674974 | 1.025883 | 1.477434 |
| C | 1.517365 | 1.377108 | -0.450741 |
| C | 2.873572 | 0.771804 | -0.099976 |
| H | 3.645676 | 1.172451 | -0.759140 |
| H | 3.143976 | 1.055162 | 0.921970 |
| C | 1.687870 | -1.294447 | 0.663789 |
| C | 2.817061 | -0.748508 | -0.202191 |
| H | 3.767873 | -1.193841 | 0.095033 |
| H | 2.641800 | -1.033732 | -1.244794 |
| H | 1.295802 | 1.152543 | -1.498435 |
| H | 1.896524 | -1.073780 | 1.716100 |
| H | 1.626760 | -2.381259 | 0.570313 |
| H | 1.556425 | 2.465126 | -0.363534 |
| C | 0.325837 | -0.697760 | 0.303838 |
| C | -0.846416 | -1.410821 | 1.048313 |
| C | -0.253404 | -1.221197 | -1.053540 |
| H | -1.376800 | -0.911533 | 1.852560 |
| H | -0.529668 | -2.402161 | 1.382533 |
| H | -0.329557 | -0.553746 | -1.907677 |
| H | 0.237968 | -2.148727 | -1.357567 |
| C | -0.888721 | 1.714037 | 0.227771 |
| H | -0.509235 | 2.725311 | 0.403364 |
| C | -2.008590 | 1.509006 | 1.252049 |
| H | -1.617413 | 1.397386 | 2.264661 |
| H | -2.670033 | 2.377269 | 1.243280 |
| H | -2.623687 | 0.638731 | 1.022446 |
| C | -1.529783 | -1.541582 | -0.297608 |
| O | -2.669719 | -1.715760 | -0.635181 |
| C | -1.490403 | 1.729349 | -1.181486 |
| H | -2.048477 | 0.818335 | -1.398420 |
| H | -2.194339 | 2.560044 | -1.259693 |
| H | -0.737027 | 1.863399 | -1.957593 |

eq4

| | | | |
|---|-----------|-----------|-----------|
| C | -1.594847 | -1.390315 | 0.726643 |
| H | -1.763415 | -1.124850 | 1.776060 |
| C | -2.764628 | -0.900005 | -0.112911 |
| C | -2.832005 | 0.618224 | -0.046372 |
| H | -3.640116 | 0.999908 | -0.672918 |
| H | -3.055353 | 0.920488 | 0.981842 |
| C | -0.291639 | 0.757908 | 0.330174 |
| C | -1.510173 | 1.249574 | -0.475280 |
| H | -1.601254 | 2.328637 | -0.377097 |
| H | -1.336219 | 1.043218 | -1.538014 |
| H | -2.623679 | -1.215326 | -1.152027 |
| H | -0.457984 | 1.034614 | 1.380036 |
| H | -3.696511 | -1.348670 | 0.234919 |
| C | -0.260071 | -0.792721 | 0.282499 |
| C | 0.942890 | -1.483156 | 1.000289 |
| C | 0.268075 | -1.355973 | -1.080207 |
| H | 0.636413 | -2.471080 | 1.353662 |
| H | 1.490988 | -0.975163 | 1.786843 |
| H | -0.227840 | -2.292651 | -1.344214 |
| H | 0.312242 | -0.706664 | -1.952217 |
| C | 1.006817 | 1.486608 | -0.126866 |
| H | -1.517328 | -2.478961 | 0.680821 |
| C | 0.766229 | 2.984191 | -0.363396 |
| H | 1.713358 | 3.476845 | -0.583674 |
| H | 0.095469 | 3.179541 | -1.197080 |
| H | 0.346342 | 3.454846 | 0.530065 |
| C | 2.175244 | 1.365226 | 0.864092 |
| H | 2.667644 | 0.397792 | 0.844581 |
| H | 2.936971 | 2.108490 | 0.625604 |
| H | 1.836150 | 1.557028 | 1.885113 |
| H | 1.323878 | 1.061980 | -1.084158 |
| C | 1.578083 | -1.637539 | -0.366922 |
| O | 2.707050 | -1.795268 | -0.746076 |



(3*R*,4*S*)-4-isopropyl-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -467.048026 | -466.769854 | -466.817988 |
| ax2 | -467.042430 | -466.764015 | -466.811775 |
| ax3 | -467.041618 | -466.763073 | -466.810607 |
| ax4 | -467.041370 | -466.762891 | -466.811473 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| eq1 | | -467.046226 | | -466.767849 | | -466.815384 |
| eq2 | | -467.044448 | | -466.766181 | | -466.813856 |
| eq3 | | -467.041228 | | -466.762715 | | -466.810103 |

ax1

```

=====
C  0.735314    0.790682   -0.045626
C -0.427041   -0.001132   -0.616200
H -0.776150    0.532157   -1.506625
C  0.841375    2.232574   -0.267991
C  0.125475   -1.372234   -1.042750
C  0.807695   -2.103141    0.116510
H  1.204230   -3.057633   -0.233179
H  0.076730   -2.333429    0.896172
C  1.445459    0.135320    1.114507
C  1.938180   -1.256802    0.706390
H  2.387724   -1.759914    1.563399
H  2.722933   -1.140892   -0.046491
H  1.404609    2.839976    0.431868
H  0.060932    2.743754   -0.819965
H -0.662264   -1.987124   -1.476726
H  2.278018    0.766015    1.428240
H  0.754519    0.055739    1.957922
H  0.864179   -1.205895   -1.831849
O  1.623739    1.320507   -1.042178
C -1.616028   -0.086364    0.363284
H -1.298216   -0.626996    1.257978
C -2.786479   -0.850352   -0.255354
H -2.545416   -1.895440   -0.446062
H -3.649266   -0.828018    0.411904
H -3.084254   -0.392844   -1.202634
C -2.081087    1.303601    0.799035
H -1.307997    1.844192    1.345367
H -2.362436    1.904157   -0.070084
H -2.954964    1.225217    1.447363

```

ax2

```

=====
C -0.872885   -0.768260    0.134387
C  0.411189   -0.326159   -0.549118
H  0.565460   -1.063545   -1.340944
C -1.101622   -2.198686    0.344733
C  0.204480    1.040403   -1.232318
C -0.549507    2.075210   -0.387914
H -0.749008    2.954232   -1.003492
H  0.062897    2.410755    0.449574
C -1.601236    0.248319    0.977538
C -1.861140    1.509361    0.153427
H -2.377105    2.255130    0.759337
H -2.522466    1.257202   -0.680704
H -1.754540   -2.523996    1.146722
H -0.343109   -2.908483    0.032870
H  1.168100    1.443765   -1.550259

```

| | | | |
|---|-----------|-----------|-----------|
| H | -2.534459 | -0.192985 | 1.329426 |
| H | -1.000754 | 0.495365 | 1.855508 |
| H | -0.375757 | 0.871558 | -2.143663 |
| O | -1.756022 | -1.512320 | -0.724581 |
| C | 1.664027 | -0.434700 | 0.355670 |
| H | 1.529529 | -1.334093 | 0.964386 |
| C | 1.916711 | 0.737889 | 1.303663 |
| H | 1.076530 | 0.939442 | 1.965854 |
| H | 2.785380 | 0.519575 | 1.927257 |
| H | 2.136634 | 1.649611 | 0.744750 |
| C | 2.907047 | -0.647287 | -0.511085 |
| H | 3.067275 | 0.204466 | -1.176232 |
| H | 3.798327 | -0.753273 | 0.109274 |
| H | 2.812857 | -1.542709 | -1.126914 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.408354 | 0.921180 | -0.085264 |
| C | 0.380789 | -0.009702 | 0.822788 |
| H | 0.615379 | 0.597633 | 1.701393 |
| C | -0.094364 | 2.351537 | -0.127939 |
| C | -0.540887 | -1.154279 | 1.290615 |
| C | -1.388167 | -1.797477 | 0.184273 |
| H | -2.088391 | -2.499648 | 0.640549 |
| H | -0.763775 | -2.376344 | -0.496101 |
| C | -1.192635 | 0.286512 | -1.207545 |
| C | -2.152940 | -0.751196 | -0.624437 |
| H | -2.722210 | -1.229475 | -1.422394 |
| H | -2.870366 | -0.239229 | 0.022957 |
| H | -0.360866 | 2.926189 | -1.008277 |
| H | 0.733316 | 2.736286 | 0.455377 |
| H | 0.056583 | -1.914895 | 1.798991 |
| H | -1.736181 | 1.065839 | -1.743029 |
| H | -0.510996 | -0.189490 | -1.915052 |
| H | -1.227733 | -0.745076 | 2.036520 |
| O | -1.198547 | 1.881462 | 0.643824 |
| C | 1.759242 | -0.486413 | 0.297592 |
| H | 2.258600 | -0.887098 | 1.185417 |
| C | 2.609471 | 0.676357 | -0.212890 |
| H | 2.674208 | 1.480635 | 0.521018 |
| H | 3.622850 | 0.333972 | -0.427524 |
| H | 2.197158 | 1.092940 | -1.134596 |
| C | 1.757767 | -1.616668 | -0.732845 |
| H | 1.300407 | -2.524259 | -0.342285 |
| H | 1.242090 | -1.339166 | -1.652621 |
| H | 2.788766 | -1.859618 | -0.997024 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.893035 | -0.720346 | -0.002722 |
| C | 0.396353 | -0.265848 | -0.670360 |
| H | 0.479852 | -0.875194 | -1.574325 |
| C | -1.193109 | -2.152986 | 0.059647 |
| C | 0.251033 | 1.194459 | -1.142378 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.363086 | 2.146473 | -0.113819 |
| H | -0.485828 | 3.131946 | -0.566555 |
| H | 0.302317 | 2.273190 | 0.742551 |
| C | -1.550244 | 0.225753 | 0.977508 |
| C | -1.712606 | 1.616729 | 0.365427 |
| H | -2.157589 | 2.293718 | 1.095677 |
| H | -2.399534 | 1.561030 | -0.484197 |
| H | -1.842607 | -2.528255 | 0.842413 |
| H | -0.484058 | -2.863621 | -0.350167 |
| H | 1.211263 | 1.573262 | -1.491886 |
| H | -2.515255 | -0.194205 | 1.264064 |
| H | -0.943357 | 0.303147 | 1.880196 |
| H | -0.410349 | 1.186764 | -2.014079 |
| O | -1.834767 | -1.321683 | -0.909430 |
| C | 1.664185 | -0.619235 | 0.147771 |
| H | 1.695688 | -1.712991 | 0.154812 |
| C | 1.690912 | -0.176835 | 1.611236 |
| H | 0.900923 | -0.648066 | 2.194953 |
| H | 2.643363 | -0.468421 | 2.058398 |
| H | 1.598092 | 0.904554 | 1.714698 |
| C | 2.928783 | -0.135705 | -0.561998 |
| H | 3.050100 | 0.944560 | -0.462857 |
| H | 3.810127 | -0.605718 | -0.123533 |
| H | 2.909871 | -0.377002 | -1.626598 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.665630 | 0.860864 | -0.165218 |
| C | 0.339722 | -0.256170 | -0.403614 |
| H | 0.261110 | -0.475435 | -1.476126 |
| C | -0.410835 | 1.977692 | 0.755033 |
| C | -0.112958 | -1.517881 | 0.346837 |
| C | -1.540327 | -1.923965 | -0.013191 |
| H | -1.824409 | -2.819249 | 0.542084 |
| H | -1.592967 | -2.174183 | -1.077146 |
| C | -2.096545 | 0.478139 | -0.468961 |
| C | -2.511186 | -0.783900 | 0.285076 |
| H | -3.530202 | -1.060917 | 0.012404 |
| H | -2.508705 | -0.581285 | 1.360421 |
| H | 0.529361 | 2.054216 | 1.285077 |
| H | -1.254778 | 2.476969 | 1.217703 |
| H | 0.581315 | -2.333254 | 0.133935 |
| H | -2.750922 | 1.317753 | -0.232191 |
| H | -2.172057 | 0.294710 | -1.545610 |
| H | -0.066136 | -1.332444 | 1.423376 |
| O | -0.309078 | 2.153214 | -0.660046 |
| C | 1.809701 | 0.124356 | -0.125376 |
| H | 1.916069 | 1.187636 | -0.352684 |
| C | 2.740530 | -0.644071 | -1.064059 |
| H | 3.785044 | -0.400543 | -0.862355 |
| H | 2.620029 | -1.721916 | -0.930800 |
| H | 2.532657 | -0.408121 | -2.108573 |
| C | 2.250647 | -0.105508 | 1.322866 |
| H | 2.340428 | -1.172397 | 1.536500 |

| | | | |
|---|----------|----------|----------|
| H | 3.230010 | 0.346012 | 1.488630 |
| H | 1.558066 | 0.319406 | 2.049363 |

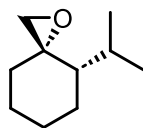
eq2

```
=====
C -0.576524    0.848158   -0.026334
C  0.350064   -0.339770   -0.257846
H  0.363464   -0.521429   -1.340919
C -0.511775    1.657817    1.196359
C -0.341428   -1.555953    0.382417
C -1.738868   -1.779431   -0.201434
H -2.212218   -2.633163    0.286214
H -1.636925   -2.034331   -1.260825
C -1.932476    0.684316   -0.670227
C -2.624592   -0.541765   -0.071881
H -3.586492   -0.707825   -0.558439
H -2.826698   -0.350141    0.986169
H  0.251980    1.479833    1.942409
H -1.421357    2.123890    1.558701
H  0.256702   -2.451760    0.221919
H -2.521899    1.587614   -0.509610
H -1.805872    0.551492   -1.748630
H -0.409109   -1.402140    1.464947
O -0.032475    2.167069   -0.052304
C  1.812175   -0.103460    0.172331
H  1.818617    0.464263    1.105478
C  2.555344    0.709059   -0.890720
H  3.557861    0.970555   -0.547621
H  2.660542    0.117045   -1.803794
H  2.026677    1.627186   -1.137441
C  2.575147   -1.405021    0.421291
H  2.180643   -1.964039    1.269098
H  2.537306   -2.051930   -0.458957
H  3.624184   -1.185376    0.626007
```

eq3

```
=====
C -0.355164    0.867572   -0.020050
C  0.195633   -0.459846   -0.526657
H  0.022798   -0.431547   -1.610382
C  0.248840    1.654203    1.065198
C -0.673066   -1.597666    0.038530
C -2.155715   -1.432310   -0.280351
H -2.722432   -2.264622    0.139995
H -2.303475   -1.455384   -1.364282
C -1.836077    1.046913   -0.286054
C -2.667163   -0.105111    0.271220
H -3.719151    0.041384    0.023422
H -2.590194   -0.114626    1.362695
H  1.170524    1.338048    1.533859
H -0.390882    2.288585    1.669045
H -0.300067   -2.548830   -0.348025
```


| | | | |
|---|-----------|-----------|-----------|
| H | -2.153361 | 2.004372 | 0.128391 |
| H | -1.974568 | 1.097255 | -1.371016 |
| H | -0.554793 | -1.628432 | 1.125434 |
| O | 0.385384 | 2.057950 | -0.297666 |
| C | 1.697343 | -0.788662 | -0.349209 |
| H | 1.848960 | -1.644594 | -1.014791 |
| C | 2.099988 | -1.271548 | 1.048425 |
| H | 3.175735 | -1.455126 | 1.071344 |
| H | 1.876390 | -0.542668 | 1.826921 |
| H | 1.604978 | -2.204579 | 1.315012 |
| C | 2.649964 | 0.306275 | -0.833305 |
| H | 2.337912 | 0.711144 | -1.796480 |
| H | 2.707800 | 1.135671 | -0.129698 |
| H | 3.653259 | -0.108576 | -0.946598 |



(3S,4S)-4-isopropyl-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -467.047130 | -466.768898 | -466.816984 |
| ax2 | -467.042131 | -466.763551 | -466.811114 |
| ax3 | -467.040225 | -466.761664 | -466.809078 |
| ax4 | -467.040847 | -466.762171 | -466.81068 |
| ax5 | -467.040294 | -466.761691 | -466.809593 |
| eq1 | -467.044830 | -466.766559 | -466.81482 |
| eq2 | -467.045298 | -466.766817 | -466.814022 |
| eq3 | -467.042156 | -466.76372 | -466.811425 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | -0.770897 | 0.755401 | 0.091715 |
| C | 0.417363 | -0.013462 | 0.637968 |
| H | 0.769931 | 0.513581 | 1.530684 |
| C | -1.588367 | 1.549666 | 1.015685 |
| C | -0.120337 | -1.396968 | 1.050862 |
| C | -0.796096 | -2.123543 | -0.115857 |
| H | -1.192632 | -3.079736 | 0.229074 |
| H | -0.058938 | -2.351688 | -0.889645 |
| C | -1.442283 | 0.121040 | -1.101394 |
| C | -1.924967 | -1.282545 | -0.717348 |
| H | -2.351867 | -1.782761 | -1.587383 |
| H | -2.725396 | -1.183715 | 0.022189 |
| H | -1.298697 | 1.620721 | 2.058036 |
| H | -2.640330 | 1.700866 | 0.801454 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.676832 | -2.008893 | 1.471476 |
| H | -2.276288 | 0.746286 | -1.421912 |
| H | -0.734621 | 0.060992 | -1.932672 |
| H | -0.857575 | -1.251606 | 1.846043 |
| O | -0.690198 | 2.180846 | 0.098636 |
| C | 1.601575 | -0.086954 | -0.347766 |
| H | 1.296214 | -0.664566 | -1.223309 |
| C | 2.798937 | -0.794926 | 0.286480 |
| H | 2.589290 | -1.838033 | 0.520779 |
| H | 3.654206 | -0.775165 | -0.390568 |
| H | 3.093868 | -0.292283 | 1.211551 |
| C | 2.020706 | 1.301317 | -0.830955 |
| H | 1.224952 | 1.799499 | -1.383095 |
| H | 2.286665 | 1.939362 | 0.015310 |
| H | 2.892167 | 1.226231 | -1.483425 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.896959 | -0.752541 | 0.076735 |
| C | 0.400168 | -0.312684 | -0.581707 |
| H | 0.584018 | -1.038349 | -1.377956 |
| C | -1.721754 | -1.763258 | -0.599608 |
| C | 0.190458 | 1.057212 | -1.256997 |
| C | -0.560355 | 2.088702 | -0.405487 |
| H | -0.769785 | 2.966452 | -1.019589 |
| H | 0.059538 | 2.427574 | 0.424499 |
| C | -1.599127 | 0.249417 | 0.958474 |
| C | -1.865137 | 1.521600 | 0.152106 |
| H | -2.367453 | 2.263499 | 0.773818 |
| H | -2.541306 | 1.281506 | -0.674477 |
| H | -1.388051 | -2.183409 | -1.541117 |
| H | -2.790418 | -1.785426 | -0.418631 |
| H | 1.153948 | 1.460808 | -1.575333 |
| H | -2.528446 | -0.188042 | 1.325108 |
| H | -0.979892 | 0.481067 | 1.827562 |
| H | -0.392331 | 0.891550 | -2.167764 |
| O | -0.913728 | -2.105908 | 0.530860 |
| C | 1.635851 | -0.421923 | 0.347054 |
| H | 1.475493 | -1.308673 | 0.966500 |
| C | 1.898790 | 0.763691 | 1.276538 |
| H | 1.059252 | 0.989207 | 1.931188 |
| H | 2.760810 | 0.542819 | 1.908607 |
| H | 2.135862 | 1.662865 | 0.704212 |
| C | 2.887088 | -0.669176 | -0.498850 |
| H | 3.063652 | 0.165364 | -1.181996 |
| H | 3.770242 | -0.770228 | 0.133849 |
| H | 2.790544 | -1.577560 | -1.094907 |

ax3

```
=====
```

| | | | |
|---|-----------|----------|-----------|
| C | -0.502882 | 0.892931 | -0.039894 |
| C | 0.360316 | 0.018148 | 0.853998 |
| H | 0.564021 | 0.622938 | 1.741890 |
| C | -1.222491 | 2.015703 | 0.579562 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.497976 | -1.182737 | 1.302719 |
| C | -1.271264 | -1.880976 | 0.174539 |
| H | -1.942765 | -2.620644 | 0.614462 |
| H | -0.591177 | -2.426888 | -0.478219 |
| C | -1.171445 | 0.219468 | -1.212058 |
| C | -2.073238 | -0.894198 | -0.674119 |
| H | -2.563923 | -1.415740 | -1.496714 |
| H | -2.860252 | -0.441064 | -0.063553 |
| H | -1.082055 | 2.226253 | 1.633516 |
| H | -2.160060 | 2.347562 | 0.147894 |
| H | 0.133282 | -1.903693 | 1.827418 |
| H | -1.749633 | 0.959673 | -1.766508 |
| H | -0.424006 | -0.194492 | -1.891767 |
| H | -1.228036 | -0.816302 | 2.030313 |
| O | -0.071590 | 2.239707 | -0.236796 |
| C | 1.765251 | -0.368003 | 0.321498 |
| H | 2.315164 | -0.669666 | 1.218888 |
| C | 2.497273 | 0.832707 | -0.276962 |
| H | 2.480015 | 1.691192 | 0.394175 |
| H | 3.537550 | 0.573503 | -0.480603 |
| H | 2.036721 | 1.140904 | -1.217497 |
| C | 1.852936 | -1.555245 | -0.639521 |
| H | 1.480066 | -2.474176 | -0.189432 |
| H | 1.309018 | -1.381331 | -1.568090 |
| H | 2.899911 | -1.722460 | -0.900375 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.916883 | -0.696874 | -0.059600 |
| C | 0.389508 | -0.245137 | -0.696070 |
| H | 0.507254 | -0.835700 | -1.608798 |
| C | -1.795634 | -1.598097 | -0.819309 |
| C | 0.246932 | 1.221402 | -1.151168 |
| C | -0.379665 | 2.163563 | -0.121321 |
| H | -0.502565 | 3.151337 | -0.569025 |
| H | 0.278583 | 2.287400 | 0.740646 |
| C | -1.566875 | 0.230121 | 0.944364 |
| C | -1.730535 | 1.627330 | 0.346538 |
| H | -2.179067 | 2.295878 | 1.082165 |
| H | -2.414096 | 1.579427 | -0.506921 |
| H | -1.494746 | -1.933572 | -1.804729 |
| H | -2.861479 | -1.592289 | -0.621684 |
| H | 1.212275 | 1.602868 | -1.483410 |
| H | -2.529881 | -0.190191 | 1.237011 |
| H | -0.953828 | 0.298449 | 1.843328 |
| H | -0.402678 | 1.223587 | -2.032073 |
| O | -0.988583 | -2.088835 | 0.254933 |
| C | 1.641769 | -0.608039 | 0.140873 |
| H | 1.659856 | -1.701061 | 0.148571 |
| C | 1.660178 | -0.164760 | 1.604108 |
| H | 0.867608 | -0.636252 | 2.183280 |
| H | 2.610287 | -0.457407 | 2.055903 |
| H | 1.568144 | 0.916654 | 1.708304 |
| C | 2.917448 | -0.137206 | -0.558105 |

| | | | |
|---|----------|-----------|-----------|
| H | 3.048445 | 0.942120 | -0.459553 |
| H | 3.790778 | -0.614702 | -0.111666 |
| H | 2.906315 | -0.379678 | -1.622663 |

ax5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.310448 | 0.930664 | 0.013883 |
| C | -0.353746 | -0.174400 | -0.795488 |
| H | -0.788485 | 0.307598 | -1.674251 |
| C | 0.464084 | 2.255313 | -0.605849 |
| C | 0.742775 | -1.121698 | -1.319734 |
| C | 1.729696 | -1.592479 | -0.251976 |
| H | 2.487049 | -2.228444 | -0.713361 |
| H | 1.218728 | -2.202080 | 0.496665 |
| C | 1.339600 | 0.524659 | 1.047333 |
| C | 2.392305 | -0.394177 | 0.425284 |
| H | 3.096483 | -0.721516 | 1.191006 |
| H | 2.964203 | 0.164967 | -0.321800 |
| H | 0.076167 | 2.427989 | -1.602820 |
| H | 1.281387 | 2.895154 | -0.293594 |
| H | 0.270862 | -1.973295 | -1.812730 |
| H | 1.798936 | 1.426903 | 1.453200 |
| H | 0.854404 | 0.008035 | 1.874801 |
| H | 1.311371 | -0.587350 | -2.087488 |
| O | -0.530965 | 2.022317 | 0.394289 |
| C | -1.541209 | -0.893150 | -0.098772 |
| H | -1.631674 | -1.868306 | -0.586706 |
| C | -2.844234 | -0.129895 | -0.353532 |
| H | -3.031260 | -0.011048 | -1.421884 |
| H | -3.693730 | -0.659342 | 0.081644 |
| H | -2.795816 | 0.864005 | 0.093240 |
| C | -1.406291 | -1.140556 | 1.404697 |
| H | -0.525627 | -1.725423 | 1.663543 |
| H | -1.363678 | -0.196021 | 1.950770 |
| H | -2.282175 | -1.686046 | 1.760380 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.653344 | 0.822871 | -0.347599 |
| C | 0.354802 | -0.315354 | -0.435105 |
| H | 0.226093 | -0.723936 | -1.444434 |
| C | -0.292499 | 2.241481 | -0.433032 |
| C | -0.095595 | -1.405870 | 0.549762 |
| C | -1.512275 | -1.887824 | 0.229480 |
| H | -1.818143 | -2.653172 | 0.944674 |
| H | -1.514113 | -2.355255 | -0.760198 |
| C | -2.061324 | 0.393001 | -0.696055 |
| C | -2.509528 | -0.729931 | 0.241808 |
| H | -3.504655 | -1.077605 | -0.038791 |
| H | -2.582363 | -0.330330 | 1.257149 |
| H | -1.029587 | 2.947820 | -0.798527 |
| H | 0.741672 | 2.541944 | -0.547650 |
| H | 0.597531 | -2.247302 | 0.523378 |
| H | -2.729153 | 1.251928 | -0.620489 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.080129 | 0.042800 | -1.731478 |
| H | -0.073758 | -1.000903 | 1.565464 |
| O | -0.604792 | 1.645014 | 0.827949 |
| C | 1.842523 | 0.068686 | -0.322359 |
| H | 2.011407 | 0.889828 | -1.023265 |
| C | 2.733657 | -1.088890 | -0.779000 |
| H | 3.774314 | -0.765780 | -0.833885 |
| H | 2.688441 | -1.926916 | -0.081537 |
| H | 2.440910 | -1.452773 | -1.765509 |
| C | 2.276656 | 0.531576 | 1.069002 |
| H | 1.700050 | 1.386394 | 1.416357 |
| H | 2.158643 | -0.272558 | 1.798454 |
| H | 3.332731 | 0.807223 | 1.055279 |

eq2

```
=====
```

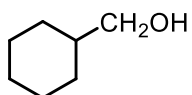
| | | | |
|---|-----------|-----------|-----------|
| C | 0.555969 | 0.874487 | 0.091499 |
| C | -0.357591 | -0.328647 | 0.306544 |
| H | -0.373481 | -0.517594 | 1.387075 |
| C | 0.079299 | 2.224740 | -0.230353 |
| C | 0.334024 | -1.535522 | -0.348169 |
| C | 1.735049 | -1.758958 | 0.225169 |
| H | 2.203878 | -2.614655 | -0.263556 |
| H | 1.644821 | -2.008385 | 1.287264 |
| C | 1.935119 | 0.705189 | 0.688002 |
| C | 2.614701 | -0.520024 | 0.075502 |
| H | 3.588401 | -0.681838 | 0.539804 |
| H | 2.791207 | -0.328533 | -0.986418 |
| H | 0.711011 | 3.069898 | 0.020495 |
| H | -0.977756 | 2.439732 | -0.312442 |
| H | -0.262777 | -2.433906 | -0.196610 |
| H | 2.521538 | 1.606645 | 0.506989 |
| H | 1.839838 | 0.577537 | 1.769637 |
| H | 0.397344 | -1.368050 | -1.428305 |
| O | 0.593901 | 1.373088 | -1.254525 |
| C | -1.811273 | -0.080857 | -0.141804 |
| H | -1.781733 | 0.538279 | -1.042864 |
| C | -2.581861 | 0.660593 | 0.954377 |
| H | -3.545311 | 1.016987 | 0.586399 |
| H | -2.773747 | -0.016490 | 1.790655 |
| H | -2.030307 | 1.515359 | 1.345450 |
| C | -2.568130 | -1.361772 | -0.493083 |
| H | -2.143965 | -1.868823 | -1.358877 |
| H | -2.563263 | -2.060654 | 0.346892 |
| H | -3.608747 | -1.125585 | -0.721493 |

eq3

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.344149 | 0.826656 | -0.209270 |
| C | 0.231674 | -0.570947 | -0.399516 |
| H | 0.072196 | -0.804732 | -1.458707 |
| C | 0.439280 | 2.057523 | -0.051201 |
| C | -0.655921 | -1.538529 | 0.402269 |
| C | -2.115055 | -1.472441 | -0.050290 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.723825 | -2.156633 | 0.543153 |
| H | -2.179749 | -1.806138 | -1.090691 |
| C | -1.774414 | 0.939515 | -0.695420 |
| C | -2.664089 | -0.051061 | 0.057613 |
| H | -3.684841 | -0.003479 | -0.324109 |
| H | -2.699813 | 0.241403 | 1.110630 |
| H | -0.013937 | 2.999192 | -0.341784 |
| H | 1.519735 | 2.039640 | -0.060926 |
| H | -0.273482 | -2.554640 | 0.288252 |
| H | -2.123518 | 1.962054 | -0.547309 |
| H | -1.803456 | 0.727203 | -1.767457 |
| H | -0.593404 | -1.286603 | 1.464850 |
| O | -0.159698 | 1.427270 | 1.081227 |
| C | 1.731363 | -0.812745 | -0.136903 |
| H | 1.836778 | -1.900995 | -0.188632 |
| C | 2.235428 | -0.398436 | 1.247513 |
| H | 3.237327 | -0.802333 | 1.404724 |
| H | 2.291750 | 0.683228 | 1.359322 |
| H | 1.592993 | -0.779856 | 2.041082 |
| C | 2.623641 | -0.251340 | -1.245833 |
| H | 2.596543 | 0.836632 | -1.293841 |
| H | 3.661481 | -0.546615 | -1.081103 |
| H | 2.318263 | -0.634653 | -2.221036 |



cyclohexylmethanol

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -350.362673 | -350.149083 | -350.190686 |
| ax2 | -350.363120 | -350.149386 | -350.19067 |
| ax3 | -350.363213 | -350.14958 | -350.191004 |
| ax4 | -350.359268 | -350.14555 | -350.186883 |
| ax5 | -350.359268 | -350.145549 | -350.186879 |
| ax6 | -350.359160 | -350.145562 | -350.187037 |
| eq | -350.365104 | -350.151839 | -350.193555 |
| eq2 | -350.365742 | -350.152367 | -350.193884 |
| eq3 | -350.365532 | -350.152194 | -350.193769 |
| eq4 | -350.365058 | -350.151638 | -350.193131 |
| eq5 | -350.365058 | -350.151637 | -350.193128 |
| eq6 | -350.364362 | -350.151039 | -350.192627 |

ax

| | | | |
|---|-----------|-----------|----------|
| C | -0.562331 | -1.362016 | 0.586154 |
| C | 0.601862 | -0.367065 | 0.688176 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.182215 | -0.607139 | 1.583525 |
| C | 0.069912 | 1.065896 | 0.827506 |
| C | -0.925162 | 1.432755 | -0.275477 |
| H | -0.417753 | 1.452205 | -1.244215 |
| H | -1.307885 | 2.440464 | -0.104276 |
| C | -1.560855 | -0.995138 | -0.514828 |
| C | -2.079038 | 0.431370 | -0.331510 |
| H | -2.643869 | 0.486942 | 0.604961 |
| H | -2.769427 | 0.690299 | -1.136259 |
| C | 1.552675 | -0.519937 | -0.489659 |
| H | 1.062111 | -0.254864 | -1.429544 |
| H | 0.904444 | 1.767758 | 0.838001 |
| H | -2.391928 | -1.702629 | -0.506070 |
| H | -1.084986 | -1.083057 | -1.495414 |
| H | -0.434489 | 1.152063 | 1.794663 |
| H | 1.870662 | -1.565039 | -0.560436 |
| O | 2.682505 | 0.323618 | -0.276535 |
| H | 3.254819 | 0.261687 | -1.046334 |
| H | -1.090341 | -1.371333 | 1.543989 |
| H | -0.175990 | -2.371485 | 0.427524 |

ax2

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.573618 | -1.370569 | 0.573765 |
| C | 0.604247 | -0.392226 | 0.690620 |
| H | 1.180177 | -0.649049 | 1.583833 |
| C | 0.084235 | 1.043226 | 0.848673 |
| C | -0.893549 | 1.438802 | -0.259537 |
| H | -0.378945 | 1.455593 | -1.224890 |
| H | -1.259824 | 2.451541 | -0.083268 |
| C | -1.568716 | -0.976597 | -0.521653 |
| C | -2.063405 | 0.456883 | -0.328256 |
| H | -2.630201 | 0.515608 | 0.606759 |
| H | -2.746227 | 0.733712 | -1.133358 |
| C | 1.554985 | -0.547834 | -0.493533 |
| H | 1.052961 | -0.325070 | -1.438304 |
| H | 0.917132 | 1.748943 | 0.896144 |
| H | -2.411728 | -1.669799 | -0.515474 |
| H | -1.098276 | -1.065662 | -1.504411 |
| H | -0.430672 | 1.116496 | 1.811054 |
| H | 1.898257 | -1.581933 | -0.542196 |
| O | 2.732259 | 0.245166 | -0.372780 |
| H | 2.484162 | 1.169830 | -0.464171 |
| H | -1.101239 | -1.389921 | 1.531683 |
| H | -0.198722 | -2.381738 | 0.398363 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.544516 | -1.361094 | 0.591712 |
| C | 0.612659 | -0.355938 | 0.671215 |
| H | 1.206391 | -0.591608 | 1.561361 |
| C | 0.074612 | 1.073660 | 0.814719 |
| C | -0.942309 | 1.428980 | -0.272198 |
| H | -0.451391 | 1.449575 | -1.249258 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.330049 | 2.434067 | -0.097247 |
| C | -1.560719 | -1.004032 | -0.496158 |
| C | -2.088470 | 0.418031 | -0.306509 |
| H | -2.638350 | 0.470490 | 0.638992 |
| H | -2.793976 | 0.669681 | -1.100338 |
| C | 1.548945 | -0.508335 | -0.524196 |
| H | 1.051670 | -0.237440 | -1.454820 |
| H | 0.904752 | 1.781428 | 0.805025 |
| H | -2.385134 | -1.718951 | -0.476342 |
| H | -1.096710 | -1.087953 | -1.482832 |
| H | -0.411624 | 1.163328 | 1.790729 |
| H | 1.857809 | -1.555557 | -0.608949 |
| O | 2.692022 | 0.336290 | -0.444285 |
| H | 3.159312 | 0.125749 | 0.370548 |
| H | -1.058584 | -1.373393 | 1.557059 |
| H | -0.151498 | -2.367362 | 0.428841 |

ax4

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.153966 | -1.219768 | 0.869611 |
| C | 0.691980 | 0.062443 | 0.957475 |
| H | 1.089047 | 0.112905 | 1.976660 |
| C | -0.171755 | 1.315262 | 0.743367 |
| C | -1.094141 | 1.233608 | -0.475064 |
| H | -0.497523 | 1.208183 | -1.388520 |
| H | -1.719167 | 2.127761 | -0.518195 |
| C | -1.106492 | -1.275590 | -0.329962 |
| C | -1.968346 | -0.017194 | -0.410136 |
| H | -2.607103 | 0.036226 | 0.477976 |
| H | -2.629847 | -0.066817 | -1.276787 |
| C | 1.948534 | 0.030961 | 0.091795 |
| H | 2.573002 | -0.813815 | 0.400854 |
| H | 0.473925 | 2.194094 | 0.674403 |
| H | -1.738211 | -2.161710 | -0.243374 |
| H | -0.553824 | -1.383334 | -1.266311 |
| H | -0.797193 | 1.453105 | 1.631014 |
| H | 2.520499 | 0.943803 | 0.265496 |
| O | 1.733863 | -0.019861 | -1.315975 |
| H | 1.399948 | -0.893228 | -1.538564 |
| H | -0.763133 | -1.283515 | 1.776073 |
| H | 0.503784 | -2.093098 | 0.874548 |

ax5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.172002 | -1.315520 | 0.743168 |
| C | 0.692051 | -0.063088 | 0.957604 |
| H | 1.089356 | -0.114078 | 1.976720 |
| C | -0.153725 | 1.219263 | 0.870344 |
| C | -1.106324 | 1.275824 | -0.329161 |
| H | -0.553599 | 1.384165 | -1.265358 |
| H | -1.738173 | 2.161804 | -0.241986 |
| C | -1.093681 | -1.233348 | -0.475734 |
| C | -1.968023 | 0.017377 | -0.410404 |
| H | -2.607131 | -0.036650 | 0.477406 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.629164 | 0.067463 | -1.277311 |
| C | 1.948282 | -0.031440 | 0.091473 |
| H | 2.519765 | -0.944813 | 0.263965 |
| H | 0.504120 | 2.092525 | 0.875625 |
| H | -1.718586 | -2.127536 | -0.519822 |
| H | -0.496515 | -1.207240 | -1.388828 |
| H | -0.762860 | 1.282705 | 1.776863 |
| H | 2.573385 | 0.812603 | 0.401195 |
| O | 1.732955 | 0.020894 | -1.316178 |
| H | 1.400922 | 0.895214 | -1.537823 |
| H | -0.797957 | -1.453106 | 1.630515 |
| H | 0.473328 | -2.194615 | 0.674520 |

ax6

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=====
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| | | | |
|---|-----------|-----------|-----------|
| C | 0.175503 | 1.268034 | 0.814252 |
| C | -0.679853 | 0.000108 | 0.969797 |
| H | -1.073491 | 0.000169 | 1.991055 |
| C | 0.175507 | -1.267789 | 0.814496 |
| C | 1.089716 | -1.257325 | -0.413262 |
| H | 0.486181 | -1.292342 | -1.321143 |
| H | 1.719234 | -2.149573 | -0.403364 |
| C | 1.089770 | 1.257208 | -0.413492 |
| C | 1.957649 | -0.000077 | -0.437459 |
| H | 2.616280 | -0.000035 | 0.437996 |
| H | 2.600865 | -0.000126 | -1.319510 |
| C | -1.934182 | 0.000041 | 0.109013 |
| H | -2.530145 | 0.885576 | 0.353509 |
| H | -0.474956 | -2.145774 | 0.797412 |
| H | 1.719331 | 2.149438 | -0.403842 |
| H | 0.486235 | 1.292027 | -1.321367 |
| H | 0.805416 | -1.360149 | 1.704922 |
| H | -2.530276 | -0.885354 | 0.353661 |
| O | -1.619163 | -0.000167 | -1.282283 |
| H | -2.446407 | -0.000325 | -1.772622 |
| H | 0.805375 | 1.360628 | 1.704654 |
| H | -0.474994 | 2.145977 | 0.796834 |

eq

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```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.376288 | -1.355224 | 0.162549 |
| C | -0.580105 | -0.233701 | -0.249652 |
| H | -0.608486 | -0.190945 | -1.344936 |
| C | -0.079585 | 1.114487 | 0.272932 |
| C | 1.350028 | 1.400915 | -0.185991 |
| H | 1.363529 | 1.497682 | -1.276343 |
| H | 1.691132 | 2.354396 | 0.221207 |
| C | 1.807237 | -1.072958 | -0.294642 |
| C | 2.298784 | 0.276559 | 0.227615 |
| H | 2.353441 | 0.238865 | 1.320397 |
| H | 3.308111 | 0.477806 | -0.135714 |
| C | -1.983219 | -0.540321 | 0.236637 |
| H | -1.995010 | -0.548841 | 1.332540 |
| H | -0.109705 | 1.093510 | 1.368735 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.471196 | -1.873132 | 0.036961 |
| H | 1.837651 | -1.065787 | -1.388742 |
| H | -0.751492 | 1.909984 | -0.050502 |
| H | -2.287004 | -1.531995 | -0.113200 |
| O | -2.879781 | 0.450667 | -0.258325 |
| H | -3.761167 | 0.251185 | 0.069444 |
| H | 0.359685 | -1.448646 | 1.254309 |
| H | 0.029804 | -2.307963 | -0.244250 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.381079 | -1.355447 | 0.166296 |
| C | -0.582016 | -0.245782 | -0.262226 |
| H | -0.606744 | -0.212113 | -1.357648 |
| C | -0.093215 | 1.110418 | 0.251906 |
| C | 1.339306 | 1.402543 | -0.196102 |
| H | 1.360830 | 1.490221 | -1.286886 |
| H | 1.669623 | 2.361497 | 0.206653 |
| C | 1.813717 | -1.068405 | -0.282284 |
| C | 2.291267 | 0.287834 | 0.234925 |
| H | 2.336177 | 0.258457 | 1.328345 |
| H | 3.302101 | 0.494536 | -0.120860 |
| C | -1.987415 | -0.563760 | 0.225853 |
| H | -1.993423 | -0.604510 | 1.321346 |
| H | -0.135926 | 1.104019 | 1.347525 |
| H | 2.480061 | -1.861667 | 0.060810 |
| H | 1.853145 | -1.068713 | -1.376047 |
| H | -0.753688 | 1.910209 | -0.091709 |
| H | -2.294705 | -1.542897 | -0.143507 |
| O | -2.974424 | 0.351152 | -0.237483 |
| H | -2.798362 | 1.210497 | 0.156720 |
| H | 0.357464 | -1.439246 | 1.258741 |
| H | 0.042498 | -2.313914 | -0.233829 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.373671 | -1.355074 | 0.162440 |
| C | -0.584884 | -0.230772 | -0.236917 |
| H | -0.618145 | -0.185731 | -1.333820 |
| C | -0.078405 | 1.114526 | 0.285203 |
| C | 1.347025 | 1.401460 | -0.186224 |
| H | 1.350788 | 1.501299 | -1.276411 |
| H | 1.692900 | 2.353332 | 0.220635 |
| C | 1.801472 | -1.073233 | -0.305090 |
| C | 2.298305 | 0.274927 | 0.215849 |
| H | 2.362719 | 0.234653 | 1.307957 |
| H | 3.304497 | 0.476316 | -0.155975 |
| C | -1.988784 | -0.540142 | 0.259462 |
| H | -1.999950 | -0.542173 | 1.351443 |
| H | -0.098071 | 1.089190 | 1.381047 |
| H | 2.467472 | -1.874427 | 0.019876 |
| H | 1.823386 | -1.064178 | -1.399399 |
| H | -0.752795 | 1.912710 | -0.027328 |
| H | -2.290299 | -1.537119 | -0.078312 |

| | | | |
|---|-----------|-----------|-----------|
| O | -2.956819 | 0.425584 | -0.136239 |
| H | -2.985347 | 0.438908 | -1.098211 |
| H | 0.364631 | -1.451384 | 1.254095 |
| H | 0.022360 | -2.306224 | -0.244024 |

eq4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.036024 | 1.249296 | -0.022867 |
| C | 0.566133 | -0.026708 | -0.618162 |
| H | 0.327362 | -0.040570 | -1.688646 |
| C | -0.059319 | -1.266268 | 0.024729 |
| C | -1.583082 | -1.255351 | -0.099410 |
| H | -1.857300 | -1.319341 | -1.157291 |
| H | -2.007146 | -2.132545 | 0.392524 |
| C | -1.559585 | 1.263560 | -0.152134 |
| C | -2.176651 | 0.022757 | 0.492295 |
| H | -1.979717 | 0.043941 | 1.569016 |
| H | -3.260716 | 0.030681 | 0.366037 |
| C | 2.086577 | -0.038362 | -0.525169 |
| H | 2.496616 | 0.818044 | -1.070357 |
| H | 0.217850 | -1.291813 | 1.082607 |
| H | -1.967127 | 2.169024 | 0.300703 |
| H | -1.827921 | 1.287636 | -1.212980 |
| H | 0.353134 | -2.167371 | -0.435762 |
| H | 2.477295 | -0.946009 | -0.986899 |
| O | 2.579750 | -0.046413 | 0.811275 |
| H | 2.343044 | 0.789104 | 1.224761 |
| H | 0.221218 | 1.310490 | 1.040626 |
| H | 0.397114 | 2.126484 | -0.510227 |

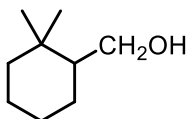
eq5

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```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.059318 | 1.266227 | 0.024807 |
| C | 0.566118 | 0.026722 | -0.618077 |
| H | 0.327300 | 0.040596 | -1.688569 |
| C | -0.036041 | -1.249341 | -0.022855 |
| C | -1.559587 | -1.263552 | -0.152066 |
| H | -1.827949 | -1.287722 | -1.212900 |
| H | -1.967150 | -2.168973 | 0.300857 |
| C | -1.583103 | 1.255363 | -0.099514 |
| C | -2.176668 | -0.022708 | 0.492259 |
| H | -1.979769 | -0.043795 | 1.568990 |
| H | -3.260729 | -0.030704 | 0.365981 |
| C | 2.086568 | 0.038326 | -0.525181 |
| H | 2.477219 | 0.945924 | -0.987065 |
| H | 0.221282 | -1.310626 | 1.040612 |
| H | -2.007183 | 2.132608 | 0.392309 |
| H | -1.857204 | 1.319256 | -1.157429 |
| H | 0.397073 | -2.126456 | -0.510358 |
| H | 2.496491 | -0.818137 | -1.070377 |
| O | 2.579939 | 0.046421 | 0.811170 |
| H | 2.342442 | -0.788677 | 1.225052 |
| H | 0.217600 | 1.291727 | 1.082760 |
| H | 0.353253 | 2.167395 | -0.435463 |

eq6

| | | | |
|---|-----------|-----------|-----------|
| C | 0.050581 | 1.258179 | -0.003431 |
| C | -0.561513 | -0.000042 | 0.617881 |
| H | -0.321062 | -0.000018 | 1.687786 |
| C | 0.050606 | -1.258229 | -0.003437 |
| C | 1.574128 | -1.259643 | 0.122880 |
| H | 1.846717 | -1.303434 | 1.182292 |
| H | 1.990218 | -2.151271 | -0.349614 |
| C | 1.574107 | 1.259676 | 0.122978 |
| C | 2.179600 | 0.000038 | -0.495768 |
| H | 1.981860 | 0.000090 | -1.572530 |
| H | 3.263875 | 0.000017 | -0.370366 |
| C | -2.077023 | -0.000043 | 0.527265 |
| H | -2.474862 | 0.886437 | 1.031569 |
| H | -0.224775 | -1.298312 | -1.060942 |
| H | 1.990192 | 2.151345 | -0.349438 |
| H | 1.846652 | 1.303384 | 1.182405 |
| H | -0.371781 | -2.146974 | 0.472099 |
| H | -2.474886 | -0.886611 | 1.031406 |
| O | -2.470891 | 0.000067 | -0.843315 |
| H | -3.431302 | 0.000068 | -0.879422 |
| H | -0.224697 | 1.298222 | -1.060965 |
| H | -0.371928 | 2.146910 | 0.472027 |



(2,2-dimethylcyclohexyl)methanol

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -428.975688 | -428.703174 | -428.749743 |
| ax2 | -428.975962 | -428.70347 | -428.750112 |
| ax3 | -428.976253 | -428.703661 | -428.750125 |
| ax4 | -428.975668 | -428.703108 | -428.749013 |
| ax5 | -428.973366 | -428.700907 | -428.747193 |
| ax6 | -428.975133 | -428.702808 | -428.749198 |
| ax7 | -428.973490 | -428.701006 | -428.74727 |
| ax8 | -428.974644 | -428.702362 | -428.748681 |
| ax9 | -428.973397 | -428.70091 | -428.74715 |
| eq | -428.977615 | -428.705533 | -428.752741 |
| eq2 | -428.978034 | -428.705818 | -428.75299 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| eq3 | | -428.978025 | | -428.705901 | | -428.753052 |
| eq4 | | -428.976402 | | -428.704209 | | -428.751274 |
| eq5 | | -428.976498 | | -428.704212 | | -428.750805 |
| eq6 | | -428.975871 | | -428.703572 | | -428.750785 |
| eq7 | | -428.976588 | | -428.704324 | | -428.751142 |
| eq8 | | -428.975575 | | -428.703435 | | -428.750798 |
| eq9 | | -428.975628 | | -428.703513 | | -428.750707 |

ax

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.720055 | 1.079809 | 0.970056 |
| C | -0.544817 | -0.391307 | 0.559152 |
| H | -0.708284 | -1.013765 | 1.445705 |
| C | 0.898162 | -0.674259 | 0.055525 |
| C | 1.303894 | 0.348590 | -1.023833 |
| H | 0.711801 | 0.166058 | -1.925455 |
| H | 2.347676 | 0.169061 | -1.295927 |
| C | -0.330882 | 2.047323 | -0.147620 |
| C | 1.108284 | 1.803651 | -0.598407 |
| H | 1.788827 | 2.048732 | 0.221440 |
| H | 1.365353 | 2.465387 | -1.427605 |
| C | -1.604729 | -0.806475 | -0.458732 |
| H | -1.563286 | -1.885206 | -0.616398 |
| H | -0.452754 | 3.076416 | 0.194936 |
| H | -1.003969 | 1.917853 | -1.000488 |
| H | -1.435414 | -0.318080 | -1.422831 |
| O | -2.891977 | -0.451924 | 0.045934 |
| H | -3.553164 | -0.801721 | -0.557710 |
| H | -0.101305 | 1.284869 | 1.846090 |
| H | -1.753793 | 1.244491 | 1.271010 |
| C | 1.870514 | -0.599068 | 1.240081 |
| H | 1.624967 | -1.363543 | 1.980510 |
| H | 2.892005 | -0.778702 | 0.898138 |
| H | 1.854275 | 0.367210 | 1.741306 |
| C | 1.013395 | -2.081659 | -0.538683 |
| H | 0.645690 | -2.835763 | 0.161519 |
| H | 0.455150 | -2.180047 | -1.470425 |
| H | 2.059441 | -2.307478 | -0.756516 |

ax2

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.720177 | 1.086614 | 0.960086 |
| C | -0.561598 | -0.382606 | 0.537342 |
| H | -0.746922 | -1.012313 | 1.416811 |
| C | 0.885676 | -0.685430 | 0.057347 |
| C | 1.320512 | 0.338470 | -1.009180 |
| H | 0.733557 | 0.173838 | -1.917753 |
| H | 2.363420 | 0.142388 | -1.272954 |
| C | -0.294165 | 2.059268 | -0.139872 |
| C | 1.146439 | 1.792916 | -0.572730 |
| H | 1.820505 | 2.017703 | 0.258177 |
| H | 1.426544 | 2.457514 | -1.392063 |
| C | -1.616696 | -0.773911 | -0.502182 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.567420 | -1.846152 | -0.698222 |
| H | -0.401272 | 3.086235 | 0.213712 |
| H | -0.956322 | 1.953926 | -1.004335 |
| H | -1.450765 | -0.257491 | -1.447597 |
| O | -2.941367 | -0.428143 | -0.106100 |
| H | -3.125488 | -0.869474 | 0.729532 |
| H | -0.117703 | 1.274152 | 1.851149 |
| H | -1.757457 | 1.267919 | 1.240870 |
| C | 1.839939 | -0.631458 | 1.257749 |
| H | 1.573950 | -1.399852 | 1.987061 |
| H | 2.864641 | -0.820129 | 0.930465 |
| H | 1.826893 | 0.330209 | 1.767693 |
| C | 0.992236 | -2.090977 | -0.543567 |
| H | 0.596070 | -2.843749 | 0.142478 |
| H | 0.455943 | -2.175298 | -1.489195 |
| H | 2.039770 | -2.331596 | -0.736974 |

ax3

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.761600 | 1.033242 | 0.982089 |
| C | -0.524286 | -0.426735 | 0.564856 |
| H | -0.656427 | -1.059063 | 1.449458 |
| C | 0.929862 | -0.636084 | 0.056195 |
| C | 1.276777 | 0.404840 | -1.026805 |
| H | 0.692979 | 0.189527 | -1.926426 |
| H | 2.327722 | 0.281156 | -1.302245 |
| C | -0.439373 | 2.019708 | -0.140781 |
| C | 1.006705 | 1.848999 | -0.603893 |
| H | 1.679146 | 2.132479 | 0.210121 |
| H | 1.221494 | 2.520908 | -1.436758 |
| C | -1.564917 | -0.892591 | -0.459903 |
| H | -1.483731 | -1.967619 | -0.604443 |
| H | -0.611084 | 3.041245 | 0.202229 |
| H | -1.112288 | 1.855168 | -0.988425 |
| H | -1.403004 | -0.417332 | -1.431369 |
| O | -2.907148 | -0.678530 | -0.033143 |
| H | -3.078589 | 0.267637 | -0.030657 |
| H | -0.136709 | 1.266221 | 1.846274 |
| H | -1.790733 | 1.160351 | 1.323338 |
| C | 1.905047 | -0.511325 | 1.234145 |
| H | 1.697600 | -1.280901 | 1.980923 |
| H | 2.931039 | -0.649056 | 0.886229 |
| H | 1.851078 | 0.456772 | 1.729309 |
| C | 1.109934 | -2.037432 | -0.536708 |
| H | 0.783144 | -2.806761 | 0.167255 |
| H | 0.552232 | -2.165196 | -1.465076 |
| H | 2.164422 | -2.213022 | -0.759765 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|----------|
| C | -0.723641 | -1.305805 | 1.002997 |
| C | 0.480659 | -0.425793 | 0.629573 |
| H | 1.061371 | -0.238275 | 1.538514 |
| C | 0.019818 | 0.950066 | 0.072327 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.003017 | 0.751161 | -1.062779 |
| H | -0.491422 | 0.315265 | -1.926431 |
| H | -1.364969 | 1.732743 | -1.380421 |
| C | -1.676550 | -1.502999 | -0.176005 |
| C | -2.176533 | -0.153261 | -0.687655 |
| H | -2.783786 | 0.321813 | 0.087534 |
| H | -2.825004 | -0.290636 | -1.554705 |
| C | 1.419907 | -1.192913 | -0.312579 |
| H | 1.146251 | -1.040981 | -1.360432 |
| H | -2.516282 | -2.132538 | 0.122909 |
| H | -1.159147 | -2.027805 | -0.985620 |
| H | 1.340453 | -2.261435 | -0.110878 |
| O | 2.799435 | -0.887003 | -0.120739 |
| H | 2.943472 | 0.034881 | -0.349844 |
| H | -1.273750 | -0.849565 | 1.828462 |
| H | -0.360157 | -2.269641 | 1.364584 |
| C | -0.600452 | 1.780040 | 1.203334 |
| H | 0.134061 | 1.953128 | 1.993003 |
| H | -0.921136 | 2.752799 | 0.824308 |
| H | -1.466584 | 1.298435 | 1.654126 |
| C | 1.202116 | 1.749112 | -0.484041 |
| H | 1.975975 | 1.896328 | 0.274120 |
| H | 1.645004 | 1.266554 | -1.359092 |
| H | 0.866330 | 2.737310 | -0.805255 |

ax5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.942790 | -0.883467 | 1.207104 |
| C | 0.271362 | 0.470849 | 0.905668 |
| H | -0.074574 | 0.869519 | 1.867253 |
| C | -0.993738 | 0.313068 | 0.015886 |
| C | -0.715953 | -0.602016 | -1.192697 |
| H | -0.024602 | -0.089859 | -1.865267 |
| H | -1.652657 | -0.743629 | -1.739374 |
| C | 1.172476 | -1.771376 | -0.019027 |
| C | -0.119831 | -1.955378 | -0.810757 |
| H | -0.833488 | -2.524036 | -0.208533 |
| H | 0.069052 | -2.543440 | -1.710661 |
| C | 1.271138 | 1.528330 | 0.434152 |
| H | 2.098621 | 1.564013 | 1.150312 |
| H | 1.558874 | -2.739230 | 0.306162 |
| H | 1.936713 | -1.346834 | -0.676098 |
| H | 0.799482 | 2.509713 | 0.442213 |
| O | 1.781179 | 1.367180 | -0.886682 |
| H | 2.354231 | 0.595983 | -0.900042 |
| H | 0.314227 | -1.440249 | 1.906045 |
| H | 1.888226 | -0.702259 | 1.724406 |
| C | -2.122133 | -0.285662 | 0.868337 |
| H | -2.407483 | 0.409648 | 1.660661 |
| H | -3.004097 | -0.474049 | 0.252103 |
| H | -1.838100 | -1.226117 | 1.339296 |
| C | -1.475314 | 1.670338 | -0.500962 |
| H | -1.633470 | 2.372706 | 0.321114 |
| H | -0.759536 | 2.110633 | -1.196063 |

H -2.425626 1.551938 -1.026301

ax6

```
=====
C -0.705298 -1.305950 1.009006
C 0.488398 -0.416266 0.624742
H 1.069519 -0.219860 1.533990
C 0.014700 0.954719 0.068625
C -1.010110 0.741973 -1.062559
H -0.496628 0.311381 -1.927723
H -1.383855 1.719096 -1.380229
C -1.660798 -1.516313 -0.165743
C -2.173846 -0.173631 -0.683006
H -2.785872 0.298335 0.090298
H -2.821572 -0.321766 -1.548923
C 1.422566 -1.182694 -0.321360
H 1.131244 -1.051131 -1.363312
H -2.494179 -2.151360 0.139298
H -1.141708 -2.041332 -0.974088
H 1.359822 -2.253041 -0.100527
O 2.781828 -0.763032 -0.249032
H 3.071887 -0.861340 0.663098
H -1.255348 -0.851354 1.835204
H -0.332489 -2.265682 1.372292
C -0.615147 1.777511 1.200182
H 0.114790 1.951082 1.994096
H -0.936428 2.750699 0.822623
H -1.482644 1.293157 1.645630
C 1.187153 1.764808 -0.489611
H 1.951643 1.929166 0.272108
H 1.661265 1.263505 -1.333062
H 0.830218 2.739758 -0.830172
```

ax7

```
=====
C 0.911052 -0.915484 1.207634
C 0.292891 0.461799 0.905135
H -0.039021 0.884158 1.861476
C -0.982539 0.348584 0.020161
C -0.761277 -0.589501 -1.183910
H -0.086778 -0.116328 -1.902775
H -1.717660 -0.714303 -1.699457
C 1.122406 -1.786765 -0.031924
C -0.184087 -1.951676 -0.803880
H -0.902273 -2.503082 -0.190937
H -0.021007 -2.544792 -1.705555
C 1.340679 1.469015 0.428464
H 2.154737 1.480231 1.154630
H 1.508349 -2.762470 0.269994
H 1.868517 -1.326702 -0.681706
H 0.912519 2.474291 0.411872
O 1.958236 1.186003 -0.824343
H 1.312366 1.332707 -1.521374
H 0.258029 -1.455357 1.897967
```


| | | | |
|---|-----------|-----------|-----------|
| H | 1.858523 | -0.768471 | 1.731375 |
| C | -2.127575 | -0.202138 | 0.883375 |
| H | -2.370345 | 0.500538 | 1.683118 |
| H | -3.024414 | -0.345597 | 0.276867 |
| H | -1.880464 | -1.157663 | 1.344219 |
| C | -1.421934 | 1.720360 | -0.497772 |
| H | -1.549989 | 2.429810 | 0.322842 |
| H | -0.706554 | 2.148138 | -1.203712 |
| H | -2.378115 | 1.631702 | -1.017791 |

ax8

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.694122 | -1.307951 | 1.013804 |
| C | 0.488608 | -0.403217 | 0.632433 |
| H | 1.067573 | -0.194600 | 1.537804 |
| C | -0.003119 | 0.957331 | 0.064614 |
| C | -1.018487 | 0.723991 | -1.070973 |
| H | -0.493220 | 0.299441 | -1.932074 |
| H | -1.407648 | 1.693404 | -1.393884 |
| C | -1.635525 | -1.541799 | -0.167490 |
| C | -2.168307 | -0.210705 | -0.694906 |
| H | -2.793875 | 0.253561 | 0.072239 |
| H | -2.807596 | -0.374022 | -1.564396 |
| C | 1.440347 | -1.152675 | -0.302078 |
| H | 1.175799 | -0.993632 | -1.351006 |
| H | -2.460030 | -2.190569 | 0.132842 |
| H | -1.099458 | -2.060894 | -0.968866 |
| H | 1.373570 | -2.226824 | -0.104426 |
| O | 2.776077 | -0.709443 | -0.062693 |
| H | 3.351352 | -1.132531 | -0.706788 |
| H | -1.258501 | -0.854417 | 1.830906 |
| H | -0.309665 | -2.258287 | 1.389064 |
| C | -0.651088 | 1.777255 | 1.187863 |
| H | 0.070469 | 1.962223 | 1.986752 |
| H | -0.980839 | 2.745102 | 0.803895 |
| H | -1.516503 | 1.284606 | 1.628245 |
| C | 1.161633 | 1.780400 | -0.490677 |
| H | 1.916977 | 1.961262 | 0.275900 |
| H | 1.649591 | 1.279094 | -1.326627 |
| H | 0.793747 | 2.746853 | -0.843568 |

ax9

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.814736 | -0.991121 | 1.217107 |
| C | 0.313777 | 0.432856 | 0.911982 |
| H | 0.010300 | 0.877188 | 1.867288 |
| C | -0.955085 | 0.425579 | 0.012523 |
| C | -0.779670 | -0.512588 | -1.197921 |
| H | -0.036922 | -0.077590 | -1.868912 |
| H | -1.727751 | -0.551875 | -1.742227 |
| C | 0.972184 | -1.873692 | -0.022283 |
| C | -0.329051 | -1.922736 | -0.819943 |
| H | -1.101967 | -2.419445 | -0.226636 |
| H | -0.196505 | -2.520320 | -1.723966 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.437838 | 1.350451 | 0.444226 |
| H | 2.251775 | 1.290477 | 1.173998 |
| H | 1.268272 | -2.879650 | 0.282389 |
| H | 1.765517 | -1.475930 | -0.656638 |
| H | 1.087485 | 2.385326 | 0.427874 |
| O | 1.919167 | 0.983255 | -0.847667 |
| H | 2.617644 | 1.599079 | -1.088207 |
| H | 0.109730 | -1.476450 | 1.896740 |
| H | 1.763251 | -0.922800 | 1.755058 |
| C | -2.151467 | -0.039651 | 0.855721 |
| H | -2.350780 | 0.673729 | 1.658365 |
| H | -3.048024 | -0.106997 | 0.235487 |
| H | -1.989005 | -1.015528 | 1.311962 |
| C | -1.272030 | 1.830719 | -0.503289 |
| H | -1.361492 | 2.543991 | 0.319715 |
| H | -0.500797 | 2.188933 | -1.186369 |
| H | -2.221454 | 1.822921 | -1.043327 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.412264 | 0.939055 | -0.032367 |
| C | 0.634103 | -0.178806 | -0.280491 |
| H | 0.718015 | -0.290712 | -1.368631 |
| C | 0.197936 | -1.532216 | 0.294757 |
| C | -1.170701 | -1.967988 | -0.219601 |
| H | -1.113970 | -2.131327 | -1.300657 |
| H | -1.458454 | -2.919030 | 0.232123 |
| C | -1.785446 | 0.442258 | -0.524744 |
| C | -2.218245 | -0.896278 | 0.068257 |
| H | -2.354100 | -0.801339 | 1.149178 |
| H | -3.185630 | -1.186068 | -0.346074 |
| C | 2.021679 | 0.177749 | 0.232772 |
| H | 2.036536 | 0.136271 | 1.326395 |
| H | 0.169417 | -1.465108 | 1.387067 |
| H | -2.530813 | 1.212963 | -0.311335 |
| H | -1.739289 | 0.339699 | -1.614604 |
| H | 0.953265 | -2.278436 | 0.046802 |
| H | 2.306600 | 1.186400 | -0.073710 |
| O | 2.951358 | -0.765811 | -0.300437 |
| H | 3.819633 | -0.568351 | 0.061634 |
| C | -0.065721 | 2.193855 | -0.841429 |
| H | 0.836550 | 2.685634 | -0.477736 |
| H | 0.078610 | 1.950246 | -1.896305 |
| H | -0.881599 | 2.917028 | -0.772932 |
| C | -0.489384 | 1.326439 | 1.449788 |
| H | 0.441638 | 1.788541 | 1.782543 |
| H | -1.290324 | 2.053517 | 1.601620 |
| H | -0.688683 | 0.472146 | 2.096458 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.423145 | 0.936001 | -0.029812 |
| C | 0.639741 | -0.164619 | -0.290780 |
| H | 0.717020 | -0.271197 | -1.379736 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.222526 | -1.525398 | 0.282373 |
| C | -1.144337 | -1.977078 | -0.225543 |
| H | -1.088464 | -2.139090 | -1.306637 |
| H | -1.417307 | -2.931827 | 0.227146 |
| C | -1.789672 | 0.425367 | -0.525372 |
| C | -2.204723 | -0.919383 | 0.065640 |
| H | -2.341540 | -0.828064 | 1.146621 |
| H | -3.167859 | -1.222527 | -0.348837 |
| C | 2.028848 | 0.217215 | 0.214919 |
| H | 2.043963 | 0.221038 | 1.309217 |
| H | 0.204657 | -1.467551 | 1.375314 |
| H | -2.544641 | 1.186011 | -0.309713 |
| H | -1.741865 | 0.326138 | -1.615416 |
| H | 0.969535 | -2.278798 | 0.020895 |
| H | 2.306769 | 1.213017 | -0.125502 |
| O | 3.051363 | -0.645209 | -0.278917 |
| H | 2.927159 | -1.516244 | 0.108579 |
| C | -0.091744 | 2.202201 | -0.827038 |
| H | 0.804810 | 2.700805 | -0.458404 |
| H | 0.055181 | 1.970627 | -1.884265 |
| H | -0.915853 | 2.915165 | -0.751045 |
| C | -0.507647 | 1.310261 | 1.455824 |
| H | 0.411407 | 1.792291 | 1.792563 |
| H | -1.325845 | 2.016910 | 1.612230 |
| H | -0.687116 | 0.447567 | 2.097057 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.408570 | 0.939340 | -0.033289 |
| C | 0.638606 | -0.181206 | -0.268028 |
| H | 0.726522 | -0.294791 | -1.357697 |
| C | 0.194384 | -1.531878 | 0.305678 |
| C | -1.170028 | -1.966727 | -0.220649 |
| H | -1.103628 | -2.132640 | -1.300813 |
| H | -1.463697 | -2.916175 | 0.230552 |
| C | -1.778569 | 0.444356 | -0.536197 |
| C | -2.218466 | -0.892587 | 0.055238 |
| H | -2.364031 | -0.795425 | 1.134659 |
| H | -3.182414 | -1.181829 | -0.367351 |
| C | 2.026817 | 0.175844 | 0.257095 |
| H | 2.038031 | 0.134077 | 1.347053 |
| H | 0.155408 | -1.461378 | 1.397354 |
| H | -2.524374 | 1.216649 | -0.330027 |
| H | -1.723727 | 0.340298 | -1.625548 |
| H | 0.950815 | -2.280916 | 0.068619 |
| H | 2.313608 | 1.186517 | -0.041224 |
| O | 3.024198 | -0.750427 | -0.167801 |
| H | 3.055253 | -0.729503 | -1.129575 |
| C | -0.051832 | 2.191673 | -0.841949 |
| H | 0.847466 | 2.683269 | -0.470860 |
| H | 0.101963 | 1.945505 | -1.894956 |
| H | -0.867293 | 2.916152 | -0.783142 |
| C | -0.496637 | 1.329305 | 1.447554 |
| H | 0.433820 | 1.786701 | 1.788114 |

| | | | |
|---|-----------|----------|----------|
| H | -1.294856 | 2.061031 | 1.590920 |
| H | -0.706675 | 0.477158 | 2.093610 |

eq4

```
=====
C  0.073354    0.832010    0.021001
C  0.391277   -0.654193   -0.303054
H  0.435670   -0.734819   -1.397902
C -0.711965   -1.608799    0.182862
C -2.097989   -1.229244   -0.327473
H -2.120651   -1.330351   -1.417197
H -2.845411   -1.916127    0.073388
C -1.350388    1.150085   -0.480666
C -2.430556    0.211145    0.045952
H -2.507372    0.298320    1.133256
H -3.401039    0.497700   -0.363233
C  1.712357   -1.185133    0.249633
H  1.775234   -2.252873    0.014993
H -0.722180   -1.620249    1.277354
H -1.583510    2.185759   -0.220013
H -1.346186    1.094066   -1.575088
H -0.463111   -2.623688   -0.134279
H  1.729792   -1.094127    1.336425
O  2.884434   -0.526283   -0.214873
H  2.854687   -0.511025   -1.176893
C  1.023323    1.783681   -0.716714
H  2.037907    1.725010   -0.329757
H  1.050155    1.556839   -1.785406
H  0.672612    2.812681   -0.603872
C  0.178929    1.118363    1.523223
H  1.211752    1.035495    1.864681
H -0.154757    2.137824    1.729227
H -0.429114    0.442339    2.124719
```

eq5

```
=====
C -0.096244    0.945579   -0.037354
C  0.463310   -0.359071   -0.667131
H  0.214559   -0.297458   -1.734174
C -0.210206   -1.621132   -0.114153
C -1.729212   -1.576117   -0.250337
H -1.999761   -1.562155   -1.311031
H -2.173065   -2.474965    0.181487
C -1.632668    0.923848   -0.162892
C -2.287132   -0.324582    0.421582
H -2.102140   -0.375627    1.498492
H -3.369262   -0.270047    0.289661
C  1.985675   -0.512812   -0.618375
H  2.483122    0.419082   -0.898553
H  0.051863   -1.744393    0.938729
H -2.033677    1.824291    0.309734
H -1.888507    0.983263   -1.226459
H  0.194986   -2.492046   -0.635676
H  2.278430   -1.267575   -1.348991
```

| | | | |
|---|-----------|-----------|-----------|
| O | 2.500969 | -0.988991 | 0.622910 |
| H | 2.293287 | -0.349900 | 1.309110 |
| C | 0.407656 | 2.170351 | -0.806536 |
| H | 1.484995 | 2.304117 | -0.706131 |
| H | 0.170479 | 2.088462 | -1.869492 |
| H | -0.071460 | 3.074477 | -0.423756 |
| C | 0.305060 | 1.109495 | 1.435446 |
| H | 1.362276 | 1.373075 | 1.526706 |
| H | -0.257767 | 1.930476 | 1.885249 |
| H | 0.116457 | 0.215501 | 2.030326 |

eq6

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.017605 | 0.849050 | 0.040591 |
| C | 0.433589 | -0.630126 | -0.187355 |
| H | 0.499163 | -0.772712 | -1.273001 |
| C | -0.637517 | -1.600882 | 0.328239 |
| C | -1.997162 | -1.341742 | -0.318545 |
| H | -1.922488 | -1.565546 | -1.387468 |
| H | -2.747366 | -2.017112 | 0.096484 |
| C | -1.347160 | 1.065410 | -0.641255 |
| C | -2.433364 | 0.111546 | -0.148055 |
| H | -2.650862 | 0.307864 | 0.904763 |
| H | -3.359276 | 0.292264 | -0.697053 |
| C | 1.804531 | -1.013743 | 0.372058 |
| H | 1.847907 | -2.096543 | 0.491141 |
| H | -0.720123 | -1.523386 | 1.416274 |
| H | -1.656262 | 2.102890 | -0.489075 |
| H | -1.217647 | 0.927051 | -1.720303 |
| H | -0.318422 | -2.622786 | 0.113396 |
| H | 1.963250 | -0.575047 | 1.361448 |
| O | 2.897531 | -0.700026 | -0.488632 |
| H | 2.945662 | 0.253233 | -0.592733 |
| C | 1.024056 | 1.808946 | -0.601503 |
| H | 1.965124 | 1.840967 | -0.045498 |
| H | 1.232504 | 1.537627 | -1.638832 |
| H | 0.627220 | 2.826624 | -0.594762 |
| C | -0.086731 | 1.207519 | 1.528950 |
| H | 0.885658 | 1.157982 | 2.020005 |
| H | -0.451360 | 2.232257 | 1.631003 |
| H | -0.770008 | 0.558713 | 2.074512 |

eq7

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.092773 | 0.945713 | -0.023146 |
| C | 0.461680 | -0.358744 | -0.653298 |
| H | 0.200313 | -0.306918 | -1.718234 |
| C | -0.214798 | -1.615623 | -0.091129 |
| C | -1.731878 | -1.569660 | -0.257346 |
| H | -1.975436 | -1.571137 | -1.324450 |
| H | -2.187268 | -2.461426 | 0.176761 |
| C | -1.626602 | 0.937264 | -0.183224 |
| C | -2.304123 | -0.308058 | 0.384034 |
| H | -2.158286 | -0.352743 | 1.466711 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.380876 | -0.251594 | 0.214085 |
| C | 1.982316 | -0.516279 | -0.630213 |
| H | 2.475575 | 0.401624 | -0.946390 |
| H | 0.016511 | -1.722335 | 0.972849 |
| H | -2.032250 | 1.837674 | 0.285770 |
| H | -1.859950 | 1.003930 | -1.251687 |
| H | 0.194637 | -2.496181 | -0.594278 |
| H | 2.257034 | -1.296676 | -1.347588 |
| O | 2.533474 | -0.830081 | 0.645646 |
| H | 2.180505 | -1.680255 | 0.924331 |
| C | 0.442944 | 2.167560 | -0.775193 |
| H | 1.514002 | 2.304362 | -0.623296 |
| H | 0.257952 | 2.080010 | -1.848353 |
| H | -0.055884 | 3.072605 | -0.421182 |
| C | 0.278275 | 1.093722 | 1.457445 |
| H | 1.354413 | 1.210648 | 1.577686 |
| H | -0.211760 | 1.979063 | 1.870344 |
| H | -0.027269 | 0.234633 | 2.054180 |

eq8

```
=====
```

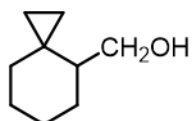
| | | | |
|---|-----------|-----------|-----------|
| C | 0.058213 | 0.836456 | 0.016733 |
| C | 0.396855 | -0.644358 | -0.315382 |
| H | 0.443360 | -0.721198 | -1.408446 |
| C | -0.691190 | -1.615423 | 0.174552 |
| C | -2.086560 | -1.252393 | -0.321954 |
| H | -2.117269 | -1.348230 | -1.411945 |
| H | -2.820342 | -1.952222 | 0.081764 |
| C | -1.373917 | 1.135789 | -0.472248 |
| C | -2.436384 | 0.181102 | 0.061321 |
| H | -2.503900 | 0.262767 | 1.149723 |
| H | -3.414673 | 0.455642 | -0.337440 |
| C | 1.721663 | -1.156038 | 0.234723 |
| H | 1.795073 | -2.223027 | 0.004312 |
| H | -0.693289 | -1.634123 | 1.269032 |
| H | -1.618712 | 2.167788 | -0.207692 |
| H | -1.378353 | 1.081599 | -1.566704 |
| H | -0.432065 | -2.624943 | -0.151200 |
| H | 1.736167 | -1.054711 | 1.324586 |
| O | 2.830827 | -0.469404 | -0.339630 |
| H | 3.634603 | -0.892560 | -0.024024 |
| C | 0.987603 | 1.804399 | -0.724671 |
| H | 2.011268 | 1.737310 | -0.365294 |
| H | 0.991485 | 1.594936 | -1.796715 |
| H | 0.635890 | 2.829794 | -0.584460 |
| C | 0.170155 | 1.119980 | 1.519273 |
| H | 1.207921 | 1.063295 | 1.851156 |
| H | -0.188114 | 2.129687 | 1.732068 |
| H | -0.414274 | 0.426340 | 2.124239 |

eq9

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.089638 | 0.939578 | -0.029444 |
| C | 0.453865 | -0.376177 | -0.648428 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.189977 | -0.327774 | -1.712748 |
| C | -0.230061 | -1.622049 | -0.072517 |
| C | -1.746568 | -1.565273 | -0.238253 |
| H | -1.992583 | -1.579704 | -1.305034 |
| H | -2.209474 | -2.447298 | 0.208148 |
| C | -1.622583 | 0.941423 | -0.197840 |
| C | -2.311423 | -0.290770 | 0.384405 |
| H | -2.168766 | -0.321113 | 1.467971 |
| H | -3.387364 | -0.227992 | 0.210939 |
| C | 1.967817 | -0.544171 | -0.631642 |
| H | 2.463140 | 0.360795 | -0.992060 |
| H | 0.019326 | -1.720465 | 0.985637 |
| H | -2.023277 | 1.851597 | 0.256344 |
| H | -1.850285 | 0.994638 | -1.268345 |
| H | 0.172419 | -2.507710 | -0.571002 |
| H | 2.226409 | -1.358274 | -1.316249 |
| O | 2.424767 | -0.865496 | 0.681613 |
| H | 3.373056 | -1.016302 | 0.635731 |
| C | 0.460517 | 2.151409 | -0.786909 |
| H | 1.531992 | 2.279391 | -0.629855 |
| H | 0.281018 | 2.058224 | -1.860594 |
| H | -0.032239 | 3.063280 | -0.441878 |
| C | 0.271467 | 1.096624 | 1.452719 |
| H | 1.346286 | 1.217395 | 1.578906 |
| H | -0.224299 | 1.982598 | 1.857516 |
| H | -0.033827 | 0.239114 | 2.051120 |



spiro[2.5]octan-4-ylmethanol

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -427.747984 | -427.498747 | -427.543544 |
| ax2 | -427.747098 | -427.498049 | -427.543592 |
| ax3 | -427.743829 | -427.494609 | -427.53986 |
| ax4 | -427.747554 | -427.498361 | -427.543577 |
| ax5 | -427.747544 | -427.4984 | -427.543646 |
| ax6 | -427.746221 | -427.497143 | -427.542546 |
| ax7 | -427.745554 | -427.49648 | -427.541821 |
| ax8 | -427.743771 | -427.494608 | -427.539765 |
| ax9 | -427.743928 | -427.494701 | -427.54005 |
| eq | -427.745458 | -427.496301 | -427.541676 |
| eq2 | -427.745023 | -427.495985 | -427.541363 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| eq3 | | -427.744254 | | -427.495104 | | -427.540507 |
| eq4 | | -427.745948 | | -427.496635 | | -427.541873 |
| eq5 | | -427.745861 | | -427.496697 | | -427.54207 |
| eq6 | | -427.745114 | | -427.495887 | | -427.541134 |
| eq7 | | -427.743223 | | -427.494025 | | -427.539397 |
| eq8 | | -427.744801 | | -427.495584 | | -427.540412 |
| eq9 | | -427.745613 | | -427.496504 | | -427.54169 |

ax1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.282019 | 0.787952 | 0.019747 |
| C | 0.365108 | -0.570311 | 0.701458 |
| H | 0.992807 | -0.467721 | 1.591493 |
| C | 0.333517 | 2.001635 | 0.901861 |
| C | 1.494736 | 1.677750 | -0.005126 |
| C | -1.043714 | -1.009180 | 1.130167 |
| C | -2.053348 | -0.964904 | -0.022049 |
| H | -1.799360 | -1.719239 | -0.770967 |
| H | -3.045070 | -1.221219 | 0.354323 |
| C | -0.688281 | 0.837956 | -1.144106 |
| C | -2.085034 | 0.412808 | -0.685767 |
| H | -2.458521 | 1.148459 | 0.033358 |
| H | -2.775970 | 0.409896 | -1.530346 |
| C | 1.012189 | -1.633761 | -0.183611 |
| H | 0.411914 | -1.813607 | -1.079374 |
| H | 0.474390 | 1.850155 | 1.963329 |
| H | -0.291937 | 2.842221 | 0.634828 |
| H | 1.643570 | 2.303529 | -0.874556 |
| H | 2.400309 | 1.321117 | 0.466084 |
| H | -1.386185 | -0.337340 | 1.921975 |
| H | -0.710391 | 1.848631 | -1.556196 |
| H | -0.347944 | 0.174093 | -1.945342 |
| H | -1.004196 | -2.013398 | 1.558183 |
| H | 1.066672 | -2.573223 | 0.367626 |
| O | 2.348755 | -1.317712 | -0.554804 |
| H | 2.336717 | -0.450330 | -0.971428 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.867686 | -0.568829 | -0.056733 |
| C | -0.557057 | -0.444175 | 0.460651 |
| H | -0.703445 | -1.195631 | 1.242395 |
| C | 1.904146 | -1.074326 | 0.905706 |
| C | 1.439254 | -1.941148 | -0.240559 |
| C | -0.769478 | 0.949180 | 1.069281 |
| C | -0.366109 | 2.072473 | 0.110702 |
| H | -1.030448 | 2.077467 | -0.758078 |
| H | -0.492153 | 3.037330 | 0.604695 |
| C | 1.291263 | 0.535742 | -1.005552 |
| C | 1.079144 | 1.907076 | -0.361629 |
| H | 1.749721 | 2.003188 | 0.498098 |
| H | 1.342712 | 2.698866 | -1.064814 |
| C | -1.563500 | -0.757881 | -0.637529 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.335651 | -1.739404 | -1.063716 |
| H | 1.582016 | -1.346601 | 1.901407 |
| H | 2.897350 | -0.651220 | 0.842369 |
| H | 2.125430 | -2.098735 | -1.061353 |
| H | 0.806831 | -2.785565 | -0.001712 |
| H | -0.158680 | 1.023760 | 1.973770 |
| H | 2.339096 | 0.396564 | -1.278980 |
| H | 0.709755 | 0.475463 | -1.930797 |
| H | -1.810577 | 1.061825 | 1.373196 |
| H | -1.508103 | -0.020701 | -1.442577 |
| O | -2.870112 | -0.759410 | -0.066518 |
| H | -3.505054 | -0.930007 | -0.767791 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.972765 | -0.076455 | -0.058524 |
| C | -0.141373 | -0.669374 | 0.794213 |
| H | 0.331607 | -1.128788 | 1.668919 |
| C | 2.259872 | 0.260775 | 0.643574 |
| C | 2.189457 | -0.913617 | -0.303954 |
| C | -1.073744 | 0.442915 | 1.306532 |
| C | -1.508960 | 1.452502 | 0.237167 |
| H | -2.193314 | 0.993969 | -0.480153 |
| H | -2.063803 | 2.260572 | 0.717513 |
| C | 0.523556 | 0.892364 | -1.135078 |
| C | -0.308076 | 2.018043 | -0.520319 |
| H | 0.318725 | 2.587715 | 0.173279 |
| H | -0.642604 | 2.710755 | -1.294273 |
| C | -0.873234 | -1.832006 | 0.127322 |
| H | -1.543451 | -2.293889 | 0.859443 |
| H | 2.334838 | 0.045316 | 1.700600 |
| H | 2.797443 | 1.139466 | 0.314033 |
| H | 2.685318 | -0.818123 | -1.260208 |
| H | 2.216089 | -1.904644 | 0.128785 |
| H | -0.538614 | 0.994955 | 2.084601 |
| H | 1.400829 | 1.297963 | -1.643626 |
| H | -0.075566 | 0.363399 | -1.879433 |
| H | -1.948958 | -0.004018 | 1.785246 |
| H | -0.143383 | -2.585125 | -0.172243 |
| O | -1.598924 | -1.511338 | -1.055606 |
| H | -2.385336 | -1.019693 | -0.803222 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.894504 | -0.533105 | -0.051856 |
| C | -0.536252 | -0.479547 | 0.462672 |
| H | -0.648155 | -1.235617 | 1.245338 |
| C | 1.953174 | -0.992144 | 0.909904 |
| C | 1.529977 | -1.876673 | -0.238887 |
| C | -0.812444 | 0.903472 | 1.069722 |
| C | -0.471259 | 2.043167 | 0.106438 |
| H | -1.132514 | 2.007847 | -0.764379 |
| H | -0.649937 | 3.002044 | 0.595490 |
| C | 1.267403 | 0.591291 | -0.999399 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.982250 | 1.951445 | -0.360297 |
| H | 1.642928 | 2.085322 | 0.501996 |
| H | 1.206681 | 2.753815 | -1.064913 |
| C | -1.522292 | -0.847341 | -0.644206 |
| H | -1.268649 | -1.832594 | -1.035990 |
| H | 1.643570 | -1.281970 | 1.904632 |
| H | 2.925428 | -0.522604 | 0.848624 |
| H | 2.223007 | -1.999454 | -1.059860 |
| H | 0.938102 | -2.750658 | -0.002542 |
| H | -0.199679 | 1.009040 | 1.969580 |
| H | 2.322873 | 0.504887 | -1.264972 |
| H | 0.697113 | 0.501126 | -1.928893 |
| H | -1.852019 | 0.977312 | 1.398011 |
| H | -1.466454 | -0.139341 | -1.474878 |
| O | -2.864728 | -0.947290 | -0.179241 |
| H | -3.174836 | -0.064229 | 0.042143 |

ax5

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.855295 | -0.580542 | -0.055374 |
| C | -0.572558 | -0.430014 | 0.446383 |
| H | -0.738104 | -1.185673 | 1.222920 |
| C | 1.873481 | -1.111698 | 0.912773 |
| C | 1.402151 | -1.962454 | -0.242709 |
| C | -0.766117 | 0.961938 | 1.062908 |
| C | -0.327792 | 2.083858 | 0.117920 |
| H | -0.981752 | 2.109073 | -0.758205 |
| H | -0.439730 | 3.047226 | 0.618089 |
| C | 1.307493 | 0.521767 | -0.993563 |
| C | 1.118679 | 1.891899 | -0.340024 |
| H | 1.782149 | 1.966028 | 0.527367 |
| H | 1.406272 | 2.683866 | -1.033480 |
| C | -1.575137 | -0.718569 | -0.668877 |
| H | -1.347665 | -1.690736 | -1.116916 |
| H | 1.537435 | -1.383646 | 1.904014 |
| H | 2.875118 | -0.707312 | 0.861157 |
| H | 2.092051 | -2.127922 | -1.058793 |
| H | 0.752356 | -2.796616 | -0.014653 |
| H | -0.168765 | 1.019367 | 1.977482 |
| H | 2.353833 | 0.363002 | -1.261830 |
| H | 0.730016 | 0.480200 | -1.922410 |
| H | -1.809830 | 1.093741 | 1.351282 |
| H | -1.512377 | 0.029516 | -1.458385 |
| O | -2.925027 | -0.685951 | -0.218275 |
| H | -3.023765 | -1.349615 | 0.471936 |

ax6

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```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.215357 | 0.822368 | -0.000551 |
| C | 0.417503 | -0.527862 | 0.669160 |
| H | 1.055320 | -0.380650 | 1.548368 |
| C | 0.200022 | 2.031777 | 0.894158 |
| C | 1.351547 | 1.794792 | -0.052007 |
| C | -0.941849 | -1.071291 | 1.136539 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.973597 | -1.110163 | 0.004522 |
| H | -1.667793 | -1.836135 | -0.753636 |
| H | -2.932123 | -1.454043 | 0.396767 |
| C | -0.789959 | 0.805771 | -1.134969 |
| C | -2.135468 | 0.263721 | -0.648103 |
| H | -2.552409 | 0.960601 | 0.085712 |
| H | -2.843747 | 0.207997 | -1.476405 |
| C | 1.117930 | -1.550544 | -0.223954 |
| H | 0.561778 | -1.714138 | -1.146015 |
| H | 0.380963 | 1.882652 | 1.950115 |
| H | -0.494377 | 2.825613 | 0.655196 |
| H | 1.428238 | 2.433087 | -0.921722 |
| H | 2.296389 | 1.492901 | 0.376778 |
| H | -1.317658 | -0.421990 | 1.931926 |
| H | -0.905158 | 1.815743 | -1.533288 |
| H | -0.418722 | 0.181207 | -1.953447 |
| H | -0.816246 | -2.066605 | 1.568292 |
| H | 1.161750 | -2.507821 | 0.306713 |
| O | 2.421819 | -1.156755 | -0.632369 |
| H | 2.920335 | -0.915791 | 0.154833 |

ax7

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.172029 | 0.836942 | -0.003064 |
| C | 0.435109 | -0.504048 | 0.666828 |
| H | 1.066704 | -0.331217 | 1.543370 |
| C | 0.120376 | 2.044599 | 0.892851 |
| C | 1.270696 | 1.850535 | -0.064712 |
| C | -0.899772 | -1.107708 | 1.130230 |
| C | -1.926730 | -1.195216 | -0.002816 |
| H | -1.581840 | -1.899945 | -0.764610 |
| H | -2.867200 | -1.589823 | 0.385442 |
| C | -0.839484 | 0.782168 | -1.131038 |
| C | -2.156546 | 0.173320 | -0.645869 |
| H | -2.605154 | 0.843661 | 0.094014 |
| H | -2.862935 | 0.090034 | -1.473532 |
| C | 1.186261 | -1.484328 | -0.224628 |
| H | 0.671324 | -1.619648 | -1.179034 |
| H | 0.315695 | 1.901210 | 1.947034 |
| H | -0.604971 | 2.812555 | 0.661101 |
| H | 1.313076 | 2.493306 | -0.933689 |
| H | 2.228916 | 1.572300 | 0.348069 |
| H | -1.306702 | -0.472936 | 1.922137 |
| H | -1.002956 | 1.789063 | -1.520332 |
| H | -0.444114 | 0.183072 | -1.957290 |
| H | -0.730446 | -2.094537 | 1.566080 |
| H | 1.225351 | -2.457563 | 0.275247 |
| O | 2.506888 | -0.997529 | -0.448941 |
| H | 2.958516 | -1.616885 | -1.029175 |

ax8

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=====
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| | | | |
|---|-----------|-----------|-----------|
| C | 0.969165 | -0.088102 | -0.060675 |
| C | -0.147471 | -0.656127 | 0.806784 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.326979 | -1.121276 | 1.676991 |
| C | 2.264979 | 0.233305 | 0.632687 |
| C | 2.171448 | -0.945548 | -0.307386 |
| C | -1.050949 | 0.477317 | 1.320959 |
| C | -1.496887 | 1.459463 | 0.233368 |
| H | -2.166789 | 0.955082 | -0.463631 |
| H | -2.056684 | 2.275999 | 0.693838 |
| C | 0.528802 | 0.880162 | -1.142039 |
| C | -0.298798 | 2.014732 | -0.537037 |
| H | 0.332633 | 2.594858 | 0.144017 |
| H | -0.635334 | 2.696056 | -1.320519 |
| C | -0.910967 | -1.801573 | 0.157066 |
| H | -1.607524 | -2.217586 | 0.892311 |
| H | 2.342455 | 0.023095 | 1.690606 |
| H | 2.814250 | 1.101565 | 0.295026 |
| H | 2.663920 | -0.863431 | -1.266648 |
| H | 2.185268 | -1.934114 | 0.131592 |
| H | -0.489895 | 1.036325 | 2.076230 |
| H | 1.411002 | 1.276937 | -1.649358 |
| H | -0.071766 | 0.351913 | -1.884963 |
| H | -1.920732 | 0.049620 | 1.825165 |
| H | -0.202428 | -2.588479 | -0.119451 |
| O | -1.628381 | -1.368160 | -0.996469 |
| H | -2.074238 | -2.133057 | -1.371805 |

ax9

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.961075 | -0.033381 | -0.041099 |
| C | -0.137722 | -0.656309 | 0.814266 |
| H | 0.350041 | -1.087321 | 1.695236 |
| C | 2.240291 | 0.329738 | 0.662919 |
| C | 2.199386 | -0.839912 | -0.290993 |
| C | -1.112979 | 0.426033 | 1.305029 |
| C | -1.591768 | 1.374390 | 0.202574 |
| H | -2.201058 | 0.824917 | -0.516751 |
| H | -2.223338 | 2.149201 | 0.641277 |
| C | 0.503628 | 0.937263 | -1.115919 |
| C | -0.407555 | 2.011570 | -0.523327 |
| H | 0.167835 | 2.615825 | 0.185452 |
| H | -0.757636 | 2.683249 | -1.308849 |
| C | -0.826682 | -1.853926 | 0.163582 |
| H | -1.549041 | -2.267097 | 0.869205 |
| H | 2.318033 | 0.110224 | 1.718733 |
| H | 2.756019 | 1.223312 | 0.339042 |
| H | 2.693146 | -0.726183 | -1.246365 |
| H | 2.250242 | -1.832267 | 0.136093 |
| H | -0.601156 | 1.021847 | 2.067115 |
| H | 1.381414 | 1.391068 | -1.580769 |
| H | -0.033746 | 0.414802 | -1.912051 |
| H | -1.965978 | -0.049067 | 1.794975 |
| H | -0.081876 | -2.629827 | -0.038036 |
| O | -1.565991 | -1.575791 | -1.021708 |
| H | -0.941015 | -1.409158 | -1.732834 |

eq

```
=====
C  -0.455518    0.848768   -0.175727
C   0.637432   -0.206152   -0.320922
H   0.706806   -0.456008   -1.387016
C  -0.452881    1.792570    0.995166
C  -0.194427    2.308544   -0.402209
C   0.230699   -1.475846    0.438935
C  -1.131127   -2.003284   -0.007395
H  -1.071703   -2.307348   -1.057392
H  -1.395381   -2.892930    0.566880
C  -1.814078    0.333977   -0.616944
C  -2.208437   -0.931302    0.142556
H  -2.331149   -0.689524    1.202920
H  -3.170418   -1.301331   -0.216270
C   2.020844    0.250282    0.112595
H   2.050806    0.384735    1.198000
H   0.384264    1.774984    1.678186
H  -1.405742    2.025587    1.450713
H  -0.982389    2.875548   -0.878802
H   0.805341    2.643260   -0.634066
H   0.194338   -1.238005    1.508231
H  -2.561433    1.117155   -0.474628
H  -1.778488    0.112539   -1.689259
H   0.997899   -2.238596    0.304603
H   2.284783    1.198419   -0.360262
O   2.955880   -0.754725   -0.277110
H   3.830393   -0.476030    0.008707
```

eq2

```
=====
C  -0.017407    0.782115   -0.121803
C   0.408889   -0.681460   -0.204498
H   0.406437   -0.963583   -1.264412
C   0.260381    1.577070    1.124049
C   0.979107    1.899610   -0.164587
C  -0.644209   -1.541595    0.506526
C  -2.037973   -1.323935   -0.084004
H  -2.039352   -1.680804   -1.118769
H  -2.771994   -1.921559    0.459177
C  -1.377485    1.011582   -0.752880
C  -2.438278    0.150944   -0.066286
H  -2.546718    0.483060    0.970706
H  -3.407770    0.284859   -0.549201
C   1.801732   -0.998582    0.315005
H   1.873226   -2.075893    0.488916
H   0.834715    1.126918    1.921109
H  -0.512169    2.258297    1.454115
H   0.694092    2.803991   -0.685144
H   2.024428    1.637636   -0.228690
H  -0.650452   -1.286870    1.571924
H  -1.639953    2.069388   -0.686983
H  -1.331558    0.753843   -1.816410
H  -0.369622   -2.595576    0.429986
```

| | | | |
|---|----------|-----------|-----------|
| H | 1.990748 | -0.497815 | 1.269107 |
| O | 2.773987 | -0.605066 | -0.652878 |
| H | 3.645507 | -0.809865 | -0.301538 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.089836 | 0.861900 | -0.218046 |
| C | 0.393758 | -0.523147 | -0.640516 |
| H | 0.100927 | -0.640972 | -1.691979 |
| C | 0.499477 | 1.564032 | 0.973467 |
| C | 0.744574 | 2.090169 | -0.422428 |
| C | -0.352841 | -1.594077 | 0.164921 |
| C | -1.867332 | -1.459944 | 0.008440 |
| H | -2.136892 | -1.650952 | -1.035264 |
| H | -2.375851 | -2.214146 | 0.611595 |
| C | -1.590646 | 1.008039 | -0.395433 |
| C | -2.342662 | -0.060583 | 0.397718 |
| H | -2.163160 | 0.096765 | 1.465749 |
| H | -3.417715 | 0.034585 | 0.235350 |
| C | 1.894318 | -0.769008 | -0.632522 |
| H | 2.414527 | 0.006603 | -1.200137 |
| H | 1.330735 | 1.097998 | 1.478217 |
| H | -0.181007 | 2.120794 | 1.603966 |
| H | 0.229957 | 2.994457 | -0.717742 |
| H | 1.742468 | 1.986335 | -0.822939 |
| H | -0.082627 | -1.493417 | 1.219155 |
| H | -1.900144 | 2.007145 | -0.082050 |
| H | -1.839204 | 0.910335 | -1.457920 |
| H | -0.025296 | -2.585741 | -0.156880 |
| H | 2.077854 | -1.724034 | -1.134091 |
| O | 2.395380 | -0.825189 | 0.701629 |
| H | 3.329529 | -1.048527 | 0.658326 |

eq4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.464490 | 0.845042 | -0.175340 |
| C | 0.642634 | -0.193958 | -0.333082 |
| H | 0.707558 | -0.439279 | -1.400292 |
| C | -0.474688 | 1.778460 | 1.004288 |
| C | -0.219199 | 2.309765 | -0.387435 |
| C | 0.253317 | -1.470334 | 0.425482 |
| C | -1.106718 | -2.011520 | -0.013061 |
| H | -1.048033 | -2.314471 | -1.063183 |
| H | -1.357209 | -2.903933 | 0.562760 |
| C | -1.817939 | 0.318217 | -0.617077 |
| C | -2.195313 | -0.952176 | 0.142055 |
| H | -2.317770 | -0.712895 | 1.202931 |
| H | -3.153333 | -1.334501 | -0.214171 |
| C | 2.026135 | 0.286748 | 0.092710 |
| H | 2.054356 | 0.459616 | 1.172594 |
| H | 0.360075 | 1.766760 | 1.690037 |
| H | -1.431833 | 1.994959 | 1.459027 |
| H | -1.011304 | 2.873285 | -0.861185 |
| H | 0.777648 | 2.657225 | -0.613415 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.226528 | -1.241127 | 1.496775 |
| H | -2.573546 | 1.092689 | -0.470951 |
| H | -1.782258 | 0.099373 | -1.689835 |
| H | 1.011750 | -2.243025 | 0.279856 |
| H | 2.281499 | 1.220277 | -0.405172 |
| O | 3.054956 | -0.626216 | -0.277775 |
| H | 2.953784 | -1.426695 | 0.245181 |

eq5

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.453824 | 0.847735 | -0.176956 |
| C | 0.642344 | -0.205643 | -0.308942 |
| H | 0.715100 | -0.457791 | -1.376357 |
| C | -0.458547 | 1.794311 | 0.991534 |
| C | -0.192674 | 2.307556 | -0.405033 |
| C | 0.230883 | -1.473025 | 0.450731 |
| C | -1.125878 | -2.004863 | -0.005582 |
| H | -1.057187 | -2.312144 | -1.054093 |
| H | -1.393313 | -2.893111 | 0.569325 |
| C | -1.808732 | 0.330297 | -0.626088 |
| C | -2.206427 | -0.934460 | 0.132609 |
| H | -2.338509 | -0.690737 | 1.191361 |
| H | -3.164577 | -1.307318 | -0.233342 |
| C | 2.026521 | 0.255313 | 0.134681 |
| H | 2.054071 | 0.385209 | 1.216952 |
| H | 0.375070 | 1.778595 | 1.679065 |
| H | -1.413725 | 2.027384 | 1.442061 |
| H | -0.978593 | 2.872274 | -0.887683 |
| H | 0.807696 | 2.643869 | -0.631669 |
| H | 0.184404 | -1.231102 | 1.518634 |
| H | -2.558192 | 1.112517 | -0.489648 |
| H | -1.766053 | 0.107625 | -1.697923 |
| H | 1.001062 | -2.234937 | 0.327737 |
| H | 2.289757 | 1.208929 | -0.327620 |
| O | 3.032017 | -0.710956 | -0.157031 |
| H | 3.064856 | -0.824934 | -1.112266 |

eq6

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.094163 | 0.876522 | -0.206056 |
| C | 0.405811 | -0.492888 | -0.656159 |
| H | 0.125516 | -0.593528 | -1.712858 |
| C | 0.523647 | 1.574906 | 0.973281 |
| C | 0.712613 | 2.121332 | -0.423282 |
| C | -0.333419 | -1.592949 | 0.117722 |
| C | -1.849646 | -1.471635 | -0.029457 |
| H | -2.120741 | -1.626318 | -1.078467 |
| H | -2.346497 | -2.253084 | 0.547841 |
| C | -1.600031 | 1.008425 | -0.351205 |
| C | -2.332371 | -0.092106 | 0.415108 |
| H | -2.140946 | 0.028617 | 1.485883 |
| H | -3.409979 | -0.000784 | 0.269005 |
| C | 1.914736 | -0.726469 | -0.628364 |
| H | 2.445121 | 0.092393 | -1.111681 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.379754 | 1.115317 | 1.442288 |
| H | -0.140509 | 2.113887 | 1.635694 |
| H | 0.169623 | 3.017958 | -0.689604 |
| H | 1.697629 | 2.043953 | -0.859661 |
| H | -0.078950 | -1.516781 | 1.180189 |
| H | -1.914669 | 1.993910 | -0.001938 |
| H | -1.863936 | 0.942639 | -1.412520 |
| H | 0.004548 | -2.573718 | -0.227885 |
| H | 2.125620 | -1.632845 | -1.204329 |
| O | 2.484184 | -0.844651 | 0.671900 |
| H | 2.111876 | -1.625238 | 1.093309 |

eq7

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.071371 | 0.842195 | -0.235384 |
| C | 0.375744 | -0.566010 | -0.616432 |
| H | 0.064697 | -0.710166 | -1.660139 |
| C | 0.475084 | 1.539224 | 0.979734 |
| C | 0.823874 | 2.032111 | -0.405982 |
| C | -0.396767 | -1.583082 | 0.230604 |
| C | -1.907089 | -1.415600 | 0.054714 |
| H | -2.170664 | -1.658632 | -0.979585 |
| H | -2.441648 | -2.121426 | 0.692892 |
| C | -1.560249 | 1.028526 | -0.464858 |
| C | -2.355754 | 0.014395 | 0.358989 |
| H | -2.198448 | 0.222499 | 1.421722 |
| H | -3.424240 | 0.124248 | 0.165658 |
| C | 1.872578 | -0.855469 | -0.635528 |
| H | 2.389313 | -0.160708 | -1.300817 |
| H | 1.241964 | 1.060373 | 1.567746 |
| H | -0.222557 | 2.133352 | 1.554697 |
| H | 0.373397 | 2.957839 | -0.737089 |
| H | 1.836266 | 1.875641 | -0.751399 |
| H | -0.128009 | -1.444464 | 1.281503 |
| H | -1.849349 | 2.047680 | -0.200241 |
| H | -1.784551 | 0.891552 | -1.527955 |
| H | -0.096885 | -2.596365 | -0.047541 |
| H | 2.007353 | -1.855929 | -1.050337 |
| O | 2.503218 | -0.873608 | 0.643148 |
| H | 2.841315 | 0.005634 | 0.830563 |

eq8

```
=====
```

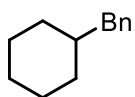
| | | | |
|---|-----------|-----------|-----------|
| C | -0.011100 | 0.778101 | -0.118531 |
| C | 0.425231 | -0.684222 | -0.167467 |
| H | 0.420311 | -0.992225 | -1.220210 |
| C | 0.186363 | 1.579915 | 1.136421 |
| C | 0.965181 | 1.919191 | -0.111285 |
| C | -0.629995 | -1.528416 | 0.556967 |
| C | -2.011177 | -1.339175 | -0.074143 |
| H | -1.984958 | -1.737798 | -1.093153 |
| H | -2.756834 | -1.917553 | 0.473939 |
| C | -1.347006 | 0.983885 | -0.807245 |
| C | -2.421481 | 0.133124 | -0.126956 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.569473 | 0.502675 | 0.892112 |
| H | -3.374760 | 0.238968 | -0.647486 |
| C | 1.833633 | -0.961686 | 0.343324 |
| H | 1.919290 | -2.014351 | 0.612268 |
| H | 0.734967 | 1.141399 | 1.957965 |
| H | -0.615223 | 2.244344 | 1.428609 |
| H | 0.693250 | 2.814018 | -0.653936 |
| H | 2.028053 | 1.721259 | -0.078862 |
| H | -0.658789 | -1.238174 | 1.612446 |
| H | -1.621319 | 2.040257 | -0.778471 |
| H | -1.262863 | 0.696690 | -1.860424 |
| H | -0.346014 | -2.582001 | 0.519464 |
| H | 2.052717 | -0.378087 | 1.243153 |
| O | 2.839467 | -0.742561 | -0.643330 |
| H | 2.688021 | 0.116766 | -1.047285 |

eq9

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.011074 | 0.782011 | -0.124474 |
| C | 0.409522 | -0.682862 | -0.198103 |
| H | 0.403303 | -0.971487 | -1.258395 |
| C | 0.269298 | 1.580110 | 1.118678 |
| C | 0.989862 | 1.896217 | -0.170359 |
| C | -0.648887 | -1.536695 | 0.512763 |
| C | -2.040616 | -1.316602 | -0.081551 |
| H | -2.041571 | -1.677571 | -1.114925 |
| H | -2.778096 | -1.909077 | 0.462567 |
| C | -1.369646 | 1.014269 | -0.757872 |
| C | -2.434877 | 0.160023 | -0.070029 |
| H | -2.543764 | 0.496226 | 0.965561 |
| H | -3.402959 | 0.296115 | -0.555123 |
| C | 1.802093 | -1.006732 | 0.331506 |
| H | 1.869374 | -2.085403 | 0.501754 |
| H | 0.842118 | 1.130209 | 1.916959 |
| H | -0.500832 | 2.264998 | 1.446678 |
| H | 0.707182 | 2.799676 | -0.693800 |
| H | 2.034823 | 1.632339 | -0.231508 |
| H | -0.656110 | -1.276598 | 1.576803 |
| H | -1.628277 | 2.073259 | -0.695949 |
| H | -1.323501 | 0.752907 | -1.820577 |
| H | -0.377208 | -2.591965 | 0.442405 |
| H | 1.985184 | -0.518530 | 1.289075 |
| O | 2.859039 | -0.589945 | -0.527646 |
| H | 2.743962 | -1.033968 | -1.373706 |



(cyclohexylmethyl)benzene

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -506.170807 | -505.877184 | -505.927701 |
| ax2 | -506.164437 | -505.870745 | -505.921025 |
| eq | -506.173096 | -505.879783 | -505.930537 |
| eq2 | -506.172033 | -505.878657 | -505.928887 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -2.436130 | -1.384546 | 0.058269 |
| C | -1.048434 | -0.846116 | 0.433990 |
| H | -0.575571 | -1.566081 | 1.107900 |
| C | -1.192306 | 0.484502 | 1.185201 |
| C | -2.018136 | 1.510177 | 0.406279 |
| H | -2.123124 | 2.422735 | 0.995732 |
| H | -1.495027 | 1.789544 | -0.512861 |
| C | -3.273057 | -0.366105 | -0.719612 |
| C | -3.395441 | 0.948103 | 0.052101 |
| H | -3.966120 | 1.676364 | -0.526927 |
| H | -3.953056 | 0.767125 | 0.976920 |
| H | -1.692358 | 0.287195 | 2.138262 |
| H | -2.814224 | -0.171753 | -1.692851 |
| H | -4.263208 | -0.779999 | -0.918524 |
| H | -0.207804 | 0.891319 | 1.424844 |
| H | -2.331297 | -2.307754 | -0.516265 |
| H | -2.968866 | -1.640449 | 0.979235 |
| C | -0.140394 | -0.737115 | -0.807420 |
| H | -0.127548 | -1.712140 | -1.300727 |
| H | -0.556711 | -0.024067 | -1.519482 |
| C | 1.271120 | -0.331180 | -0.470933 |
| C | 1.729003 | 0.962489 | -0.716832 |
| C | 2.144026 | -1.239115 | 0.131691 |
| C | 3.021428 | 1.342890 | -0.370195 |
| H | 1.064533 | 1.678759 | -1.185375 |
| C | 3.436010 | -0.865265 | 0.479375 |
| H | 1.806460 | -2.250721 | 0.324771 |
| C | 3.879321 | 0.429776 | 0.230535 |
| H | 3.357351 | 2.351873 | -0.570147 |
| H | 4.099083 | -1.584903 | 0.941299 |
| H | 4.885423 | 0.721990 | 0.499512 |

ax2

| | | | |
|---|----------|-----------|-----------|
| C | 1.853134 | -1.165524 | 0.784198 |
| C | 1.611886 | -0.988109 | -0.725893 |
| H | 2.251916 | -1.718489 | -1.227644 |
| C | 2.084486 | 0.394310 | -1.212908 |
| C | 1.699907 | 1.572042 | -0.313550 |
| H | 2.170384 | 2.480807 | -0.694303 |
| H | 0.621622 | 1.738693 | -0.337896 |
| C | 1.465584 | 0.039194 | 1.647204 |
| C | 2.122986 | 1.316242 | 1.130432 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.854020 | 2.164837 | 1.761837 |
| H | 3.212179 | 1.211280 | 1.178143 |
| H | 3.177527 | 0.369503 | -1.266479 |
| H | 0.382709 | 0.179105 | 1.647462 |
| H | 1.761384 | -0.151563 | 2.680803 |
| H | 1.728419 | 0.561260 | -2.232628 |
| H | 1.337876 | -2.064352 | 1.132504 |
| H | 2.922680 | -1.343816 | 0.932903 |
| C | 0.193071 | -1.388953 | -1.193834 |
| H | 0.165337 | -1.277570 | -2.280245 |
| H | 0.076570 | -2.453788 | -0.979951 |
| C | -0.990637 | -0.663807 | -0.605196 |
| C | -1.624429 | -1.148696 | 0.539538 |
| C | -1.493198 | 0.496194 | -1.195110 |
| C | -2.705547 | -0.478549 | 1.099289 |
| H | -1.260783 | -2.060002 | 0.999349 |
| C | -2.573961 | 1.171922 | -0.640864 |
| H | -1.027148 | 0.875980 | -2.096812 |
| C | -3.180894 | 0.689446 | 0.513479 |
| H | -3.179647 | -0.870197 | 1.989645 |
| H | -2.945661 | 2.071955 | -1.112774 |
| H | -4.023713 | 1.212079 | 0.945389 |

eq

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.196111 | 1.009687 | 0.129949 |
| C | 1.050361 | -0.511309 | 0.044128 |
| H | 0.862540 | -0.775400 | -1.003731 |
| C | 2.350394 | -1.192541 | 0.477646 |
| C | 3.551494 | -0.696304 | -0.326653 |
| H | 4.464301 | -1.181550 | 0.023503 |
| H | 3.421835 | -0.980326 | -1.375807 |
| C | 2.395895 | 1.511856 | -0.673714 |
| C | 3.686555 | 0.822873 | -0.233425 |
| H | 4.526474 | 1.167213 | -0.839416 |
| H | 3.904785 | 1.099608 | 0.803076 |
| H | 2.516649 | -0.982794 | 1.540491 |
| H | 2.225254 | 1.306896 | -1.735378 |
| H | 2.488821 | 2.594429 | -0.570483 |
| H | 2.248644 | -2.275841 | 0.379479 |
| H | 0.282517 | 1.495671 | -0.218209 |
| H | 1.323470 | 1.287648 | 1.183029 |
| C | -0.129810 | -1.025870 | 0.882300 |
| H | -0.133714 | -2.117896 | 0.840488 |
| H | 0.031155 | -0.742187 | 1.925458 |
| C | -1.466626 | -0.507007 | 0.418659 |
| C | -2.134950 | 0.502332 | 1.110018 |
| C | -2.049451 | -1.009642 | -0.746212 |
| C | -3.351055 | 0.999310 | 0.652008 |
| H | -1.697153 | 0.903056 | 2.016406 |
| C | -3.263343 | -0.517427 | -1.208370 |
| H | -1.545813 | -1.798413 | -1.292796 |
| C | -3.918943 | 0.491577 | -0.509893 |
| H | -3.854050 | 1.782624 | 1.203611 |

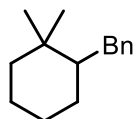
H -3.700354 -0.923039 -2.111331
H -4.865156 0.875080 -0.867046

eq2

```

=====
C -1.452702 1.254500 0.168306
C -1.207018 0.000116 1.009701
H -1.945882 0.000224 1.819353
C -1.452750 -1.254444 0.168585
C -2.861901 -1.259677 -0.425616
H -3.007915 -2.151199 -1.038124
H -3.593998 -1.307207 0.386776
C -2.861842 1.259657 -0.425917
C -3.114402 -0.000100 -1.253642
H -4.134171 -0.000133 -1.642700
H -2.442223 -0.000212 -2.117719
H -0.723339 -1.289796 -0.646940
H -3.593961 1.307437 0.386433
H -3.007760 2.151046 -1.038646
H -1.293644 -2.147810 0.777921
H -1.293579 2.147997 0.777452
H -0.723283 1.289660 -0.647219
C 0.173046 0.000157 1.696519
H 0.233444 0.879919 2.340787
H 0.233410 -0.879484 2.340970
C 1.351735 0.000042 0.755643
C 1.907456 -1.197363 0.302300
C 1.907653 1.197392 0.302265
C 2.977602 -1.200838 -0.584929
H 1.498396 -2.137119 0.653374
C 2.977759 1.200687 -0.584931
H 1.498656 2.137186 0.653318
C 3.515046 -0.000140 -1.034652
H 3.393850 -2.141003 -0.922049
H 3.394183 2.140756 -0.922100
H 4.349718 -0.000181 -1.722681

```



((2,2-dimethylcyclohexyl)methyl)benzene

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -584.783671 | -584.431218 | -584.486693 |
| ax2 | -584.781414 | -584.429069 | -584.484469 |
| ax3 | -584.777118 | -584.424438 | -584.478472 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| eq | | -584.785787 | | -584.433625 | | -584.489819 |
| eq2 | | -584.781347 | | -584.428874 | | -584.483939 |
| eq3 | | -584.783286 | | -584.431043 | | -584.486228 |

ax

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -2.239235 | -0.703555 | -0.044878 |
| C | -0.757531 | -0.454108 | 0.356916 |
| H | -0.470796 | -1.263455 | 1.037500 |
| C | -0.608608 | 0.876206 | 1.113832 |
| C | -1.161586 | 2.063008 | 0.323794 |
| H | -1.052358 | 2.978915 | 0.907222 |
| H | -0.580371 | 2.202697 | -0.592461 |
| C | -2.802374 | 0.518174 | -0.795486 |
| C | -2.628118 | 1.836138 | -0.040746 |
| H | -2.999524 | 2.660955 | -0.651666 |
| H | -3.229430 | 1.826348 | 0.872170 |
| H | -1.136502 | 0.811863 | 2.067243 |
| H | -2.299620 | 0.600388 | -1.763849 |
| H | -3.859876 | 0.339253 | -1.008670 |
| H | 0.441780 | 1.042859 | 1.357903 |
| C | 0.208009 | -0.531892 | -0.847974 |
| H | -0.075656 | 0.194971 | -1.610385 |
| H | 0.122509 | -1.519816 | -1.300108 |
| C | -3.069390 | -0.973734 | 1.218110 |
| H | -4.115531 | -1.137517 | 0.950783 |
| H | -2.708206 | -1.872731 | 1.722683 |
| H | -3.035951 | -0.154319 | 1.933647 |
| C | -2.374463 | -1.936122 | -0.943680 |
| H | -1.886429 | -2.805099 | -0.494894 |
| H | -3.429885 | -2.179356 | -1.083042 |
| H | -1.941542 | -1.774011 | -1.930874 |
| C | 1.649658 | -0.312167 | -0.465413 |
| C | 2.342954 | -1.287680 | 0.253978 |
| C | 2.317184 | 0.867322 | -0.791549 |
| C | 3.662148 | -1.088729 | 0.640582 |
| H | 1.841693 | -2.214011 | 0.509579 |
| C | 3.638618 | 1.072101 | -0.407415 |
| H | 1.795247 | 1.633931 | -1.351657 |
| C | 4.315357 | 0.095149 | 0.312282 |
| H | 4.182943 | -1.858624 | 1.194653 |
| H | 4.138739 | 1.994731 | -0.671218 |
| H | 5.343028 | 0.251362 | 0.611328 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.459620 | -0.930042 | 0.327529 |
| C | -0.845647 | 0.485685 | 0.517399 |
| H | -0.307247 | 0.472190 | 1.469116 |
| C | -1.949316 | 1.552356 | 0.620641 |
| C | -2.876889 | 1.536821 | -0.593803 |
| H | -3.643911 | 2.306042 | -0.488914 |
| H | -2.306952 | 1.778968 | -1.496325 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.453309 | -0.929485 | -0.849933 |
| C | -3.520654 | 0.160935 | -0.757186 |
| H | -4.147196 | 0.137591 | -1.650693 |
| H | -4.179918 | -0.031154 | 0.093548 |
| H | -2.544556 | 1.385313 | 1.520747 |
| H | -1.897069 | -0.793831 | -1.782466 |
| H | -2.921577 | -1.915768 | -0.910391 |
| H | -1.484245 | 2.534030 | 0.731752 |
| C | 0.169035 | 0.880523 | -0.583764 |
| H | 0.139564 | 1.968544 | -0.690837 |
| H | -0.132446 | 0.474466 | -1.550025 |
| C | -2.175323 | -1.352883 | 1.617950 |
| H | -2.604482 | -2.350046 | 1.498757 |
| H | -1.466906 | -1.390515 | 2.448584 |
| H | -2.981771 | -0.677522 | 1.898344 |
| C | -0.374587 | -1.971847 | 0.047046 |
| H | 0.392685 | -1.964658 | 0.825045 |
| H | -0.817369 | -2.970137 | 0.019237 |
| H | 0.113883 | -1.799261 | -0.911929 |
| C | 1.607468 | 0.493958 | -0.320256 |
| C | 2.345549 | -0.223548 | -1.260747 |
| C | 2.247936 | 0.885644 | 0.857230 |
| C | 3.676989 | -0.553097 | -1.031708 |
| H | 1.867702 | -0.533851 | -2.182303 |
| C | 3.577757 | 0.559385 | 1.092577 |
| H | 1.701954 | 1.457697 | 1.597645 |
| C | 4.298273 | -0.165477 | 0.149137 |
| H | 4.227263 | -1.114258 | -1.775534 |
| H | 4.053490 | 0.874223 | 2.012117 |
| H | 5.333127 | -0.421636 | 0.331857 |

ax3

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```

| | | | |
|---|-----------|-----------|-----------|
| C | -2.052068 | -0.530844 | -0.059607 |
| C | -1.200738 | 0.033150 | 1.116797 |
| H | -1.836293 | -0.085348 | 2.000252 |
| C | -0.943581 | 1.545240 | 0.958329 |
| C | -0.455170 | 1.969940 | -0.430989 |
| H | -0.388131 | 3.059208 | -0.468982 |
| H | 0.549438 | 1.584861 | -0.615897 |
| C | -1.523785 | -0.061823 | -1.426712 |
| C | -1.382377 | 1.454942 | -1.528825 |
| H | -0.987782 | 1.724728 | -2.510141 |
| H | -2.362279 | 1.931629 | -1.441828 |
| H | -1.870885 | 2.083436 | 1.167691 |
| H | -0.546590 | -0.515864 | -1.607979 |
| H | -2.195345 | -0.436505 | -2.204437 |
| H | -0.228209 | 1.866738 | 1.719166 |
| C | 0.086631 | -0.744324 | 1.510942 |
| H | -0.134631 | -1.811170 | 1.533741 |
| H | 0.300958 | -0.452804 | 2.541200 |
| C | -3.497405 | -0.037872 | 0.124105 |
| H | -4.108995 | -0.331146 | -0.732011 |
| H | -3.936401 | -0.483727 | 1.019154 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.564681 | 1.044205 | 0.226040 |
| C | -2.100324 | -2.060010 | -0.044480 |
| H | -2.390007 | -2.435691 | 0.939974 |
| H | -2.839158 | -2.412611 | -0.767499 |
| H | -1.141723 | -2.506149 | -0.308318 |
| C | 1.351672 | -0.517660 | 0.717657 |
| C | 2.257749 | 0.469525 | 1.110786 |
| C | 1.667016 | -1.284813 | -0.404199 |
| C | 3.416134 | 0.715198 | 0.383786 |
| H | 2.047603 | 1.056365 | 1.996779 |
| C | 2.824513 | -1.045724 | -1.136094 |
| H | 0.999701 | -2.079389 | -0.712249 |
| C | 3.699820 | -0.036777 | -0.750738 |
| H | 4.099164 | 1.490406 | 0.705477 |
| H | 3.045290 | -1.651493 | -2.005172 |
| H | 4.600433 | 0.151433 | -1.319511 |

eq

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| | | | |
|---|-----------|-----------|-----------|
| C | -2.118795 | -0.761277 | 0.054264 |
| C | -0.713642 | -0.117161 | -0.088599 |
| H | -0.436384 | -0.228048 | -1.144433 |
| C | -0.724740 | 1.383715 | 0.226109 |
| C | -1.749047 | 2.148974 | -0.607364 |
| H | -1.745804 | 3.204955 | -0.331350 |
| H | -1.465373 | 2.093500 | -1.663255 |
| C | -3.124331 | 0.062846 | -0.774006 |
| C | -3.141879 | 1.550659 | -0.434523 |
| H | -3.860579 | 2.065981 | -1.074393 |
| H | -3.476448 | 1.696909 | 0.596168 |
| H | -0.939873 | 1.527916 | 1.289925 |
| H | -2.865972 | -0.048530 | -1.832965 |
| H | -4.119829 | -0.370108 | -0.644890 |
| H | 0.273101 | 1.792355 | 0.054366 |
| C | 0.365738 | -0.828326 | 0.750235 |
| H | 0.266567 | -1.908596 | 0.637309 |
| H | 0.209977 | -0.597204 | 1.805853 |
| C | -2.569749 | -0.827837 | 1.518015 |
| H | -3.592042 | -1.208560 | 1.573938 |
| H | -1.935059 | -1.503286 | 2.093514 |
| H | -2.550945 | 0.146030 | 2.006874 |
| C | -2.115972 | -2.183203 | -0.516064 |
| H | -1.516405 | -2.868273 | 0.083481 |
| H | -3.134525 | -2.577191 | -0.540733 |
| H | -1.727784 | -2.192829 | -1.537247 |
| C | 1.767085 | -0.432644 | 0.357748 |
| C | 2.536280 | 0.414320 | 1.153877 |
| C | 2.317736 | -0.897452 | -0.838338 |
| C | 3.819133 | 0.790439 | 0.767985 |
| H | 2.125059 | 0.783251 | 2.085835 |
| C | 3.597801 | -0.526094 | -1.228641 |
| H | 1.734539 | -1.560855 | -1.466752 |
| C | 4.354125 | 0.321879 | -0.425352 |
| H | 4.399860 | 1.448666 | 1.400742 |

| | | | |
|---|----------|-----------|-----------|
| H | 4.007665 | -0.900553 | -2.157430 |
| H | 5.351798 | 0.611436 | -0.726630 |

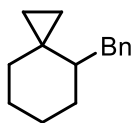
eq2

```
=====
C -1.446998    0.937888   -0.141440
C -1.049072   -0.104187    0.939629
H -1.757883    0.064432    1.760330
C -1.299324   -1.538998    0.460308
C -2.767130   -1.749592    0.087704
H -2.921713   -2.765028   -0.281627
H -3.379671   -1.639907    0.988305
C -2.932872    0.694918   -0.479378
C -3.225048   -0.728271   -0.951546
H -4.293278   -0.841321   -1.145868
H -2.712530   -0.916931   -1.898485
H -0.671043   -1.770609   -0.402472
H -3.528985    0.899266    0.416608
H -3.242956    1.417051   -1.239204
H -1.012841   -2.236103    1.251745
C  0.333372    0.075238    1.608127
H  0.386016   -0.669173    2.407137
H  0.363297    1.051159    2.093509
C -0.619107    0.845808   -1.432652
H -1.083743    1.466688   -2.202872
H  0.395897    1.209540   -1.285705
H -0.554793   -0.168761   -1.823984
C -1.314308    2.356958    0.414841
H -0.271580    2.625571    0.589273
H -1.728525    3.079062   -0.292607
H -1.855651    2.460656    1.358454
C  1.567573   -0.067464    0.749931
C  2.344740    1.047770    0.433867
C  1.982473   -1.312454    0.272310
C  3.478873    0.933967   -0.361361
H  2.049788    2.020156    0.809839
C  3.113362   -1.432523   -0.527091
H  1.421782   -2.199507    0.537184
C  3.863018   -0.307884   -0.853538
H  4.062598    1.814518   -0.595528
H  3.414390   -2.407175   -0.888231
H  4.744111   -0.400629   -1.474069
```

eq3

```
=====
C -1.233688   -0.834554   -0.139665
C -0.938016    0.685254    0.016307
H -0.743657    1.067899   -0.992863
C -2.148388    1.455145    0.571922
C -3.430968    1.229651   -0.220376
H -4.256145    1.777154    0.238676
H -3.305975    1.627094   -1.232731
C -2.561609   -1.004434   -0.908370
C -3.746681   -0.258792   -0.305605
```


| | | | |
|---|-----------|-----------|-----------|
| H | -4.637822 | -0.429000 | -0.912525 |
| H | -3.965701 | -0.644487 | 0.694078 |
| H | -2.313379 | 1.159810 | 1.613084 |
| H | -2.410464 | -0.642622 | -1.931678 |
| H | -2.779672 | -2.072971 | -0.981955 |
| H | -1.902573 | 2.519132 | 0.589298 |
| C | 0.270959 | 1.044838 | 0.903690 |
| H | 0.104994 | 0.657230 | 1.910661 |
| H | 0.278949 | 2.134766 | 0.994381 |
| C | -1.320348 | -1.535628 | 1.220840 |
| H | -1.650678 | -2.568078 | 1.086150 |
| H | -0.344142 | -1.563827 | 1.707885 |
| H | -2.019753 | -1.048544 | 1.900786 |
| C | -0.161771 | -1.543761 | -0.978358 |
| H | 0.791352 | -1.625385 | -0.459508 |
| H | -0.497754 | -2.556785 | -1.213860 |
| H | 0.007482 | -1.019837 | -1.921797 |
| C | 1.633798 | 0.612509 | 0.424130 |
| C | 2.123176 | 1.043250 | -0.810462 |
| C | 2.440235 | -0.216046 | 1.201850 |
| C | 3.370477 | 0.636926 | -1.264905 |
| H | 1.515906 | 1.697249 | -1.424981 |
| C | 3.692092 | -0.624982 | 0.753007 |
| H | 2.078592 | -0.554183 | 2.165552 |
| C | 4.159094 | -0.205243 | -0.486047 |
| H | 3.730130 | 0.977745 | -2.226942 |
| H | 4.300027 | -1.272967 | 1.370657 |
| H | 5.130117 | -0.524191 | -0.840109 |



4-benzylspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -583.555416 | -583.226313 | -583.280622 |
| ax2 | -583.555172 | -583.226152 | -583.279779 |
| ax3 | -583.549319 | -583.220017 | -583.27393 |
| eq1 | -583.553941 | -583.224843 | -583.279275 |
| eq2 | -583.549833 | -583.220409 | -583.273616 |
| eq3 | -583.551602 | -583.222463 | -583.277043 |

ax1

```

=====
C   2.185060   -0.663982   -0.106547
C   0.754624   -0.374703    0.323674
H   0.422684   -1.200442    0.960370
C   3.030546   -1.483294    0.826211
C   2.540474   -2.069644   -0.477726
C   0.723171    0.919506    1.149161
C   1.383135    2.092635    0.420083
H   0.808096    2.346939   -0.474897
H   1.370653    2.975882    1.060851
C   2.865752    0.481209   -0.829758
C   2.819504    1.754452    0.017009
H   3.417488    1.601657    0.920921
H   3.267882    2.586935   -0.527779
C  -0.193951   -0.333020   -0.891473
H   0.069625    0.496746   -1.547866
H  -0.049160   -1.253444   -1.461852
C  -1.643309   -0.214099   -0.497260
C  -2.317597   -1.308323    0.047964
C  -2.334958    0.988836   -0.632323
C  -3.643849   -1.204092    0.447381
H  -1.796046   -2.252402    0.155255
C  -3.663355    1.099287   -0.233958
H  -1.826801    1.847309   -1.055304
C  -4.322066    0.002878    0.308610
H  -4.150020   -2.064926    0.864072
H  -4.182712    2.041629   -0.348431
H  -5.355295    0.085613    0.617718
H   2.575373   -1.844321    1.738390
H   4.081137   -1.238136    0.902368
H   3.266244   -2.219567   -1.265305
H   1.758786   -2.815901   -0.425186
H   1.262456    0.741570    2.084200
H   3.897894    0.206178   -1.055803
H   2.367505    0.663613   -1.786981
H  -0.304864    1.169193    1.418966

```

ax2

```

=====
C  -1.167831    0.815898    0.315863
C  -0.943389   -0.639445    0.700429
H  -0.498852   -0.658834    1.700230
C  -1.491358    1.774210    1.429614
C  -0.162388    1.850872    0.718829
C  -2.303160   -1.353647    0.754195
C  -3.098454   -1.195226   -0.544988
H  -2.583303   -1.707633   -1.361813
H  -4.071295   -1.678267   -0.438873
C  -1.934539    1.002822   -0.978419
C  -3.281413    0.279381   -0.908874
H  -3.901078    0.760955   -0.145963
H  -3.811419    0.372445   -1.858299
C   0.026935   -1.380133   -0.244038
H   0.072419   -2.422871    0.079200

```

| | | | |
|---|-----------|-----------|-----------|
| H | -0.364554 | -1.377687 | -1.261529 |
| C | 1.416267 | -0.798577 | -0.247474 |
| C | 1.852314 | 0.022666 | -1.285726 |
| C | 2.282746 | -1.033263 | 0.821022 |
| C | 3.113463 | 0.607885 | -1.253387 |
| H | 1.192014 | 0.212722 | -2.123551 |
| C | 3.544234 | -0.452263 | 0.859051 |
| H | 1.961517 | -1.675569 | 1.632830 |
| C | 3.962843 | 0.375412 | -0.177918 |
| H | 3.432360 | 1.245362 | -2.067592 |
| H | 4.202005 | -0.646222 | 1.696098 |
| H | 4.944289 | 0.829282 | -0.150444 |
| H | -1.495348 | 1.390783 | 2.441001 |
| H | -2.216641 | 2.551252 | 1.230230 |
| H | 0.002417 | 2.680812 | 0.044861 |
| H | 0.714191 | 1.521749 | 1.259634 |
| H | -2.885888 | -0.925470 | 1.575034 |
| H | -2.081620 | 2.068743 | -1.163717 |
| H | -1.352196 | 0.610646 | -1.818145 |
| H | -2.156647 | -2.411744 | 0.981726 |

ax3

```

=====
C -1.767502 -0.586616 0.113663
C -1.284453 0.156548 -1.128903
H -2.001222 -0.071528 -1.922682
C -3.208740 -1.025236 0.117715
C -2.101217 -2.040866 -0.025173
C -1.352290 1.679222 -0.905544
C -0.820030 2.161225 0.447091
H 0.259916 2.016291 0.507161
H -1.002296 3.233602 0.540030
C -1.234903 -0.092268 1.446930
C -1.480516 1.407344 1.598994
H -2.557897 1.601842 1.594348
H -1.092249 1.759319 2.556172
C 0.056882 -0.353382 -1.708639
H -0.101030 -1.388198 -2.018511
H 0.251790 0.222767 -2.615966
C 1.286774 -0.310846 -0.837678
C 2.128854 0.801358 -0.829529
C 1.624982 -1.399922 -0.033442
C 3.257036 0.840214 -0.018493
H 1.893071 1.648320 -1.463221
C 2.751717 -1.368664 0.779277
H 0.990807 -2.278864 -0.040712
C 3.570032 -0.244294 0.793547
H 3.894821 1.714361 -0.024837
H 2.993652 -2.222888 1.397882
H 4.449262 -0.217906 1.423091
H -3.807732 -0.813403 -0.757109
H -3.740792 -0.991251 1.058590
H -1.899975 -2.688884 0.817082
H -1.968404 -2.498132 -0.996377

```

| | | | |
|---|-----------|-----------|-----------|
| H | -2.404165 | 1.974764 | -0.969225 |
| H | -1.720273 | -0.649003 | 2.251423 |
| H | -0.162253 | -0.283499 | 1.525402 |
| H | -0.834792 | 2.189387 | -1.721444 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -2.152790 | -0.661689 | -0.146873 |
| C | -0.731001 | -0.102491 | -0.181076 |
| H | -0.463225 | 0.012497 | -1.239004 |
| C | -2.435405 | -2.128565 | -0.277663 |
| C | -2.638803 | -1.432660 | 1.048394 |
| C | -0.718298 | 1.292124 | 0.459154 |
| C | -1.726724 | 2.240096 | -0.187039 |
| H | -1.699928 | 3.210355 | 0.311906 |
| H | -1.440706 | 2.409592 | -1.229972 |
| C | -3.159488 | 0.273583 | -0.793458 |
| C | -3.136432 | 1.655573 | -0.144449 |
| H | -3.842039 | 2.320191 | -0.645864 |
| H | -3.460168 | 1.568287 | 0.897389 |
| C | 0.328625 | -1.008075 | 0.467772 |
| H | 0.160013 | -1.049797 | 1.545244 |
| H | 0.232674 | -2.023021 | 0.080667 |
| C | 1.736626 | -0.531588 | 0.209289 |
| C | 2.307288 | -0.675541 | -1.056735 |
| C | 2.491907 | 0.077242 | 1.209925 |
| C | 3.594464 | -0.222596 | -1.316009 |
| H | 1.736236 | -1.152620 | -1.844654 |
| C | 3.781710 | 0.532908 | 0.956178 |
| H | 2.064023 | 0.195887 | 2.198117 |
| C | 4.336978 | 0.385493 | -0.308676 |
| H | 4.020282 | -0.347000 | -2.302947 |
| H | 4.351319 | 1.002787 | 1.747090 |
| H | 5.340071 | 0.737556 | -0.508217 |
| H | -1.615301 | -2.826586 | -0.354859 |
| H | -3.318213 | -2.406705 | -0.836960 |
| H | -3.654372 | -1.258397 | 1.376989 |
| H | -1.939438 | -1.663643 | 1.838979 |
| H | -0.951483 | 1.183674 | 1.524695 |
| H | -2.919792 | 0.372719 | -1.857854 |
| H | -4.156774 | -0.165931 | -0.727944 |
| H | 0.284874 | 1.717271 | 0.394794 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.540038 | 0.921296 | 0.060566 |
| C | -1.082252 | -0.216705 | 0.970643 |
| H | -1.769984 | -0.199995 | 1.825312 |
| C | -0.971188 | 2.303921 | 0.154900 |
| C | -0.673912 | 1.443238 | -1.052056 |
| C | -1.327092 | -1.547825 | 0.248484 |
| C | -2.802805 | -1.709883 | -0.121646 |
| H | -2.955245 | -2.651957 | -0.651221 |
| H | -3.395170 | -1.760845 | 0.797396 |

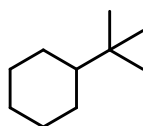
| | | | |
|---|-----------|-----------|-----------|
| C | -3.014972 | 0.794566 | -0.279597 |
| C | -3.297448 | -0.539518 | -0.970976 |
| H | -4.364736 | -0.642602 | -1.174426 |
| H | -2.782990 | -0.553741 | -1.936665 |
| C | 0.314676 | -0.111607 | 1.620208 |
| H | 0.356372 | 0.805149 | 2.209598 |
| H | 0.375485 | -0.938723 | 2.332173 |
| C | 1.537380 | -0.168993 | 0.733425 |
| C | 1.925984 | -1.356109 | 0.107996 |
| C | 2.334108 | 0.961076 | 0.545381 |
| C | 3.047769 | -1.400597 | -0.711322 |
| H | 1.350807 | -2.258106 | 0.271001 |
| C | 3.459549 | 0.922053 | -0.269613 |
| H | 2.065396 | 1.886469 | 1.040058 |
| C | 3.815462 | -0.258512 | -0.910576 |
| H | 3.326717 | -2.330680 | -1.188866 |
| H | 4.058229 | 1.813583 | -0.402334 |
| H | 4.688948 | -0.292199 | -1.547664 |
| H | -0.160678 | 2.484580 | 0.845771 |
| H | -1.651250 | 3.134983 | 0.025496 |
| H | -1.172570 | 1.696325 | -1.978175 |
| H | 0.330009 | 1.064240 | -1.165774 |
| H | -0.721446 | -1.583656 | -0.661709 |
| H | -3.605404 | 0.859556 | 0.640570 |
| H | -3.316841 | 1.627504 | -0.917786 |
| H | -1.006972 | -2.378302 | 0.882340 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.347008 | 0.766811 | -0.239629 |
| C | 0.939967 | -0.648774 | 0.170440 |
| H | 0.731992 | -1.199846 | -0.753813 |
| C | 0.359686 | 1.873582 | -0.466960 |
| C | 1.262923 | 1.900642 | 0.743851 |
| C | 2.141426 | -1.330993 | 0.843326 |
| C | 3.385612 | -1.330457 | -0.042433 |
| H | 4.218215 | -1.803059 | 0.481567 |
| H | 3.186936 | -1.932947 | -0.934515 |
| C | 2.570291 | 0.771803 | -1.140767 |
| C | 3.758895 | 0.086532 | -0.470515 |
| H | 4.616076 | 0.068616 | -1.145762 |
| H | 4.054589 | 0.664217 | 0.410666 |
| C | -0.287755 | -0.777366 | 1.085466 |
| H | -0.301514 | -1.809951 | 1.445697 |
| H | -0.158696 | -0.153429 | 1.971481 |
| C | -1.637524 | -0.490577 | 0.468971 |
| C | -2.533533 | 0.377909 | 1.091680 |
| C | -2.034284 | -1.107179 | -0.718614 |
| C | -3.784162 | 0.636217 | 0.541439 |
| H | -2.241117 | 0.867165 | 2.013213 |
| C | -3.282007 | -0.851245 | -1.274147 |
| H | -1.363021 | -1.796298 | -1.215622 |
| C | -4.162164 | 0.024645 | -0.647650 |
| H | -4.460658 | 1.317997 | 1.039850 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.568544 | -1.338462 | -2.196900 |
| H | -5.132588 | 0.225638 | -1.080971 |
| H | -0.690174 | 1.692932 | -0.301244 |
| H | 0.580150 | 2.564518 | -1.269494 |
| H | 2.076495 | 2.613255 | 0.753571 |
| H | 0.804430 | 1.724494 | 1.706477 |
| H | 2.359304 | -0.807040 | 1.780742 |
| H | 2.329446 | 0.247896 | -2.072262 |
| H | 2.820615 | 1.800925 | -1.405921 |
| H | 1.871796 | -2.355918 | 1.106501 |



tert-butylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -393.053126 | -392.756973 | -392.803118 |
| eq | -393.060569 | -392.764864 | -392.812421 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.697218 | -1.259608 | -0.776082 |
| C | -0.172502 | 0.012962 | -0.849206 |
| H | -0.613118 | 0.027009 | -1.851327 |
| C | 0.742996 | 1.251124 | -0.797460 |
| C | 1.749412 | 1.255032 | 0.352433 |
| H | 2.367767 | 2.152989 | 0.292464 |
| H | 1.232317 | 1.292787 | 1.314353 |
| C | 1.769280 | -1.257860 | 0.322452 |
| C | 2.625914 | 0.006148 | 0.286777 |
| H | 3.346656 | -0.004510 | 1.106467 |
| H | 3.200756 | 0.029406 | -0.645031 |
| H | 1.316966 | 1.260130 | -1.730367 |
| H | 1.309933 | -1.340509 | 1.307420 |
| H | 2.400757 | -2.140301 | 0.198711 |
| H | 0.154013 | 2.167187 | -0.797729 |
| C | -1.417123 | 0.008556 | 0.096942 |
| C | -1.144366 | -0.491166 | 1.520804 |
| H | -0.384357 | 0.099079 | 2.031334 |
| H | -2.064715 | -0.424238 | 2.105788 |
| H | -0.829536 | -1.535300 | 1.524971 |
| C | -2.029087 | 1.410052 | 0.188540 |
| H | -1.394313 | 2.092120 | 0.756379 |
| H | -2.188499 | 1.839180 | -0.803380 |
| H | -2.996431 | 1.359660 | 0.692580 |
| C | -2.472522 | -0.919994 | -0.522026 |

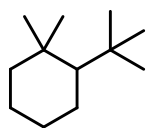
| | | | |
|---|-----------|-----------|-----------|
| H | -3.347482 | -0.989208 | 0.127586 |
| H | -2.801524 | -0.541835 | -1.492179 |
| H | -2.085522 | -1.929900 | -0.666385 |
| H | 0.068342 | -2.146035 | -0.674229 |
| H | 1.212670 | -1.359189 | -1.736471 |

eq

```

=====
C  0.665695    1.256612    0.171331
C -0.071298    0.006200   -0.330278
H  0.009852    0.009309   -1.425793
C  0.663824   -1.242862    0.177159
C  2.130621   -1.256098   -0.255511
H  2.622490   -2.154790    0.121496
H  2.183993   -1.297826   -1.348136
C  2.139039    1.252631   -0.243092
C  2.857408   -0.006442    0.234689
H  3.893843   -0.006814   -0.107884
H  2.881428   -0.013333    1.329239
H  0.625392   -1.260249    1.270866
H  2.200119    1.304436   -1.334994
H  2.635802    2.144258    0.144211
H  0.171685   -2.150554   -0.173235
C -1.594405   -0.001124   -0.018308
C -1.877537   -0.194763    1.475316
H -1.370070    0.556397    2.083061
H -2.949550   -0.103691    1.663615
H -1.565260   -1.181076    1.820462
C -2.232189    1.318528   -0.470147
H -1.932051    2.154203    0.162120
H -1.957243    1.555608   -1.501025
H -3.320192    1.242858   -0.421214
C -2.274094   -1.133812   -0.797835
H -3.352153   -1.114225   -0.625542
H -2.103971   -1.023412   -1.871444
H -1.912109   -2.116230   -0.495438
H  0.192856    2.159641   -0.213902
H  0.602759    1.302282    1.263592

```



2-(*tert*-butyl)-1,1-dimethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -471.658496 | -471.303011 | -471.353765 |
| eq | -471.663250 | -471.308237 | -471.359237 |

eq2 | -471.661531 | -471.306305 | -471.357508

ax

```
=====
C -0.926850 0.919674 -0.093120
C 0.217906 0.041104 -0.709625
H 0.469243 0.519512 -1.663127
C -0.378392 -1.336204 -1.084760
C -1.047471 -2.066824 0.078604
H -1.458896 -3.015085 -0.273933
H -0.310305 -2.313822 0.845351
C -1.648087 0.183074 1.055876
C -2.157965 -1.209673 0.683340
H -2.577265 -1.694414 1.567161
H -2.972660 -1.123273 -0.040437
H -1.129691 -1.183662 -1.861147
H -0.975274 0.097590 1.910067
H -2.485894 0.805501 1.383653
H 0.379186 -1.968299 -1.540597
C 1.610168 -0.042749 0.030805
C -1.951033 1.236668 -1.201034
H -2.744225 1.869269 -0.796822
H -1.470850 1.783669 -2.015390
H -2.423437 0.354066 -1.625263
C -0.467407 2.287378 0.425038
H 0.022651 2.863942 -0.361555
H -1.343289 2.853449 0.750907
H 0.208861 2.219948 1.273839
C 1.567388 -0.224101 1.556031
H 1.027722 -1.121625 1.852865
H 2.592041 -0.322972 1.923268
H 1.121811 0.624759 2.069764
C 2.426273 -1.220424 -0.528957
H 2.013312 -2.184734 -0.231133
H 2.477244 -1.190775 -1.619589
H 3.446400 -1.166172 -0.144801
C 2.442873 1.216809 -0.271122
H 3.446577 1.099160 0.143184
H 2.543558 1.364610 -1.348609
H 2.018762 2.120968 0.155892
```

eq

```
=====
C 0.752290 0.953349 -0.018728
C -0.169877 -0.264175 -0.371035
H -0.110026 -0.336865 -1.464951
C 0.429848 -1.570077 0.192405
C 1.845429 -1.852828 -0.295275
H 2.203386 -2.795564 0.123152
H 1.845818 -1.962732 -1.384572
C 2.198519 0.602059 -0.453653
C 2.759154 -0.701429 0.096996
H 3.771132 -0.856512 -0.282208
```

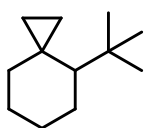

| | | | |
|---|-----------|-----------|-----------|
| H | 2.832498 | -0.651123 | 1.187232 |
| H | 0.450434 | -1.518161 | 1.283765 |
| H | 2.215119 | 0.548176 | -1.548158 |
| H | 2.843022 | 1.438725 | -0.172962 |
| H | -0.216899 | -2.409913 | -0.059772 |
| C | -1.707642 | -0.217089 | -0.045227 |
| C | 0.741079 | 1.309374 | 1.472242 |
| H | 1.486835 | 2.083772 | 1.669258 |
| H | -0.228457 | 1.703088 | 1.777479 |
| H | 0.973556 | 0.456495 | 2.109998 |
| C | 0.417463 | 2.223737 | -0.820710 |
| H | -0.432655 | 2.772281 | -0.427732 |
| H | 1.275903 | 2.899007 | -0.790854 |
| H | 0.220736 | 1.987512 | -1.868703 |
| C | -2.029248 | -0.662334 | 1.390654 |
| H | -1.488207 | -0.077487 | 2.134231 |
| H | -3.097296 | -0.530906 | 1.577126 |
| H | -1.797277 | -1.714730 | 1.552696 |
| C | -2.361548 | 1.152919 | -0.258970 |
| H | -2.045438 | 1.881372 | 0.486188 |
| H | -2.151782 | 1.553099 | -1.251020 |
| H | -3.444405 | 1.042323 | -0.167745 |
| C | -2.420714 | -1.181859 | -1.008584 |
| H | -3.484485 | -1.232801 | -0.767215 |
| H | -2.327564 | -0.834083 | -2.039646 |
| H | -2.022469 | -2.194843 | -0.956272 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.738483 | 0.926526 | -0.016032 |
| C | -0.176222 | -0.313896 | -0.321216 |
| H | -0.106954 | -0.443554 | -1.409819 |
| C | 0.465420 | -1.579881 | 0.284345 |
| C | 1.883301 | -1.827407 | -0.234720 |
| H | 2.306951 | -2.708011 | 0.252322 |
| H | 1.821115 | -2.056563 | -1.303709 |
| C | 2.125774 | 0.622745 | -0.630047 |
| C | 2.790415 | -0.618738 | -0.048298 |
| H | 3.754272 | -0.788921 | -0.532033 |
| H | 2.994632 | -0.466812 | 1.014626 |
| H | 0.470213 | -1.520252 | 1.376222 |
| H | 2.008055 | 0.492316 | -1.711229 |
| H | 2.764811 | 1.496937 | -0.482801 |
| H | -0.127372 | -2.453989 | 0.029137 |
| C | -1.720460 | -0.218618 | -0.042545 |
| C | 0.943463 | 1.226123 | 1.481508 |
| H | 1.814791 | 1.876258 | 1.595680 |
| H | 0.094259 | 1.749352 | 1.913246 |
| H | 1.125408 | 0.334797 | 2.078893 |
| C | 0.251161 | 2.218529 | -0.678738 |
| H | -0.646703 | 2.611902 | -0.204556 |
| H | 1.027251 | 2.982577 | -0.587116 |
| H | 0.049147 | 2.072885 | -1.741864 |
| C | -2.432625 | 0.594054 | -1.137284 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.233097 | 0.168967 | -2.123730 |
| H | -3.511934 | 0.557985 | -0.973221 |
| H | -2.142617 | 1.639676 | -1.155082 |
| C | -2.358214 | -1.618657 | -0.097487 |
| H | -2.081949 | -2.150016 | -1.011051 |
| H | -2.077567 | -2.235352 | 0.756040 |
| H | -3.444594 | -1.516516 | -0.085551 |
| C | -2.067962 | 0.382791 | 1.323122 |
| H | -3.132699 | 0.240206 | 1.522423 |
| H | -1.510920 | -0.098324 | 2.129271 |
| H | -1.869694 | 1.453018 | 1.358257 |



4-(*tert*-butyl)spiro[2.5]octane
(Chair Conformations)

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -470.436059 | -470.104485 | -470.154307 |
| ax2 | -470.435040 | -470.103285 | -470.153494 |
| eq | -470.433291 | -470.101512 | -470.150987 |
| eq2 | -470.430844 | -470.098836 | -470.148435 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.926103 | 0.797311 | -0.013210 |
| C | 0.250007 | 0.104525 | 0.672490 |
| H | 0.467639 | 0.714806 | 1.555257 |
| C | -1.874122 | 1.541662 | 0.894506 |
| C | -0.991380 | 2.293381 | -0.066695 |
| C | -0.248990 | -1.263593 | 1.188744 |
| C | -1.031981 | -2.101010 | 0.165216 |
| H | -1.459119 | -2.966151 | 0.676937 |
| H | -0.363529 | -2.495056 | -0.598853 |
| C | -1.609500 | -0.000524 | -1.106022 |
| C | -2.145020 | -1.307328 | -0.519663 |
| H | -2.613297 | -1.914977 | -1.296103 |
| H | -2.922564 | -1.065120 | 0.211015 |
| C | 1.614946 | 0.043894 | -0.095248 |
| H | -1.629009 | 1.599900 | 1.946332 |
| H | -2.931049 | 1.481184 | 0.673287 |
| H | -1.454594 | 2.745718 | -0.933437 |
| H | -0.171777 | 2.855508 | 0.355488 |
| H | 0.584045 | -1.850664 | 1.579924 |
| H | -2.426694 | 0.588169 | -1.528681 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.912748 | -0.210450 | -1.921797 |
| H | -0.913359 | -1.068701 | 2.035700 |
| C | 1.768341 | -1.144744 | -1.053203 |
| H | 1.726758 | -2.096500 | -0.523176 |
| H | 1.011508 | -1.152863 | -1.836405 |
| H | 2.744927 | -1.083412 | -1.538582 |
| C | 2.728435 | -0.076140 | 0.956324 |
| H | 3.703346 | -0.155723 | 0.470874 |
| H | 2.745392 | 0.800274 | 1.607213 |
| H | 2.595946 | -0.960339 | 1.582203 |
| C | 1.865159 | 1.326807 | -0.893533 |
| H | 1.837306 | 2.209134 | -0.253527 |
| H | 2.854054 | 1.280856 | -1.354980 |
| H | 1.128074 | 1.458970 | -1.686937 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.914794 | 0.805200 | -0.003177 |
| C | -0.244335 | 0.080032 | -0.692856 |
| H | -0.480342 | 0.661170 | -1.590078 |
| C | 1.807579 | 1.626132 | -0.899187 |
| C | 0.918292 | 2.302402 | 0.112613 |
| C | 0.310080 | -1.266598 | -1.203328 |
| C | 0.997281 | -2.107931 | -0.127625 |
| H | 1.373742 | -3.031200 | -0.572580 |
| H | 0.279315 | -2.401606 | 0.641724 |
| C | 1.668780 | 0.014910 | 1.057597 |
| C | 2.149095 | -1.328443 | 0.506295 |
| H | 2.620192 | -1.912510 | 1.298838 |
| H | 2.912196 | -1.148787 | -0.257584 |
| C | -1.604570 | 0.017530 | 0.089062 |
| H | 1.532845 | 1.719265 | -1.940914 |
| H | 2.871189 | 1.602408 | -0.705530 |
| H | 1.384993 | 2.737729 | 0.986061 |
| H | 0.074704 | 2.852970 | -0.274656 |
| H | -0.465573 | -1.842575 | -1.704321 |
| H | 2.522198 | 0.607804 | 1.394492 |
| H | 1.044165 | -0.159847 | 1.932978 |
| H | 1.057969 | -1.031410 | -1.967511 |
| C | -1.484640 | -0.241195 | 1.595591 |
| H | -0.990348 | -1.184194 | 1.824067 |
| H | -0.943602 | 0.562905 | 2.095336 |
| H | -2.487227 | -0.280574 | 2.028239 |
| C | -2.508658 | -1.066257 | -0.510563 |
| H | -3.505531 | -0.997174 | -0.070923 |
| H | -2.609585 | -0.947048 | -1.591796 |
| H | -2.127064 | -2.068931 | -0.312812 |
| C | -2.335860 | 1.359769 | -0.072199 |
| H | -2.468096 | 1.614485 | -1.125774 |
| H | -3.325233 | 1.301061 | 0.386532 |
| H | -1.797938 | 2.172762 | 0.412869 |

eq

```
=====
```

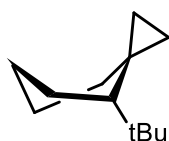
| | | | |
|---|-----------|-----------|-----------|
| C | -0.761824 | 0.838852 | -0.182368 |
| C | 0.173032 | -0.379068 | -0.287993 |
| H | 0.089362 | -0.715781 | -1.330022 |
| C | -0.879242 | 1.660514 | 1.074862 |
| C | -0.355771 | 2.285053 | -0.194833 |
| C | -0.474030 | -1.490334 | 0.560322 |
| C | -1.870472 | -1.840345 | 0.034962 |
| H | -2.322162 | -2.611377 | 0.662105 |
| H | -1.761283 | -2.270603 | -0.965784 |
| C | -2.115660 | 0.521596 | -0.803099 |
| C | -2.788543 | -0.622992 | -0.045828 |
| H | -3.733520 | -0.892594 | -0.521210 |
| H | -3.025103 | -0.281641 | 0.966198 |
| C | 1.708020 | -0.205204 | -0.081736 |
| H | -0.178425 | 1.500092 | 1.878981 |
| H | -1.878936 | 1.924389 | 1.393475 |
| H | -1.002612 | 2.972354 | -0.723752 |
| H | 0.687872 | 2.551969 | -0.211807 |
| H | 0.130871 | -2.394578 | 0.544523 |
| H | -2.747685 | 1.411728 | -0.780488 |
| H | -1.982129 | 0.243704 | -1.853467 |
| H | -0.538774 | -1.162180 | 1.602704 |
| C | 2.102025 | 0.490363 | 1.226762 |
| H | 1.868975 | 1.553924 | 1.227085 |
| H | 1.611508 | 0.028492 | 2.085715 |
| H | 3.180388 | 0.395666 | 1.373265 |
| C | 2.301750 | 0.553310 | -1.278477 |
| H | 3.368413 | 0.726829 | -1.120675 |
| H | 2.192250 | -0.038988 | -2.189890 |
| H | 1.827474 | 1.515926 | -1.451649 |
| C | 2.381038 | -1.588116 | -0.079025 |
| H | 2.028314 | -2.203413 | -0.909911 |
| H | 3.460438 | -1.464949 | -0.185928 |
| H | 2.202824 | -2.130749 | 0.849231 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.792190 | 0.873169 | -0.157592 |
| C | 0.163550 | -0.316721 | -0.371748 |
| H | 0.103175 | -0.533065 | -1.446511 |
| C | -0.676617 | 1.822350 | 1.002879 |
| C | -0.489862 | 2.327189 | -0.408779 |
| C | -0.437056 | -1.533222 | 0.367094 |
| C | -1.848531 | -1.887001 | -0.088305 |
| H | -2.202855 | -2.768040 | 0.450037 |
| H | -1.837699 | -2.142886 | -1.152623 |
| C | -2.223585 | 0.526812 | -0.564990 |
| C | -2.779173 | -0.704091 | 0.139063 |
| H | -3.786095 | -0.920393 | -0.222545 |
| H | -2.856370 | -0.506867 | 1.212889 |
| C | 1.698720 | -0.217315 | -0.059691 |
| H | 0.210751 | 1.776257 | 1.616350 |
| H | -1.580212 | 2.096167 | 1.531292 |
| H | -1.299968 | 2.901403 | -0.837579 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.487812 | 2.657138 | -0.706645 |
| H | 0.211935 | -2.400263 | 0.249419 |
| H | -2.861443 | 1.391826 | -0.374322 |
| H | -2.239603 | 0.352538 | -1.646861 |
| H | -0.468820 | -1.306838 | 1.437101 |
| C | 2.030615 | -0.473494 | 1.418559 |
| H | 1.475115 | 0.181394 | 2.089421 |
| H | 1.825465 | -1.503870 | 1.708192 |
| H | 3.094815 | -0.292893 | 1.584135 |
| C | 2.343256 | 1.114057 | -0.461663 |
| H | 3.429116 | 1.000248 | -0.437476 |
| H | 2.063591 | 1.410099 | -1.473807 |
| H | 2.089958 | 1.919811 | 0.226013 |
| C | 2.404571 | -1.299711 | -0.894996 |
| H | 2.319427 | -1.078380 | -1.960974 |
| H | 3.466277 | -1.331653 | -0.642548 |
| H | 1.993440 | -2.293858 | -0.721946 |



4-(*tert*-butyl)spiro[2.5]octane
(Twist Boat Conformations)

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -470.423180 | -470.091147 | -470.141012 |
| ax2 | -470.430321 | -470.098681 | -470.148818 |
| eq1 | -470.425838 | -470.093978 | -470.144708 |
| eq2 | -470.428177 | -470.096456 | -470.146197 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.223244 | -0.034367 | 0.758660 |
| C | -2.228605 | 0.112958 | -0.084374 |
| C | -1.799972 | 1.370112 | -0.834113 |
| C | -0.841486 | 2.208798 | 0.036700 |
| C | -0.238270 | 1.376360 | 1.174401 |
| H | -2.959571 | -0.453055 | -0.663591 |
| H | -0.997986 | 1.247495 | 1.948045 |
| H | -1.308458 | 1.067957 | -1.760717 |
| H | -2.671225 | 1.960404 | -1.119120 |
| H | -1.381572 | 3.049213 | 0.476383 |
| H | -0.050091 | 2.640049 | -0.578118 |
| H | 0.574135 | 1.922314 | 1.649348 |
| H | -2.724087 | 0.397997 | 0.848038 |
| H | 0.505122 | -0.531552 | 1.691123 |
| C | -1.026385 | -0.782450 | 0.212258 |
| C | -1.379119 | -2.131145 | 0.778976 |
| C | -0.952547 | -2.011990 | -0.658190 |
| H | -2.419501 | -2.338442 | 0.992155 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.670702 | -2.577622 | 1.464495 |
| H | -0.000814 | -2.427157 | -0.939406 |
| H | -1.715516 | -2.106323 | -1.419195 |
| C | 1.536685 | -0.064986 | -0.097934 |
| C | 2.261841 | -1.400254 | 0.145597 |
| C | 1.321685 | 0.140436 | -1.602233 |
| C | 2.505890 | 1.027430 | 0.378501 |
| H | 2.574501 | -1.470239 | 1.189801 |
| H | 1.650195 | -2.273259 | -0.069141 |
| H | 3.157966 | -1.461393 | -0.475628 |
| H | 0.907981 | 1.126127 | -1.813728 |
| H | 2.284044 | 0.074094 | -2.115195 |
| H | 0.660419 | -0.606279 | -2.037099 |
| H | 3.474894 | 0.888965 | -0.105514 |
| H | 2.150296 | 2.027744 | 0.129343 |
| H | 2.662205 | 0.977550 | 1.458232 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.518574 | 0.075765 | 1.215756 |
| C | 1.674968 | -1.434824 | 0.937457 |
| C | 1.623028 | -1.724043 | -0.562621 |
| C | 0.266416 | -1.319302 | -1.159907 |
| C | -0.247308 | 0.071990 | -0.677813 |
| H | 2.610035 | -1.799394 | 1.363689 |
| H | -0.464254 | 0.674178 | -1.564984 |
| H | 2.430187 | -1.185749 | -1.063103 |
| H | 1.792593 | -2.786377 | -0.746024 |
| H | -0.458187 | -2.091780 | -0.901834 |
| H | 0.338458 | -1.326922 | -2.248476 |
| H | 0.872781 | -1.990656 | 1.425346 |
| H | 0.925239 | 0.237936 | 2.117699 |
| H | 2.495233 | 0.524163 | 1.408670 |
| C | 0.896360 | 0.794066 | 0.029126 |
| C | 1.871125 | 1.492527 | -0.887920 |
| C | 0.963745 | 2.291632 | 0.008532 |
| H | 1.653842 | 1.493303 | -1.947623 |
| H | 2.921379 | 1.443339 | -0.636564 |
| H | 1.404261 | 2.782245 | 0.866491 |
| H | 0.154807 | 2.834082 | -0.457817 |
| C | -1.616490 | 0.001244 | 0.068443 |
| C | -2.676896 | -0.454444 | -0.944179 |
| C | -1.649300 | -0.965476 | 1.258214 |
| C | -2.022173 | 1.388396 | 0.575930 |
| H | -2.733452 | 0.240041 | -1.785329 |
| H | -2.461764 | -1.447910 | -1.340094 |
| H | -3.660263 | -0.492344 | -0.471169 |
| H | -0.963449 | -0.665654 | 2.049431 |
| H | -2.655714 | -0.973328 | 1.682839 |
| H | -1.412034 | -1.988475 | 0.966734 |
| H | -3.029156 | 1.347538 | 0.996885 |
| H | -1.345950 | 1.746080 | 1.353049 |
| H | -2.026886 | 2.120500 | -0.233924 |

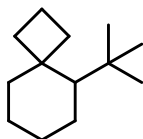
eq1

```
=====
C  -0.122482    -0.340103    -0.264379
C   2.212477     0.502028     0.411366
C   2.686198    -0.657180    -0.456226
C   1.867990    -1.915765    -0.117069
C   0.491758    -1.553877     0.459120
H   2.852475     1.376723     0.287393
H   0.586161    -1.319085     1.521566
H  -0.001725    -0.522787    -1.339842
H   2.548165    -0.387003    -1.506227
H   3.751375    -0.841477    -0.315477
H   2.408429    -2.526675     0.608327
H   1.738891    -2.528284    -1.011450
H  -0.157153    -2.423524     0.393793
H   2.276492     0.213492     1.464785
C   0.774678     0.885891     0.055474
C   0.671743     2.146389    -0.761941
C   0.327177     2.165840     0.706866
H  -0.143248     2.237510    -1.463729
H   1.594536     2.616229    -1.074080
H   1.036634     2.629617     1.379835
H  -0.702920     2.312968     0.983287
C  -1.663770    -0.246349    -0.043996
C  -2.031813    -0.181726     1.442575
C  -2.293220     0.936847    -0.795716
C  -2.326452    -1.502264    -0.639791
H  -1.732687    -1.094980     1.959075
H  -1.563575     0.659504     1.951664
H  -3.113858    -0.081095     1.552763
H  -2.023329     0.909226    -1.853767
H  -3.380680     0.864683    -0.731249
H  -2.013226     1.908587    -0.398813
H  -3.411952    -1.393695    -0.604590
H  -2.038245    -1.636998    -1.684905
H  -2.076269    -2.411317    -0.096055
```

eq2

```
=====
C  -2.091899     0.536620    -0.877395
C  -2.534193    -0.926683    -0.674163
C  -1.971903    -1.470774     0.638482
C  -0.431859    -1.497768     0.598722
C   0.156858    -0.371767    -0.283277
H  -3.621998    -0.997816    -0.690942
H   0.042003    -0.701394    -1.323331
H  -2.315563    -0.838326     1.458996
H  -2.353868    -2.473575     0.833562
H  -0.103458    -2.461929     0.209155
H  -0.037282    -1.416468     1.614553
H  -2.168223    -1.545746    -1.496690
H  -1.963284     0.740964    -1.943822
H  -2.862016     1.219083    -0.511986
C  -0.786161     0.828891    -0.143219
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.934805 | 1.554566 | 1.168244 |
| C | -0.407418 | 2.277362 | -0.045839 |
| H | -0.234364 | 1.337566 | 1.961095 |
| H | -1.938830 | 1.782920 | 1.498744 |
| H | -1.066335 | 2.982994 | -0.535111 |
| H | 0.630026 | 2.568514 | -0.039218 |
| C | 1.692412 | -0.196092 | -0.122278 |
| C | 2.245938 | 0.609065 | -1.305578 |
| C | 2.121915 | 0.459188 | 1.196141 |
| C | 2.352767 | -1.582689 | -0.182767 |
| H | 2.079129 | 0.069762 | -2.240812 |
| H | 1.783352 | 1.589119 | -1.400423 |
| H | 3.322428 | 0.754332 | -1.191869 |
| H | 1.682163 | -0.045594 | 2.057885 |
| H | 3.207556 | 0.389459 | 1.294387 |
| H | 1.860349 | 1.514807 | 1.247286 |
| H | 3.436282 | -1.470078 | -0.254597 |
| H | 2.138805 | -2.174783 | 0.707356 |
| H | 2.013211 | -2.143334 | -1.056663 |



5-(*tert*-butyl)spiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -509.737302 | -509.37498 | -509.426401 |
| ax2 | -509.735463 | -509.373229 | -509.424437 |
| ax3 | -509.736747 | -509.374502 | -509.425926 |
| ax4 | -509.732162 | -509.369769 | -509.421304 |
| eq | -509.735981 | -509.373719 | -509.425195 |
| eq2 | -509.735168 | -509.373031 | -509.424619 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.385365 | -0.052935 | -0.704737 |
| H | -0.366497 | -0.661386 | -1.615344 |
| C | -0.395714 | 1.411818 | -1.186125 |
| C | -0.189966 | 2.425095 | -0.061958 |
| H | -0.216662 | 3.438708 | -0.467277 |
| H | -1.004425 | 2.355007 | 0.662596 |
| C | 1.282483 | 0.724198 | 1.094789 |
| C | 1.150017 | 2.175248 | 0.627250 |
| H | 1.280965 | 2.849284 | 1.475859 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.951221 | 2.403495 | -0.081384 |
| H | 0.431021 | 1.526192 | -1.895472 |
| H | 0.623486 | 0.559054 | 1.945390 |
| H | 2.299105 | 0.552434 | 1.457733 |
| H | -1.303401 | 1.631936 | -1.744708 |
| C | -1.685934 | -0.532094 | 0.041276 |
| C | 0.976783 | -0.293749 | -0.017706 |
| C | 1.370908 | -1.733099 | 0.415291 |
| C | 2.188702 | -0.346462 | -1.000992 |
| C | 2.780300 | -1.505136 | -0.169881 |
| H | 0.844618 | -2.479470 | -0.175968 |
| H | 1.281027 | -1.981210 | 1.473831 |
| H | 1.875625 | -0.686974 | -1.988912 |
| H | 2.788660 | 0.556534 | -1.108499 |
| H | 3.227412 | -2.332429 | -0.716874 |
| H | 3.489773 | -1.153316 | 0.576150 |
| C | -1.893221 | -2.036486 | -0.205988 |
| H | -1.876998 | -2.268731 | -1.272712 |
| H | -1.134420 | -2.640332 | 0.288098 |
| H | -2.863091 | -2.345283 | 0.190139 |
| C | -1.694115 | -0.333889 | 1.562685 |
| H | -2.644120 | -0.700259 | 1.959573 |
| H | -0.897670 | -0.902174 | 2.043836 |
| H | -1.597186 | 0.710821 | 1.854222 |
| C | -2.917397 | 0.181561 | -0.533208 |
| H | -2.972823 | 0.068624 | -1.618248 |
| H | -3.823088 | -0.252219 | -0.105027 |
| H | -2.917420 | 1.247269 | -0.301178 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.359195 | 0.865115 | 1.133798 |
| H | -2.346685 | 0.672799 | 1.560897 |
| C | -1.338047 | 2.241634 | 0.474773 |
| C | -0.008312 | 2.470622 | -0.236372 |
| H | -0.005979 | 3.440391 | -0.738074 |
| H | 0.802867 | 2.488232 | 0.496795 |
| C | 0.279928 | -0.055872 | -0.639634 |
| C | 0.220481 | 1.358098 | -1.256320 |
| H | 1.111417 | 1.552425 | -1.849484 |
| H | -0.617301 | 1.380680 | -1.959282 |
| H | -2.146692 | 2.305285 | -0.261023 |
| H | 0.229377 | -0.741015 | -1.492303 |
| H | -1.523938 | 3.017074 | 1.220131 |
| C | -1.037942 | -0.273635 | 0.161977 |
| C | -1.268638 | -1.695652 | 0.753875 |
| C | -2.190575 | -0.606690 | -0.840871 |
| C | -1.976777 | -2.106626 | -0.549955 |
| H | -1.988676 | -1.623568 | 1.571104 |
| H | -0.423840 | -2.283766 | 1.096133 |
| H | -3.151447 | -0.261287 | -0.456730 |
| H | -2.075971 | -0.271580 | -1.870718 |
| H | -2.858869 | -2.738633 | -0.470128 |
| H | -1.282085 | -2.555441 | -1.259424 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.640828 | -0.422227 | 0.064900 |
| H | -0.654724 | 0.856947 | 1.966792 |
| C | 1.653149 | -0.221081 | 1.585997 |
| H | 2.616145 | -0.552898 | 1.981082 |
| H | 1.532092 | 0.827925 | 1.856324 |
| H | 0.874607 | -0.794082 | 2.088083 |
| C | 1.969751 | -1.894859 | -0.238666 |
| H | 1.189171 | -2.579476 | 0.085914 |
| H | 2.108141 | -2.037010 | -1.312603 |
| H | 2.897266 | -2.185467 | 0.259553 |
| C | 2.809445 | 0.393108 | -0.508372 |
| H | 3.744201 | 0.037355 | -0.069977 |
| H | 2.886219 | 0.277246 | -1.590974 |
| H | 2.720144 | 1.456263 | -0.282860 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.387791 | -0.086409 | 0.673973 |
| H | 0.358444 | -0.722226 | 1.565688 |
| C | 0.400587 | 1.373977 | 1.179722 |
| C | 0.063847 | 2.435930 | 0.121085 |
| H | -0.057971 | 3.399830 | 0.620242 |
| H | 0.890869 | 2.556386 | -0.574576 |
| C | -1.215661 | 0.658301 | -1.159704 |
| C | -1.203309 | 2.107748 | -0.669777 |
| H | -1.299289 | 2.791111 | -1.515653 |
| H | -2.077816 | 2.275492 | -0.037568 |
| H | -0.340997 | 1.450930 | 1.980438 |
| H | -0.448818 | 0.509878 | -1.925070 |
| H | -2.175989 | 0.440927 | -1.634414 |
| H | 1.364395 | 1.608664 | 1.635615 |
| C | 1.716000 | -0.514669 | -0.045895 |
| C | -0.974605 | -0.323825 | -0.010050 |
| C | -1.422533 | -1.768145 | -0.379107 |
| C | -2.180567 | -0.303557 | 0.984675 |
| C | -2.816769 | -1.470140 | 0.204237 |
| H | -0.907292 | -2.508308 | 0.230878 |
| H | -1.357795 | -2.059758 | -1.427076 |
| H | -1.860397 | -0.623764 | 1.977394 |
| H | -2.755158 | 0.615892 | 1.078953 |
| H | -3.292797 | -2.258516 | 0.783619 |
| H | -3.515072 | -1.119949 | -0.553675 |
| C | 1.544453 | -1.792101 | -0.873980 |
| H | 1.165921 | -2.618178 | -0.272625 |
| H | 0.868827 | -1.639629 | -1.716146 |
| H | 2.514640 | -2.092890 | -1.275772 |
| C | 2.341318 | 0.543830 | -0.965583 |
| H | 3.244624 | 0.126201 | -1.415921 |
| H | 1.677840 | 0.842377 | -1.776281 |
| H | 2.636672 | 1.435666 | -0.413058 |
| C | 2.747732 | -0.815411 | 1.053315 |
| H | 2.424780 | -1.656256 | 1.670220 |
| H | 3.712242 | -1.072024 | 0.610133 |
| H | 2.900429 | 0.044968 | 1.707184 |

ax4

```
=====
C  1.190885    0.808791   -1.255237
H  2.101003    0.623331   -1.831097
C  1.283107    2.171516   -0.568733
C  0.054588    2.441464    0.297845
H  0.213187    3.344041    0.892279
H -0.790468    2.649492   -0.355195
C -0.283892   -0.129122    0.600100
C -0.268643    1.278869    1.249626
H -1.223442    1.471016    1.741321
H  0.479725    1.281747    2.043901
H  2.181351    2.186252    0.055490
H -0.199976   -0.848630    1.422578
H  1.401306    2.966603   -1.307168
C  1.030065   -0.292579   -0.211960
C  1.420067   -1.738099   -0.666010
C  2.252526   -0.382327    0.766517
C  2.254397   -1.912349    0.614124
H  2.063478   -1.674882   -1.545212
H  0.650714   -2.474531   -0.853761
H  3.138080    0.060641    0.308409
H  2.136947    0.021949    1.770210
H  3.219226   -2.407634    0.524693
H  1.681378   -2.397352    1.403395
C -1.681563   -0.456864   -0.050723
H  0.357317    0.793401   -1.963111
C -2.346415    0.712974   -0.792932
H -3.304947    0.372922   -1.190646
H -2.550980    1.552984   -0.130204
H -1.751736    1.070727   -1.632491
C -1.647113   -1.637488   -1.025519
H -1.003517   -1.440748   -1.884016
H -1.312575   -2.554099   -0.540054
H -2.657379   -1.816530   -1.400057
C -2.627276   -0.851035    1.096286
H -3.629593   -1.047907    0.710088
H -2.274816   -1.754974    1.596776
H -2.708681   -0.060321    1.843575
```

eq

```
=====
C  0.370804   -0.531241    0.268628
H  0.373338   -0.923290    1.294714
C -0.064787   -1.711703   -0.620297
C -1.310131   -2.390824   -0.043427
H -1.615308   -3.223552   -0.680216
H -1.044835   -2.816128    0.929721
C -2.020057   -0.144705    0.861566
C -2.466948   -1.412515    0.134315
H -3.284911   -1.886518    0.680412
H -2.863909   -1.146985   -0.848382
H -0.267183   -1.357183   -1.636846
```

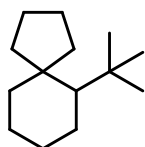
| | | | |
|---|-----------|-----------|-----------|
| H | -1.778216 | -0.382176 | 1.902708 |
| H | -2.842265 | 0.574738 | 0.884384 |
| H | 0.723017 | -2.457161 | -0.696231 |
| C | 1.844011 | -0.051715 | 0.054652 |
| C | -0.782061 | 0.505260 | 0.214923 |
| C | -0.636777 | 1.957572 | 0.753962 |
| C | -1.203636 | 1.120634 | -1.157613 |
| C | -1.480014 | 2.460293 | -0.438214 |
| H | 0.372906 | 2.345250 | 0.683128 |
| H | -1.016087 | 2.136762 | 1.761246 |
| H | -0.381058 | 1.199137 | -1.861639 |
| H | -2.047344 | 0.652670 | -1.662178 |
| H | -1.127060 | 3.363330 | -0.932141 |
| H | -2.531585 | 2.586034 | -0.189184 |
| C | 2.767816 | -1.259124 | -0.176164 |
| H | 2.600448 | -2.037482 | 0.571760 |
| H | 2.633214 | -1.698462 | -1.164605 |
| H | 3.808104 | -0.937007 | -0.097435 |
| C | 2.040910 | 0.893368 | -1.135960 |
| H | 3.107574 | 1.091821 | -1.264899 |
| H | 1.676304 | 0.443580 | -2.061334 |
| H | 1.542673 | 1.852950 | -1.003636 |
| C | 2.353292 | 0.614863 | 1.344088 |
| H | 2.416434 | -0.124800 | 2.145525 |
| H | 3.354993 | 1.021121 | 1.187362 |
| H | 1.716243 | 1.422373 | 1.695008 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -2.176148 | 0.252560 | -0.740236 |
| H | -2.094244 | -0.028147 | -1.796806 |
| C | -2.774856 | -0.904383 | 0.048127 |
| C | -1.826210 | -2.093565 | 0.024961 |
| H | -2.206421 | -2.904758 | 0.648975 |
| H | -1.753338 | -2.481127 | -0.996254 |
| C | 0.172554 | -0.536993 | -0.344270 |
| C | -0.439552 | -1.673014 | 0.504006 |
| H | 0.211165 | -2.543856 | 0.505705 |
| H | -0.517239 | -1.339137 | 1.543187 |
| H | -2.932702 | -0.590482 | 1.085207 |
| H | 0.112269 | -0.852808 | -1.394580 |
| H | -3.752822 | -1.172648 | -0.355847 |
| C | -0.788840 | 0.684143 | -0.242459 |
| C | -0.379648 | 2.041650 | -0.889282 |
| C | -0.837177 | 1.414594 | 1.135227 |
| C | -0.108219 | 2.627290 | 0.513706 |
| H | -1.252975 | 2.507617 | -1.346243 |
| H | 0.425442 | 2.052888 | -1.615835 |
| H | -1.863421 | 1.653914 | 1.416725 |
| H | -0.355733 | 0.926330 | 1.979507 |
| H | -0.531965 | 3.608298 | 0.719758 |
| H | 0.950429 | 2.649458 | 0.764782 |
| C | 1.714605 | -0.409203 | -0.074517 |
| H | -2.840593 | 1.118345 | -0.693692 |

| | | | |
|---|----------|-----------|-----------|
| C | 2.074397 | -0.125626 | 1.389421 |
| H | 3.157447 | -0.200154 | 1.513852 |
| H | 1.780464 | 0.874976 | 1.702124 |
| H | 1.616866 | -0.847324 | 2.067189 |
| C | 2.393979 | 0.651172 | -0.953433 |
| H | 3.476975 | 0.531938 | -0.883443 |
| H | 2.114957 | 0.535394 | -2.003032 |
| H | 2.164431 | 1.666674 | -0.643279 |
| C | 2.377100 | -1.748436 | -0.459974 |
| H | 2.066603 | -2.068732 | -1.457369 |
| H | 3.461430 | -1.628254 | -0.469585 |
| H | 2.151067 | -2.549540 | 0.241286 |



6-(*tert*-butyl)spiro[4.5]decane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -549.068507 | -548.674871 | -548.728109 |
| ax2 | -549.065953 | -548.672462 | -548.72622 |
| ax3 | -549.067062 | -548.673318 | -548.726266 |
| eq | -549.067547 | -548.674182 | -548.727211 |
| eq2 | -549.066914 | -548.673464 | -548.727224 |
| eq3 | -549.066908 | -548.67346 | -548.727932 |
| eq4 | -549.066909 | -548.67346 | -548.727907 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.615001 | -0.014913 | -0.717336 |
| H | -0.530992 | -0.549399 | -1.670200 |
| C | -0.883043 | 1.459475 | -1.091780 |
| C | -0.805245 | 2.418776 | 0.094751 |
| H | -0.989028 | 3.440183 | -0.245389 |
| H | -1.589393 | 2.186146 | 0.818079 |
| C | 0.946610 | 0.891659 | 1.109232 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.565889 | 2.333737 | 0.763089 |
| H | 0.588287 | 2.943720 | 1.668335 |
| H | 1.312311 | 2.757805 | 0.086254 |
| H | -0.127161 | 1.761259 | -1.820980 |
| H | 0.332566 | 0.550792 | 1.942056 |
| H | 1.979136 | 0.873075 | 1.465148 |
| H | -1.838865 | 1.561611 | -1.600474 |
| C | -1.820394 | -0.737083 | 0.001440 |
| C | 0.802179 | -0.091421 | -0.074574 |
| C | 1.264003 | -1.500232 | 0.346533 |
| C | 1.893036 | 0.227799 | -1.130999 |
| C | 2.795047 | -1.417385 | 0.455737 |
| H | 1.002607 | -2.201500 | -0.448579 |
| H | 0.800627 | -1.852552 | 1.267378 |
| C | 3.210405 | -0.317765 | -0.550999 |
| H | 1.965162 | 1.285034 | -1.376605 |
| H | 1.643120 | -0.303281 | -2.052967 |
| H | 3.094484 | -1.144421 | 1.467283 |
| H | 3.261075 | -2.376658 | 0.235144 |
| H | 3.767360 | 0.472806 | -0.048414 |
| H | 3.855078 | -0.707234 | -1.337678 |
| C | -3.150070 | -0.213559 | -0.564431 |
| H | -3.970870 | -0.823925 | -0.183727 |
| H | -3.342194 | 0.818921 | -0.270551 |
| H | -3.169818 | -0.268238 | -1.655210 |
| C | -1.892522 | -0.596533 | 1.529158 |
| H | -1.042120 | -1.061389 | 2.025107 |
| H | -1.954343 | 0.440089 | 1.855299 |
| H | -2.792538 | -1.105822 | 1.882956 |
| C | -1.788720 | -2.244344 | -0.309816 |
| H | -1.733498 | -2.422946 | -1.385765 |
| H | -0.950862 | -2.749963 | 0.163590 |
| H | -2.703179 | -2.713368 | 0.059877 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.908676 | 1.234496 | 1.256479 |
| C | -0.418690 | -0.092938 | 0.636167 |
| C | 0.635703 | 1.381151 | -1.195129 |
| H | 1.598062 | 1.625038 | -1.653981 |
| H | -0.012441 | 1.040431 | -2.004344 |
| C | -1.222494 | 2.317706 | 0.227916 |
| C | 0.035565 | 2.640339 | -0.572270 |
| H | -0.175941 | 3.373059 | -1.353496 |
| H | 0.766352 | 3.098940 | 0.100516 |
| H | -2.020028 | 1.989040 | -0.442078 |
| H | -1.585945 | 3.214393 | 0.734287 |
| H | -1.762907 | 1.060660 | 1.906377 |
| H | -0.117777 | 1.619650 | 1.905372 |
| C | 0.871526 | 0.223695 | -0.202775 |
| C | 2.026629 | 0.590348 | 0.799722 |
| C | 1.472712 | -0.983810 | -0.965152 |
| C | 3.141303 | -0.456852 | 0.617837 |
| H | 1.663388 | 0.552769 | 1.825954 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.397115 | 1.602286 | 0.634099 |
| C | 2.414904 | -1.662532 | 0.022978 |
| H | 2.075949 | -0.591094 | -1.789887 |
| H | 0.737732 | -1.646563 | -1.405397 |
| H | 3.883389 | -0.101798 | -0.100472 |
| H | 3.662722 | -0.673892 | 1.549613 |
| H | 3.084889 | -2.383359 | -0.445493 |
| H | 1.844866 | -2.183792 | 0.797129 |
| C | -1.563726 | -0.968791 | -0.005123 |
| H | -0.077784 | -0.699304 | 1.481964 |
| C | -1.845262 | -0.728592 | -1.496707 |
| H | -0.990889 | -0.945714 | -2.134127 |
| H | -2.660798 | -1.385521 | -1.808720 |
| H | -2.159314 | 0.295638 | -1.693305 |
| C | -2.893900 | -0.741208 | 0.732512 |
| H | -3.631415 | -1.460576 | 0.371068 |
| H | -2.785432 | -0.888674 | 1.808755 |
| H | -3.294250 | 0.258590 | 0.561424 |
| C | -1.235577 | -2.459711 | 0.203388 |
| H | -0.293831 | -2.764227 | -0.246292 |
| H | -1.180751 | -2.686887 | 1.270336 |
| H | -2.025055 | -3.078908 | -0.228360 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.493570 | 1.493977 | 1.239894 |
| H | -1.393243 | 1.802881 | 1.779037 |
| C | 0.102514 | 2.694270 | 0.505275 |
| C | 1.289587 | 2.274776 | -0.358151 |
| H | 1.656839 | 3.127714 | -0.932838 |
| H | 2.114328 | 1.946636 | 0.278827 |
| C | 0.325724 | -0.106452 | -0.601025 |
| C | 0.875381 | 1.154600 | -1.309387 |
| H | 1.698312 | 0.892222 | -1.969222 |
| H | 0.096109 | 1.548340 | -1.964179 |
| H | -0.660653 | 3.143245 | -0.137780 |
| H | -0.103333 | -0.721088 | -1.399872 |
| H | 0.399544 | 3.459788 | 1.224700 |
| C | -0.876919 | 0.331506 | 0.307672 |
| C | -1.551539 | -0.806030 | 1.102089 |
| C | -2.077941 | 0.731958 | -0.590783 |
| C | -2.376108 | -1.606964 | 0.083248 |
| H | -2.233429 | -0.331740 | 1.813897 |
| H | -0.869651 | -1.418087 | 1.684791 |
| C | -2.741612 | -0.586570 | -1.022408 |
| H | -1.814737 | 1.358539 | -1.439247 |
| H | -2.773904 | 1.305731 | 0.027178 |
| H | -1.790529 | -2.424659 | -0.334787 |
| H | -3.258474 | -2.049277 | 0.543967 |
| H | -2.356956 | -0.914355 | -1.988150 |
| H | -3.818653 | -0.468988 | -1.134374 |
| C | 1.447354 | -1.033868 | 0.016030 |
| H | 0.216117 | 1.152524 | 1.993758 |

| | | | |
|---|----------|-----------|-----------|
| C | 1.865171 | -0.720524 | 1.460663 |
| H | 1.047405 | -0.836621 | 2.169180 |
| H | 2.653284 | -1.418090 | 1.754801 |
| H | 2.265191 | 0.286742 | 1.566361 |
| C | 0.998223 | -2.505547 | -0.034777 |
| H | 0.151162 | -2.715983 | 0.612438 |
| H | 0.727497 | -2.792468 | -1.053206 |
| H | 1.820151 | -3.149807 | 0.285048 |
| C | 2.724610 | -0.965311 | -0.837779 |
| H | 3.431725 | -1.718818 | -0.486325 |
| H | 2.515358 | -1.169192 | -1.890038 |
| H | 3.215283 | 0.005884 | -0.767327 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.263276 | -1.885687 | 0.577719 |
| C | 0.477244 | -0.634338 | -0.299675 |
| H | 0.564665 | -0.995711 | -1.333507 |
| C | -1.977944 | -0.721167 | -0.815943 |
| H | -2.912413 | -0.153652 | -0.795835 |
| H | -1.766343 | -0.938398 | -1.868920 |
| C | -0.840646 | -2.787584 | 0.029394 |
| C | -2.159042 | -2.033914 | -0.062381 |
| H | -2.919930 | -2.640973 | -0.557218 |
| H | -2.527056 | -1.834793 | 0.947379 |
| H | -0.548079 | -3.134846 | -0.966828 |
| H | -0.948767 | -3.674412 | 0.657042 |
| H | 1.176185 | -2.470094 | 0.648525 |
| H | 0.007392 | -1.580415 | 1.597385 |
| C | 1.876399 | 0.032769 | -0.026708 |
| C | -0.851951 | 0.197307 | -0.279876 |
| C | -1.251982 | 0.731261 | 1.131617 |
| C | -0.855697 | 1.470639 | -1.176879 |
| C | -1.689931 | 2.189308 | 0.931445 |
| H | -0.411609 | 0.688466 | 1.818790 |
| H | -2.046673 | 0.134374 | 1.578000 |
| C | -0.820227 | 2.671144 | -0.229619 |
| H | -1.806091 | 1.504259 | -1.715430 |
| H | -0.074153 | 1.465677 | -1.930900 |
| H | -2.740907 | 2.227417 | 0.634337 |
| H | -1.580856 | 2.789029 | 1.835132 |
| H | -1.189423 | 3.585878 | -0.693755 |
| H | 0.192173 | 2.864479 | 0.128618 |
| C | 2.242812 | 1.093872 | -1.076611 |
| H | 2.131236 | 0.701270 | -2.089978 |
| H | 1.652992 | 2.001057 | -0.990886 |
| H | 3.288646 | 1.378816 | -0.945289 |
| C | 2.963759 | -1.055620 | -0.154902 |
| H | 3.943066 | -0.581624 | -0.234592 |
| H | 2.998674 | -1.717424 | 0.708790 |
| H | 2.812202 | -1.666001 | -1.048587 |
| C | 2.030543 | 0.661791 | 1.363589 |
| H | 3.079746 | 0.921642 | 1.524869 |
| H | 1.448520 | 1.576599 | 1.469960 |

H 1.737118 -0.029303 2.155877

eq2

```
=====
C 0.723515 0.377163 -0.386055
H 0.835179 0.578626 -1.459829
C 0.912480 1.725654 0.347236
C -0.020468 2.832797 -0.126432
H 0.185029 3.752529 0.424938
H 0.162619 3.043514 -1.185025
C -1.680048 1.074863 -0.668382
C -1.464901 2.394599 0.057811
H -2.156735 3.146151 -0.327690
H -1.679903 2.282105 1.124569
H 0.737666 1.571509 1.415394
H -1.500211 1.242769 -1.735689
H -2.721875 0.764877 -0.579685
H 1.945318 2.057904 0.250418
C 1.934762 -0.563962 -0.016997
C -0.757640 -0.093930 -0.226688
C -1.216804 -1.292919 -1.091473
C -1.141742 -0.584587 1.182109
C -2.540935 -1.769309 -0.451623
H -0.504884 -2.105884 -1.061121
H -1.338451 -1.004015 -2.137057
C -2.515171 -1.253790 1.010642
H -1.148257 0.206146 1.932569
H -0.418104 -1.334454 1.502115
H -3.404376 -1.371830 -0.983385
H -2.619303 -2.854795 -0.491072
H -3.315445 -0.532769 1.175943
H -2.660126 -2.057657 1.730915
C 2.321972 -0.496624 1.470855
H 1.486117 -0.728146 2.130338
H 3.111300 -1.225057 1.667697
H 2.708479 0.483373 1.748315
C 1.749481 -2.044046 -0.372475
H 0.990478 -2.529897 0.239776
H 1.494926 -2.179134 -1.424048
H 2.693271 -2.564445 -0.194503
C 3.150109 -0.089621 -0.834278
H 4.035664 -0.664242 -0.554872
H 2.977150 -0.238719 -1.902089
H 3.376822 0.963815 -0.672437
```

eq3

```
=====
C -2.484025 1.627076 0.135075
C -2.153776 0.384999 -0.677658
H -2.062020 0.674299 -1.730155
C 0.324973 0.691134 -0.374989
H 0.324787 0.980645 -1.434368
C -1.337088 2.618770 0.012460
C -0.030966 1.956477 0.437740
```

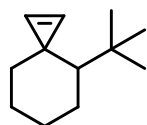
| | | | |
|---|-----------|-----------|-----------|
| H | 0.774568 | 2.684627 | 0.370149 |
| H | -0.116499 | 1.691027 | 1.494395 |
| H | -1.258449 | 2.954096 | -1.026710 |
| H | -1.518679 | 3.505477 | 0.623060 |
| H | -3.421811 | 2.065018 | -0.212309 |
| H | -2.624936 | 1.360231 | 1.187266 |
| C | -0.852638 | -0.341644 | -0.259765 |
| C | -1.028631 | -0.959731 | 1.155760 |
| C | -0.734076 | -1.578680 | -1.206075 |
| C | -0.462966 | -2.379866 | 1.089502 |
| H | -2.097399 | -1.022944 | 1.378526 |
| H | -0.579628 | -0.360670 | 1.946061 |
| C | -0.817598 | -2.842788 | -0.326888 |
| H | 0.178959 | -1.553842 | -1.788413 |
| H | -1.551352 | -1.569470 | -1.927466 |
| H | 0.617195 | -2.372605 | 1.230121 |
| H | -0.883097 | -3.029256 | 1.858003 |
| H | -0.171934 | -3.645900 | -0.683328 |
| H | -1.840528 | -3.224318 | -0.331150 |
| H | -2.969955 | -0.340184 | -0.621463 |
| C | 1.817319 | 0.281046 | -0.077888 |
| C | 2.131588 | 0.154825 | 1.420377 |
| H | 1.570330 | -0.645319 | 1.899268 |
| H | 3.193265 | -0.070015 | 1.545142 |
| H | 1.930776 | 1.081577 | 1.957509 |
| C | 2.276023 | -1.012079 | -0.768375 |
| H | 2.160992 | -0.947014 | -1.851913 |
| H | 3.338212 | -1.158646 | -0.561290 |
| H | 1.752162 | -1.898268 | -0.419437 |
| C | 2.736348 | 1.381782 | -0.646030 |
| H | 3.778082 | 1.067227 | -0.559817 |
| H | 2.527259 | 1.557520 | -1.703507 |
| H | 2.642775 | 2.328783 | -0.117653 |

eq4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 2.153929 | 0.384206 | -0.677599 |
| H | 2.062083 | 0.673223 | -1.730181 |
| C | 2.484715 | 1.626499 | 0.134727 |
| C | 1.337829 | 2.618267 | 0.012519 |
| H | 1.519792 | 3.504932 | 0.623071 |
| H | 1.258779 | 2.953633 | -1.026601 |
| C | -0.324658 | 0.691184 | -0.374638 |
| C | 0.031818 | 1.956232 | 0.438323 |
| H | -0.773508 | 2.684651 | 0.371232 |
| H | 0.117655 | 1.690598 | 1.494928 |
| H | 2.626112 | 1.359933 | 1.186926 |
| H | -0.324266 | 0.980955 | -1.433951 |
| H | 3.422375 | 2.064306 | -0.213157 |
| C | 0.852678 | -0.342005 | -0.259476 |
| C | 0.733756 | -1.578849 | -1.205967 |
| C | 1.028390 | -0.960356 | 1.155938 |
| C | 0.817092 | -2.842910 | -0.326759 |
| H | 1.550791 | -1.569768 | -1.927654 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.179459 | -1.553990 | -1.788046 |
| C | 0.461250 | -2.379841 | 1.089282 |
| H | 0.580139 | -0.360939 | 1.946375 |
| H | 2.097116 | -1.024804 | 1.378597 |
| H | 0.172123 | -3.646351 | -0.683735 |
| H | 1.840165 | -3.224143 | -0.330119 |
| H | -0.619077 | -2.371460 | 1.228727 |
| H | 0.879936 | -3.029656 | 1.858213 |
| H | 2.969852 | -0.341270 | -0.621470 |
| C | -1.817241 | 0.281654 | -0.077929 |
| C | -2.131657 | 0.154273 | 1.420167 |
| H | -1.931261 | 1.080653 | 1.958137 |
| H | -3.193310 | -0.070925 | 1.544611 |
| H | -1.570198 | -0.646122 | 1.898438 |
| C | -2.276631 | -1.010615 | -0.769671 |
| H | -2.160957 | -0.944894 | -1.853095 |
| H | -1.753860 | -1.897614 | -0.421072 |
| H | -3.339090 | -1.156403 | -0.563356 |
| C | -2.735648 | 1.383352 | -0.645298 |
| H | -2.526464 | 1.559597 | -1.702696 |
| H | -3.777537 | 1.069232 | -0.559331 |
| H | -2.641662 | 2.330081 | -0.116500 |



4-(*tert*-butyl)spiro[2.5]oct-1-ene

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -469.167658 | -468.86162 | -468.911439 |
| ax2 | -469.166854 | -468.860647 | -468.910623 |
| eq | -469.168772 | -468.86294 | -468.913879 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.906371 | 0.883980 | -0.003228 |
| C | -0.226133 | 0.090981 | -0.675228 |
| H | -0.477589 | 0.667800 | -1.570059 |
| C | 1.683319 | 1.853846 | -0.863296 |
| C | 0.895068 | 2.385268 | 0.008792 |
| C | 0.339561 | -1.259389 | -1.168970 |
| C | 1.192476 | -2.026750 | -0.150003 |
| H | 1.640482 | -2.890325 | -0.646257 |
| H | 0.570843 | -2.418964 | 0.654776 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.677923 | 0.117995 | 1.062548 |
| C | 2.283652 | -1.149427 | 0.459066 |
| H | 2.840121 | -1.708112 | 1.213956 |
| H | 2.998330 | -0.860638 | -0.318622 |
| C | -1.583575 | -0.014625 | 0.095213 |
| H | -0.467341 | -1.900195 | -1.529795 |
| H | 2.461067 | 0.759568 | 1.469474 |
| H | 1.019551 | -0.151840 | 1.893379 |
| H | 0.974068 | -1.048178 | -2.035324 |
| C | -1.661393 | -1.149669 | 1.122879 |
| H | -1.567774 | -2.126935 | 0.647990 |
| H | -0.898142 | -1.068097 | 1.895739 |
| H | -2.635693 | -1.117411 | 1.616225 |
| C | -2.690925 | -0.258264 | -0.940750 |
| H | -3.657688 | -0.368948 | -0.445171 |
| H | -2.762164 | 0.579294 | -1.637591 |
| H | -2.509087 | -1.165420 | -1.519258 |
| C | -1.894074 | 1.304665 | 0.808639 |
| H | -1.838003 | 2.149750 | 0.119131 |
| H | -2.904850 | 1.273625 | 1.221297 |
| H | -1.200131 | 1.490535 | 1.629651 |
| H | 2.399079 | 1.965197 | -1.660109 |
| H | 0.481297 | 3.267635 | 0.466586 |

ax2

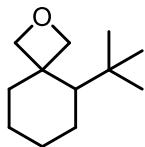
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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.867935 | 0.910579 | -0.034384 |
| C | -0.218285 | 0.049005 | -0.703724 |
| H | -0.499113 | 0.577911 | -1.619370 |
| C | 1.517244 | 1.992709 | -0.863397 |
| C | 0.718467 | 2.404989 | 0.061574 |
| C | 0.427788 | -1.268533 | -1.179020 |
| C | 1.217062 | -2.014232 | -0.105229 |
| H | 1.645984 | -2.923380 | -0.531407 |
| H | 0.557128 | -2.327801 | 0.707560 |
| C | 1.740863 | 0.186476 | 0.992285 |
| C | 2.323215 | -1.116526 | 0.442914 |
| H | 2.890852 | -1.629783 | 1.221313 |
| H | 3.023364 | -0.887136 | -0.366988 |
| C | -1.563016 | -0.075552 | 0.091363 |
| H | -0.316436 | -1.920023 | -1.634221 |
| H | 2.544731 | 0.858679 | 1.296883 |
| H | 1.164038 | -0.043216 | 1.889834 |
| H | 1.130415 | -1.005926 | -1.977161 |
| C | -1.400488 | -0.257689 | 1.604729 |
| H | -0.839892 | -1.156303 | 1.859163 |
| H | -0.901280 | 0.599830 | 2.057759 |
| H | -2.388836 | -0.343299 | 2.062482 |
| C | -2.405339 | -1.237947 | -0.444224 |
| H | -3.401851 | -1.206441 | 0.001262 |
| H | -2.520823 | -1.179299 | -1.528892 |
| H | -1.962999 | -2.205364 | -0.201123 |
| C | -2.366140 | 1.215868 | -0.128947 |
| H | -2.590003 | 1.360221 | -1.187871 |

| | | | |
|---|-----------|----------|-----------|
| H | -3.313111 | 1.169599 | 0.413297 |
| H | -1.824369 | 2.092958 | 0.224833 |
| H | 2.193558 | 2.209260 | -1.672718 |
| H | 0.252809 | 3.224625 | 0.581729 |

eq

```
=====
C  -0.739489    0.917757   -0.178278
C   0.125786   -0.347686   -0.333483
H   0.038925   -0.636394   -1.389795
C  -0.588668    1.856262    0.989473
C  -0.220737    2.327103   -0.154645
C  -0.560584   -1.458488    0.486269
C  -1.986763   -1.727220    0.003250
H  -2.442763   -2.514559    0.606659
H  -1.948858   -2.096900   -1.026462
C  -2.149580    0.670548   -0.712411
C  -2.837574   -0.461592    0.049292
H  -3.831514   -0.651810   -0.360256
H  -2.972966   -0.155913    1.091786
C   1.657348   -0.253856   -0.073669
H   0.010240   -2.385202    0.441587
H  -2.730050    1.591130   -0.635934
H  -2.094088    0.405665   -1.774219
H  -0.593103   -1.153802    1.537055
C   2.010168   -0.052162    1.404464
H   1.602298    0.876303    1.802670
H   1.646021   -0.877548    2.017947
H   3.096168   -0.011988    1.518366
C   2.290487    0.872408   -0.904289
H   3.374553    0.743514   -0.931654
H   1.925419    0.854356   -1.934103
H   2.095592    1.858583   -0.489279
C   2.314698   -1.563033   -0.541974
H   2.081987   -1.763250   -1.590504
H   3.399375   -1.484027   -0.449020
H   2.000150   -2.423214    0.047289
H  -0.717318    1.999401    2.048816
H   0.169385    3.145413   -0.734947
```



5-(*tert*-butyl)-2-oxaspiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -545.644851 | -545.306231 | -545.357863 |
| ax2 | -545.637958 | -545.299191 | -545.350653 |
| eq1 | -545.631981 | -545.293148 | -545.344836 |
| eq2 | -545.635030 | -545.296228 | -545.347911 |
| eq3 | -545.642777 | -545.30407 | -545.355808 |

ax

```

=====
C  -0.377718   -0.048536   -0.701622
H  -0.369065   -0.664892   -1.606560
C  -0.329822    1.412218   -1.193225
C  -0.088723    2.427362   -0.077570
H  -0.077203    3.436616   -0.493601
H  -0.906606    2.394215    0.645591
C   1.312185    0.689920    1.108947
C   1.240362    2.136468    0.617360
H   1.399768    2.819047    1.453635
H   2.050015    2.317401   -0.095848
H   0.503998    1.487935   -1.900709
H   0.649664    0.562273    1.962587
H   2.322882    0.467335    1.461560
H  -1.226366    1.660526   -1.757538
C  -1.692939   -0.481182    0.043073
C   0.962759   -0.317990    0.004537
C   1.359509   -1.752431    0.402896
C   2.177044   -0.460528   -0.942178
H   0.792458   -2.529281   -0.110773
H   1.429007   -1.977636    1.468567
H   1.901533   -0.734025   -1.965093
H   2.908398    0.347943   -0.956760
C  -1.939609   -1.980746   -0.192966
H  -1.932411   -2.221600   -1.257720
H  -1.195307   -2.600964    0.304407
H  -2.914911   -2.262117    0.209577
C  -1.694239   -0.271481    1.562561
H  -2.654177   -0.606693    1.962363
H  -0.915262   -0.861133    2.047973
H  -1.565132    0.771731    1.846711
C  -2.898370    0.266231   -0.541364
H  -2.953570    0.146028   -1.625563
H  -3.818821   -0.134198   -0.112617
H  -2.863643    1.333193   -0.317916
O   2.656514   -1.608441   -0.213121

```

ax2

```

=====
C   0.375894   -0.075050    0.678778

```

| | | | |
|---|-----------|-----------|-----------|
| H | 0.352071 | -0.719242 | 1.564044 |
| C | 0.344307 | 1.381128 | 1.191570 |
| C | -0.012324 | 2.437888 | 0.135306 |
| H | -0.158166 | 3.396148 | 0.637499 |
| H | 0.811776 | 2.579080 | -0.559468 |
| C | -1.235597 | 0.642358 | -1.172644 |
| C | -1.271877 | 2.081148 | -0.654136 |
| H | -2.146082 | 2.202748 | -0.010142 |
| H | -1.400838 | 2.776207 | -1.484860 |
| H | 1.296243 | 1.636100 | 1.660229 |
| H | -0.468731 | 0.530060 | -1.942407 |
| H | -2.192743 | 0.390250 | -1.636169 |
| H | -0.409987 | 1.432104 | 1.983513 |
| C | 1.706789 | -0.473186 | -0.047053 |
| C | -0.960775 | -0.335235 | -0.031433 |
| C | -1.386374 | -1.778046 | -0.367293 |
| C | -2.181258 | -0.403743 | 0.916771 |
| H | -0.830472 | -2.543004 | 0.173613 |
| H | -1.473382 | -2.044245 | -1.420571 |
| H | -1.912787 | -0.627643 | 1.952184 |
| H | -2.904829 | 0.408652 | 0.884868 |
| C | 1.542466 | -1.750367 | -0.876491 |
| H | 1.219423 | -2.591003 | -0.262932 |
| H | 0.828485 | -1.615574 | -1.691223 |
| H | 2.502825 | -2.018280 | -1.321028 |
| C | 2.305038 | 0.600986 | -0.965358 |
| H | 3.217426 | 0.204304 | -1.415269 |
| H | 1.634851 | 0.885458 | -1.775252 |
| H | 2.578747 | 1.497582 | -0.409765 |
| C | 2.749420 | -0.758653 | 1.044083 |
| H | 2.438644 | -1.598100 | 1.668419 |
| H | 3.711194 | -1.008928 | 0.592446 |
| H | 2.899454 | 0.108385 | 1.689467 |
| O | -2.680922 | -1.587053 | 0.251275 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.446069 | 0.249348 | -0.573525 |
| H | -0.492530 | -0.040764 | -1.628942 |
| C | -0.210840 | 1.779607 | -0.528043 |
| C | 1.269274 | 2.141199 | -0.584261 |
| H | 1.722786 | 1.680768 | -1.466062 |
| H | 1.392505 | 3.218106 | -0.700544 |
| C | 1.395080 | 0.325821 | 1.188467 |
| C | 1.974440 | 1.667283 | 0.694510 |
| H | 3.046244 | 1.577009 | 0.516728 |
| H | 1.848870 | 2.420100 | 1.473927 |
| H | -0.750661 | 2.254788 | -1.345716 |
| H | 0.630480 | 0.502870 | 1.943008 |
| H | 2.175914 | -0.271184 | 1.662381 |
| H | -0.623308 | 2.189629 | 0.398308 |
| C | -1.845140 | -0.122910 | 0.017121 |
| C | 0.788035 | -0.463595 | 0.023078 |
| C | 0.785637 | -1.981403 | 0.291157 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.928155 | -0.849325 | -0.948341 |
| H | 0.083087 | -2.538319 | -0.323418 |
| H | 0.740061 | -2.315705 | 1.327900 |
| H | 1.586169 | -0.999740 | -1.975574 |
| H | 2.840342 | -0.254821 | -0.934847 |
| C | -2.269488 | -1.552564 | -0.354350 |
| H | -2.059698 | -1.773865 | -1.402691 |
| H | -1.782063 | -2.303707 | 0.263371 |
| H | -3.343806 | -1.663301 | -0.196262 |
| C | -1.903506 | -0.001798 | 1.542772 |
| H | -2.917280 | -0.221977 | 1.884467 |
| H | -1.231048 | -0.714562 | 2.022875 |
| H | -1.647728 | 1.000607 | 1.888245 |
| C | -2.896311 | 0.818994 | -0.590968 |
| H | -2.864103 | 0.785362 | -1.682736 |
| H | -3.892816 | 0.508670 | -0.273780 |
| H | -2.755820 | 1.852306 | -0.277600 |
| O | 2.109850 | -2.119526 | -0.279840 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.154520 | -0.537827 | -0.359915 |
| H | -0.089785 | -0.847739 | -1.410625 |
| C | 0.487808 | -1.658139 | 0.485563 |
| C | 1.891406 | -2.028253 | 0.014251 |
| H | 2.291730 | -2.831687 | 0.634615 |
| H | 1.839895 | -2.407548 | -1.010873 |
| C | 2.183277 | 0.330803 | -0.737513 |
| C | 2.803455 | -0.811035 | 0.056591 |
| H | 3.794388 | -1.047765 | -0.333024 |
| H | 2.933558 | -0.494679 | 1.096831 |
| H | 0.547132 | -1.327700 | 1.527357 |
| H | 2.120711 | 0.050386 | -1.793979 |
| H | 2.815237 | 1.218726 | -0.677989 |
| H | -0.135598 | -2.548355 | 0.476174 |
| C | -1.696074 | -0.431156 | -0.080836 |
| C | 0.780545 | 0.696856 | -0.248469 |
| C | 0.311545 | 2.058193 | -0.793064 |
| C | 0.745995 | 1.436452 | 1.104192 |
| H | -0.513367 | 2.111751 | -1.493208 |
| H | 1.150230 | 2.643143 | -1.177464 |
| H | 0.249048 | 0.962322 | 1.946506 |
| H | 1.728076 | 1.802225 | 1.413997 |
| C | -2.392865 | 0.632539 | -0.941350 |
| H | -2.200879 | 1.641813 | -0.585229 |
| H | -2.091830 | 0.562599 | -1.988639 |
| H | -3.471983 | 0.476892 | -0.894167 |
| C | -2.335735 | -1.777254 | -0.475447 |
| H | -3.421804 | -1.678177 | -0.467446 |
| H | -2.032418 | -2.076175 | -1.481295 |
| H | -2.081701 | -2.581963 | 0.211728 |
| C | -2.058779 | -0.158650 | 1.384535 |
| H | -1.810650 | 0.858562 | 1.684393 |
| H | -3.136977 | -0.279219 | 1.511268 |

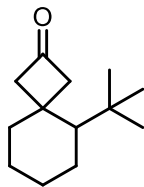
| | | | |
|---|-----------|-----------|----------|
| H | -1.568296 | -0.854789 | 2.065526 |
| O | -0.038883 | 2.516525 | 0.536788 |

eq3

```

=====
C  -0.253639   -0.507957   -0.394879
H  -0.226940   -0.729933   -1.469502
C   0.217061   -1.778479    0.343387
C   1.591359   -2.271986   -0.090487
H   1.846930   -3.183475    0.452813
H   1.577401   -2.523192   -1.155687
C   2.207217    0.084429   -0.568624
C   2.623014   -1.182638    0.161741
H   3.616866   -1.492905   -0.165028
H   2.684598   -0.986731    1.237158
H   0.260005   -1.561950    1.415668
H   2.220007   -0.105769   -1.647615
H   2.924499    0.887787   -0.383122
H  -0.518923   -2.571999    0.215311
C  -1.769800   -0.241398   -0.056454
C   0.806750    0.603151   -0.203147
C   0.643173    1.988040   -0.872851
C   0.810853    1.415213    1.109842
H  -0.285300    2.203443   -1.389745
H   1.479230    2.259684   -1.520727
H  -0.050881    1.281274    1.760713
H   1.726322    1.347049    1.701495
C  -2.604984   -1.178986   -0.943814
H  -2.474302   -0.931225   -1.998933
H  -2.330166   -2.225189   -0.804463
H  -3.665449   -1.079543   -0.703051
C  -2.135294   -0.555070    1.405370
H  -3.184995   -0.303687    1.568057
H  -2.015104   -1.612080    1.638970
H  -1.547310    0.016693    2.122159
C  -2.248967    1.184030   -0.352814
H  -2.134814    1.434630   -1.407492
H  -3.313113    1.251915   -0.117618
H  -1.730322    1.934388    0.245290
O   0.727662    2.667589    0.397717

```



5-(*tert*-butyl)spiro[3.5]nonan-2-one

Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy

| | | | |
|-----|-------------|-------------|-------------|
| ax | -583.766233 | -583.423009 | -583.476576 |
| ax3 | -583.765523 | -583.422175 | -583.475727 |
| ax4 | -583.764070 | -583.420801 | -583.474566 |
| eq | -583.765055 | -583.421855 | -583.475815 |
| eq2 | -583.764476 | -583.421315 | -583.475042 |
| eq3 | -583.764956 | -583.42184 | -583.475524 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.597915 | -0.080581 | -0.707657 |
| H | -0.429095 | -0.660811 | -1.620751 |
| C | -0.952109 | 1.344948 | -1.177431 |
| C | -0.986090 | 2.370899 | -0.046108 |
| H | -1.255109 | 3.350946 | -0.444691 |
| H | -1.755981 | 2.104688 | 0.681491 |
| C | 0.845779 | 1.065796 | 1.103444 |
| C | 0.378061 | 2.444652 | 0.636988 |
| H | 0.351132 | 3.129621 | 1.485976 |
| H | 1.101095 | 2.853246 | -0.074861 |
| H | -0.179333 | 1.655389 | -1.888548 |
| H | 0.250700 | 0.749152 | 1.957942 |
| H | 1.879558 | 1.130585 | 1.458261 |
| H | -1.888566 | 1.347783 | -1.731008 |
| C | -1.748606 | -0.857889 | 0.033965 |
| C | 0.775805 | 0.008202 | -0.009833 |
| C | 1.484591 | -1.306364 | 0.445309 |
| C | 1.966571 | 0.258945 | -1.002091 |
| H | 1.160234 | -2.168048 | -0.138892 |
| H | 1.513208 | -1.555678 | 1.504987 |
| H | 1.756685 | -0.134677 | -1.999147 |
| H | 2.391743 | 1.258093 | -1.076637 |
| C | -1.613858 | -2.364284 | -0.248775 |
| H | -1.565361 | -2.562269 | -1.321298 |
| H | -0.731329 | -2.795471 | 0.220238 |
| H | -2.481775 | -2.892599 | 0.151244 |
| C | -1.782530 | -0.694369 | 1.558764 |
| H | -2.614392 | -1.280696 | 1.956110 |
| H | -0.869170 | -1.067486 | 2.023123 |
| H | -1.930803 | 0.338850 | 1.869154 |
| C | -3.116266 | -0.430727 | -0.516374 |
| H | -3.159684 | -0.537450 | -1.602453 |
| H | -3.894192 | -1.064503 | -0.086813 |
| H | -3.353552 | 0.603610 | -0.265135 |
| C | 2.743526 | -0.760781 | -0.195053 |
| O | 3.915281 | -0.974120 | -0.038648 |

ax3

| | | | |
|---|----------|-----------|----------|
| C | 0.589030 | -0.108595 | 0.671708 |
| H | 0.405931 | -0.720945 | 1.561346 |
| C | 0.921400 | 1.314561 | 1.175705 |
| C | 0.833720 | 2.422416 | 0.114251 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.666165 | 2.351752 | -0.581606 |
| H | 0.932444 | 3.389239 | 0.612253 |
| C | -0.806517 | 0.982267 | -1.175587 |
| C | -0.475117 | 2.388734 | -0.675285 |
| H | -1.290532 | 2.740116 | -0.039066 |
| H | -0.420009 | 3.081371 | -1.516722 |
| H | 0.212281 | 1.555928 | 1.972963 |
| H | -0.098473 | 0.672175 | -1.948195 |
| H | -1.797050 | 0.981303 | -1.641098 |
| H | 1.910934 | 1.329809 | 1.635249 |
| C | 1.796160 | -0.821889 | -0.034984 |
| C | -0.780591 | -0.033983 | -0.032644 |
| C | -1.514898 | -1.355792 | -0.430726 |
| C | -1.961204 | 0.264610 | 0.962568 |
| H | -1.179668 | -2.206869 | 0.163212 |
| H | -1.572459 | -1.632442 | -1.481766 |
| H | -1.736371 | -0.093360 | 1.970103 |
| H | -2.385264 | 1.264867 | 1.012119 |
| C | 1.362845 | -2.046487 | -0.847007 |
| H | 0.824599 | -2.771005 | -0.236010 |
| H | 0.734280 | -1.770600 | -1.694409 |
| H | 2.250686 | -2.545065 | -1.241463 |
| C | 2.634892 | 0.067448 | -0.963674 |
| H | 3.426859 | -0.540124 | -1.406788 |
| H | 2.051615 | 0.493368 | -1.779207 |
| H | 3.115296 | 0.879945 | -0.419203 |
| C | 2.735104 | -1.320626 | 1.075510 |
| H | 2.234699 | -2.058102 | 1.705985 |
| H | 3.618268 | -1.792150 | 0.639832 |
| H | 3.075534 | -0.503751 | 1.713687 |
| C | -2.755639 | -0.779954 | 0.211903 |
| O | -3.931860 | -0.992714 | 0.086045 |

ax4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.367119 | 1.571297 | 1.167062 |
| H | -1.266042 | 1.957677 | 1.654070 |
| C | 0.333566 | 2.688240 | 0.399392 |
| C | 1.507844 | 2.132068 | -0.399992 |
| H | 1.985088 | 2.926798 | -0.976370 |
| H | 2.262844 | 1.736389 | 0.284698 |
| C | 0.365382 | -0.161619 | -0.616192 |
| C | 1.016925 | 1.034407 | -1.341477 |
| H | 1.819142 | 0.692984 | -1.991442 |
| H | 0.264975 | 1.477035 | -2.001297 |
| H | -0.375707 | 3.154713 | -0.292167 |
| H | -0.122844 | -0.749015 | -1.402066 |
| H | 0.663089 | 3.465340 | 1.090947 |
| C | -0.783366 | 0.406739 | 0.264878 |
| C | -1.686162 | -0.646527 | 0.990550 |
| C | -2.008239 | 0.758364 | -0.656770 |
| H | -2.136097 | -0.198428 | 1.880544 |
| H | -1.318619 | -1.635326 | 1.238890 |
| H | -2.559626 | 1.628622 | -0.294279 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.852939 | 0.838306 | -1.731007 |
| C | 1.374978 | -1.173050 | 0.051118 |
| H | 0.288262 | 1.212582 | 1.960687 |
| C | 1.602752 | -0.958075 | 1.553045 |
| H | 2.268173 | -1.739643 | 1.926347 |
| H | 2.077804 | 0.001468 | 1.756960 |
| H | 0.678378 | -1.010628 | 2.127747 |
| C | 0.857614 | -2.606051 | -0.167516 |
| H | -0.134130 | -2.771843 | 0.247383 |
| H | 0.809371 | -2.831361 | -1.234856 |
| H | 1.536121 | -3.324958 | 0.296380 |
| C | 2.752020 | -1.121942 | -0.627800 |
| H | 3.387997 | -1.901308 | -0.203274 |
| H | 2.676984 | -1.304275 | -1.701174 |
| H | 3.252573 | -0.165380 | -0.476172 |
| C | -2.651149 | -0.521429 | -0.166023 |
| O | -3.511883 | -1.234286 | -0.607775 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.247044 | -0.734223 | -0.345196 |
| H | -0.486224 | -1.054145 | -1.367539 |
| C | -1.269671 | -1.411453 | 0.591610 |
| C | -2.717704 | -1.161662 | 0.177513 |
| H | -2.888539 | -1.590862 | -0.814770 |
| H | -3.393316 | -1.670698 | 0.867288 |
| C | -2.000657 | 1.034034 | -0.754741 |
| C | -3.011851 | 0.330829 | 0.139043 |
| H | -2.943721 | 0.739228 | 1.152683 |
| H | -4.026016 | 0.522488 | -0.215445 |
| H | -1.096802 | -2.483827 | 0.629942 |
| H | -2.120786 | 0.686861 | -1.786598 |
| H | -2.182143 | 2.111181 | -0.756569 |
| H | -1.127739 | -1.033730 | 1.608667 |
| C | 1.202259 | -1.288928 | -0.096558 |
| C | -0.547838 | 0.792352 | -0.329380 |
| C | -0.161176 | 1.531563 | 0.996750 |
| C | 0.420658 | 1.744825 | -1.105031 |
| H | 0.061480 | 0.961022 | 1.894309 |
| H | -0.883997 | 2.316048 | 1.233866 |
| H | 1.076829 | 1.375317 | -1.884305 |
| H | -0.143981 | 2.598831 | -1.487940 |
| C | 1.726426 | -1.077851 | 1.330569 |
| H | 1.967074 | -0.035320 | 1.534762 |
| H | 1.017545 | -1.424354 | 2.083390 |
| H | 2.648156 | -1.650049 | 1.458951 |
| C | 1.175492 | -2.808585 | -0.359083 |
| H | 2.197213 | -3.188840 | -0.393206 |
| H | 0.654804 | -3.361165 | 0.420790 |
| H | 0.700188 | -3.035403 | -1.316274 |
| C | 2.242226 | -0.715512 | -1.071774 |
| H | 2.526936 | 0.306522 | -0.833184 |
| H | 3.151675 | -1.316273 | -1.015266 |
| H | 1.885658 | -0.748603 | -2.103513 |

| | | | |
|---|----------|----------|----------|
| C | 1.010579 | 2.124585 | 0.237191 |
| O | 2.059440 | 2.601991 | 0.578060 |

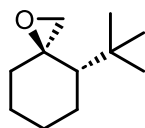
eq2

| | | | |
|---|-----------|-----------|-----------|
| C | -0.766647 | 0.344659 | -0.378438 |
| H | -0.941655 | 0.576856 | -1.436870 |
| C | -1.142482 | 1.602411 | 0.433190 |
| C | -0.407155 | 2.862820 | -0.004676 |
| H | -0.739496 | 3.713396 | 0.593088 |
| H | -0.646327 | 3.088096 | -1.048686 |
| C | 1.507020 | 1.424970 | -0.657159 |
| C | 1.092593 | 2.651780 | 0.139443 |
| H | 1.337669 | 2.509973 | 1.196585 |
| H | 1.651219 | 3.523815 | -0.204515 |
| H | -2.218225 | 1.767155 | 0.381133 |
| H | 1.323322 | 1.612980 | -1.720217 |
| H | 2.582382 | 1.250559 | -0.553955 |
| H | -0.905313 | 1.419937 | 1.485986 |
| C | -1.774295 | -0.814441 | -0.032333 |
| C | 0.763113 | 0.129038 | -0.276579 |
| C | 1.363461 | -0.449592 | 1.045720 |
| C | 1.488915 | -1.002054 | -1.085452 |
| H | 0.680736 | -1.108878 | 1.581085 |
| H | 1.836785 | 0.237109 | 1.746544 |
| H | 0.891965 | -1.858655 | -1.375624 |
| H | 2.078575 | -0.671512 | -1.940423 |
| C | -2.145953 | -0.874335 | 1.459509 |
| H | -1.278184 | -0.982420 | 2.109256 |
| H | -2.694195 | 0.011383 | 1.778207 |
| H | -2.793336 | -1.736760 | 1.629585 |
| C | -3.068502 | -0.542224 | -0.817604 |
| H | -3.828820 | -1.280392 | -0.554517 |
| H | -3.478642 | 0.445344 | -0.605490 |
| H | -2.889444 | -0.611609 | -1.892356 |
| C | -1.307863 | -2.213855 | -0.446881 |
| H | -0.443009 | -2.553950 | 0.123813 |
| H | -2.117798 | -2.922059 | -0.260408 |
| H | -1.072919 | -2.262567 | -1.510728 |
| C | 2.281072 | -1.288454 | 0.176947 |
| O | 3.295632 | -1.894018 | 0.393049 |

eq3

| | | | |
|---|-----------|----------|-----------|
| C | 0.780121 | 0.437544 | 0.262631 |
| H | 1.001013 | 0.815864 | 1.269168 |
| C | 0.889852 | 1.659130 | -0.670141 |
| C | 0.097459 | 2.844903 | -0.113041 |
| H | 0.181177 | 3.701138 | -0.784778 |
| H | 0.551542 | 3.141199 | 0.837709 |
| C | -1.514561 | 1.203043 | 0.911278 |
| C | -1.369635 | 2.498784 | 0.117241 |
| H | -1.868090 | 2.390310 | -0.849255 |
| H | -1.876728 | 3.312266 | 0.638877 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.925585 | 1.968802 | -0.782357 |
| H | -1.164488 | 1.351743 | 1.937146 |
| H | -2.570965 | 0.924240 | 0.974999 |
| H | 0.524409 | 1.398040 | -1.669227 |
| C | 1.862604 | -0.667890 | 0.032015 |
| C | -0.717340 | 0.041748 | 0.291196 |
| C | -1.431091 | -0.367031 | -1.047040 |
| C | -1.219117 | -1.291509 | 0.933678 |
| H | -0.781315 | -0.851212 | -1.773041 |
| H | -2.042753 | 0.378936 | -1.550909 |
| H | -0.513537 | -2.115800 | 0.860046 |
| H | -1.638447 | -1.252445 | 1.938302 |
| C | 1.546223 | -1.637288 | -1.111768 |
| H | 0.679796 | -2.266311 | -0.909569 |
| H | 1.373757 | -1.102698 | -2.047780 |
| H | 2.399740 | -2.301073 | -1.266370 |
| C | 3.218880 | -0.020419 | -0.292700 |
| H | 4.001694 | -0.778894 | -0.233279 |
| H | 3.244102 | 0.401093 | -1.297494 |
| H | 3.463704 | 0.770810 | 0.419237 |
| C | 2.083574 | -1.450565 | 1.337683 |
| H | 1.175696 | -1.885331 | 1.747482 |
| H | 2.795658 | -2.261580 | 1.171548 |
| H | 2.502855 | -0.790862 | 2.100595 |
| C | -2.182238 | -1.399820 | -0.230879 |
| O | -3.204099 | -2.006501 | -0.406496 |



(3R,4S)-4-(*tert*-butyl)-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -506.349117 | -506.0415 | -506.091188 |
| ax2 | -506.347485 | -506.039542 | -506.089507 |
| eq2 | -506.346617 | -506.038943 | -506.088564 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.876239 | 0.827040 | 0.023939 |
| C | -0.259515 | 0.088249 | -0.668462 |
| H | -0.481065 | 0.697305 | -1.549510 |
| C | 0.962657 | 2.286850 | -0.049786 |
| C | 0.291192 | -1.262465 | -1.175847 |
| C | 1.119958 | -2.052734 | -0.152900 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.567891 | -2.911890 | -0.655933 |
| H | 0.482660 | -2.451588 | 0.635403 |
| C | 1.629142 | 0.075698 | 1.093536 |
| C | 2.215735 | -1.198664 | 0.483571 |
| H | 2.749655 | -1.771178 | 1.243049 |
| H | 2.945985 | -0.912667 | -0.278348 |
| C | -1.613567 | 0.003709 | 0.108182 |
| H | 1.505918 | 2.824963 | 0.719419 |
| H | 0.185448 | 2.844698 | -0.558133 |
| H | -0.523822 | -1.882484 | -1.552695 |
| H | 2.417615 | 0.716109 | 1.490811 |
| H | 0.956277 | -0.171929 | 1.917122 |
| H | 0.938098 | -1.048209 | -2.030888 |
| C | -1.717742 | -1.163161 | 1.097157 |
| H | -1.646092 | -2.125677 | 0.590084 |
| H | -0.955466 | -1.124919 | 1.874342 |
| H | -2.692045 | -1.123308 | 1.588831 |
| C | -2.728235 | -0.176656 | -0.932120 |
| H | -3.696630 | -0.270937 | -0.436938 |
| H | -2.773763 | 0.680769 | -1.606242 |
| H | -2.573581 | -1.073728 | -1.533909 |
| C | -1.885455 | 1.305116 | 0.869580 |
| H | -1.863657 | 2.168526 | 0.203182 |
| H | -2.875492 | 1.261132 | 1.327798 |
| H | -1.155058 | 1.468877 | 1.664173 |
| O | 1.768083 | 1.476032 | -0.904090 |

ax2

```
=====
```

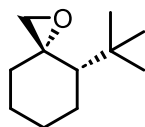
| | | | |
|---|-----------|-----------|-----------|
| C | 0.858288 | 0.839313 | 0.016017 |
| C | -0.254776 | 0.065166 | -0.679776 |
| H | -0.496866 | 0.647706 | -1.573214 |
| C | 0.885478 | 2.305969 | -0.022566 |
| C | 0.359681 | -1.256356 | -1.187716 |
| C | 1.120726 | -2.053290 | -0.127534 |
| H | 1.551577 | -2.944656 | -0.587216 |
| H | 0.442887 | -2.400859 | 0.654490 |
| C | 1.668030 | 0.102420 | 1.062115 |
| C | 2.229625 | -1.199329 | 0.486292 |
| H | 2.758699 | -1.750865 | 1.264532 |
| H | 2.960082 | -0.957452 | -0.290935 |
| C | -1.607387 | -0.029359 | 0.101705 |
| H | 1.420027 | 2.847130 | 0.750557 |
| H | 0.082134 | 2.845401 | -0.509104 |
| H | -0.398114 | -1.873408 | -1.666605 |
| H | 2.475489 | 0.756691 | 1.393654 |
| H | 1.049893 | -0.121221 | 1.930170 |
| H | 1.074774 | -0.987057 | -1.971119 |
| C | -1.493371 | -0.405440 | 1.584259 |
| H | -0.975815 | -1.350121 | 1.742267 |
| H | -0.982012 | 0.369924 | 2.155524 |
| H | -2.498678 | -0.505710 | 1.999713 |
| C | -2.520905 | -1.051520 | -0.584017 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.526833 | -0.984087 | -0.165950 |
| H | -2.588351 | -0.866301 | -1.658516 |
| H | -2.168223 | -2.072985 | -0.435980 |
| C | -2.306250 | 1.337041 | 0.041012 |
| H | -2.449639 | 1.663402 | -0.991143 |
| H | -3.287853 | 1.272431 | 0.514610 |
| H | -1.736973 | 2.102678 | 0.567631 |
| O | 1.707371 | 1.547708 | -0.907764 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.748668 | 0.828025 | -0.148257 |
| C | 0.156248 | -0.396372 | -0.275394 |
| H | 0.055818 | -0.721906 | -1.318716 |
| C | -0.744442 | 1.748113 | 0.996586 |
| C | -0.522912 | -1.490610 | 0.570895 |
| C | -1.935174 | -1.782800 | 0.050313 |
| H | -2.413897 | -2.536722 | 0.677437 |
| H | -1.849182 | -2.211694 | -0.952694 |
| C | -2.101768 | 0.593360 | -0.783440 |
| C | -2.807567 | -0.529799 | -0.018414 |
| H | -3.766937 | -0.760689 | -0.483215 |
| H | -3.017402 | -0.179884 | 0.996617 |
| C | 1.689274 | -0.231066 | -0.079412 |
| H | -0.022136 | 1.655811 | 1.793377 |
| H | -1.678214 | 2.229494 | 1.266642 |
| H | 0.056069 | -2.411572 | 0.540407 |
| H | -2.683753 | 1.514932 | -0.747833 |
| H | -1.974289 | 0.313335 | -1.832613 |
| H | -0.569122 | -1.169291 | 1.616190 |
| C | 2.101219 | 0.431433 | 1.239224 |
| H | 1.912363 | 1.503885 | 1.226409 |
| H | 1.585362 | -0.008771 | 2.094818 |
| H | 3.173531 | 0.291068 | 1.392180 |
| C | 2.255091 | 0.588922 | -1.246974 |
| H | 3.332760 | 0.718630 | -1.124875 |
| H | 2.086224 | 0.073526 | -2.195433 |
| H | 1.794612 | 1.573091 | -1.301823 |
| C | 2.348498 | -1.617324 | -0.136441 |
| H | 1.984894 | -2.196083 | -0.988762 |
| H | 3.428454 | -1.501108 | -0.243910 |
| H | 2.168086 | -2.194598 | 0.770608 |
| O | -0.217755 | 2.145907 | -0.274615 |



(3S,4S)-4-(*tert*-butyl)-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -506.347988 | -506.040362 | -506.089876 |
| ax2 | -506.346925 | -506.038984 | -506.088514 |
| eq1 | -506.347191 | -506.039359 | -506.088931 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | -0.910996 | 0.799749 | 0.018574 |
| C | 0.250259 | 0.085206 | 0.690715 |
| H | 0.484948 | 0.688719 | 1.572066 |
| C | -1.726693 | 1.707625 | 0.839032 |
| C | -0.291069 | -1.270550 | 1.197559 |
| C | -1.106074 | -2.070780 | 0.170528 |
| H | -1.555290 | -2.928726 | 0.674443 |
| H | -0.456619 | -2.472644 | -0.605611 |
| C | -1.623268 | 0.055862 | -1.082816 |
| C | -2.200641 | -1.232215 | -0.490304 |
| H | -2.705796 | -1.813081 | -1.262912 |
| H | -2.954642 | -0.962459 | 0.255405 |
| C | 1.596566 | 0.009396 | -0.100122 |
| H | -1.451307 | 1.890085 | 1.871426 |
| H | -2.772906 | 1.849605 | 0.592418 |
| H | 0.529330 | -1.882052 | 1.576824 |
| H | -2.413704 | 0.688923 | -1.487845 |
| H | -0.933452 | -0.174570 | -1.897290 |
| H | -0.943024 | -1.061912 | 2.050841 |
| C | 1.719457 | -1.176264 | -1.064771 |
| H | 1.671576 | -2.129912 | -0.538184 |
| H | 0.952797 | -1.170284 | -1.838288 |
| H | 2.690156 | -1.125288 | -1.562723 |
| C | 2.722942 | -0.126131 | 0.934507 |
| H | 3.688534 | -0.220298 | 0.433823 |
| H | 2.762099 | 0.750204 | 1.584329 |
| H | 2.585508 | -1.008537 | 1.562250 |
| C | 1.832325 | 1.299214 | -0.891882 |
| H | 1.769626 | 2.177182 | -0.249005 |
| H | 2.825556 | 1.273229 | -1.345274 |
| H | 1.098584 | 1.418532 | -1.690780 |
| O | -0.806104 | 2.215827 | -0.127755 |

ax2

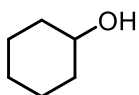
| | | | |
|---|-----------|-----------|-----------|
| C | 0.877226 | 0.829339 | -0.057541 |
| C | -0.241662 | 0.029418 | -0.717109 |
| H | -0.514976 | 0.572645 | -1.625563 |
| C | 1.524685 | 1.892447 | -0.840940 |
| C | 0.382958 | -1.298294 | -1.194062 |
| C | 1.145396 | -2.058331 | -0.110427 |
| H | 1.552871 | -2.980099 | -0.529234 |
| H | 0.469927 | -2.348546 | 0.698070 |
| C | 1.727356 | 0.130039 | 0.984146 |
| C | 2.274869 | -1.191384 | 0.442890 |
| H | 2.819991 | -1.714926 | 1.229176 |
| H | 2.987173 | -0.984759 | -0.361764 |
| C | -1.576969 | -0.061208 | 0.098978 |
| H | 1.164436 | 2.117191 | -1.838002 |
| H | 2.558877 | 2.146132 | -0.638529 |
| H | -0.375334 | -1.929892 | -1.652306 |
| H | 2.539354 | 0.799570 | 1.271015 |
| H | 1.138747 | -0.065357 | 1.879110 |
| H | 1.095284 | -1.049556 | -1.987633 |
| C | -1.400659 | -0.187236 | 1.616443 |
| H | -0.846660 | -1.081069 | 1.900945 |
| H | -0.892267 | 0.683702 | 2.032091 |
| H | -2.386349 | -0.247195 | 2.083139 |
| C | -2.423018 | -1.242330 | -0.386450 |
| H | -3.410267 | -1.198732 | 0.077744 |
| H | -2.560489 | -1.215795 | -1.469589 |
| H | -1.972470 | -2.200704 | -0.123078 |
| C | -2.376643 | 1.224637 | -0.162849 |
| H | -2.625796 | 1.316270 | -1.222239 |
| H | -3.310431 | 1.210594 | 0.403307 |
| H | -1.807243 | 2.105740 | 0.130066 |
| O | 0.611799 | 2.207774 | 0.213099 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.737091 | 0.848584 | -0.221962 |
| C | 0.170103 | -0.377730 | -0.337289 |
| H | 0.088502 | -0.694851 | -1.384264 |
| C | -0.318710 | 2.247205 | -0.057229 |
| C | -0.501552 | -1.480304 | 0.505469 |
| C | -1.918034 | -1.783116 | 0.010171 |
| H | -2.369028 | -2.559525 | 0.630563 |
| H | -1.855668 | -2.183427 | -1.006745 |
| C | -2.126234 | 0.594961 | -0.774622 |
| C | -2.796506 | -0.535818 | 0.005126 |
| H | -3.777222 | -0.756670 | -0.418496 |
| H | -2.956520 | -0.202664 | 1.034036 |
| C | 1.695133 | -0.211845 | -0.086117 |
| H | -0.992775 | 3.025623 | -0.398853 |
| H | 0.722123 | 2.529860 | -0.008957 |
| H | 0.084905 | -2.395577 | 0.467622 |
| H | -2.712517 | 1.511742 | -0.703955 |
| H | -2.047708 | 0.327739 | -1.831628 |
| H | -0.538408 | -1.160346 | 1.550934 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.034265 | 0.405062 | 1.276675 |
| H | 1.747622 | 1.450793 | 1.356259 |
| H | 1.541014 | -0.137422 | 2.084413 |
| H | 3.112356 | 0.340024 | 1.441158 |
| C | 2.318846 | 0.609718 | -1.224293 |
| H | 3.379173 | 0.779229 | -1.026312 |
| H | 2.239850 | 0.063204 | -2.166956 |
| H | 1.846322 | 1.578728 | -1.366085 |
| C | 2.368905 | -1.593393 | -0.139888 |
| H | 2.041846 | -2.160818 | -1.014309 |
| H | 3.450873 | -1.465593 | -0.206960 |
| H | 2.163480 | -2.186406 | 0.750862 |
| O | -0.787873 | 1.494551 | 1.060178 |



cyclohexanol

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -311.062057 | -310.878736 | -310.916784 |
| ax2 | -311.062032 | -310.878622 | -310.916642 |
| eq | -311.063428 | -310.880109 | -310.91815 |
| eq2 | -311.063410 | -310.880074 | -310.918178 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.350132 | 1.238662 | 0.613910 |
| C | -1.153151 | -0.046464 | 0.425892 |
| H | -1.957943 | -0.079163 | 1.166826 |
| C | -0.273839 | -1.278882 | 0.590069 |
| C | 0.955288 | -1.230933 | -0.317930 |
| H | 1.579670 | -2.107880 | -0.139255 |
| H | 0.634260 | -1.271995 | -1.361434 |
| C | 0.878212 | 1.284733 | -0.294864 |
| C | 1.756395 | 0.050589 | -0.088050 |
| H | 2.618856 | 0.083180 | -0.755982 |
| H | 2.143795 | 0.053293 | 0.936204 |
| H | 0.045842 | -1.328375 | 1.634569 |
| H | 0.555125 | 1.323717 | -1.338210 |
| H | 1.447463 | 2.195424 | -0.102007 |
| H | -0.870313 | -2.170607 | 0.389944 |
| H | -0.999290 | 2.099614 | 0.433224 |
| H | -0.034987 | 1.292124 | 1.660080 |
| O | -1.725409 | -0.110988 | -0.883933 |
| H | -2.235853 | 0.692342 | -1.026656 |

ax2

```

=====
C  -0.322327      1.259319      0.605078
C  -1.166753     -0.000120      0.417541
H  -1.979042     -0.000099      1.144695
C  -0.322194     -1.259379      0.604991
C   0.915102     -1.259143     -0.295552
H   1.509857     -2.153327     -0.104573
H   0.613154     -1.311499     -1.347139
C   0.914921      1.259233     -0.295522
C   1.753565      0.000111     -0.074699
H   2.620107      0.000168     -0.737721
H   2.133703      0.000105      0.951807
H  -0.003541     -1.303742      1.650189
H   0.612919      1.311537     -1.347097
H   1.509561      2.153513     -0.104606
H  -0.942283     -2.136660      0.414254
H  -0.942648      2.136421      0.414328
H  -0.003674      1.303605      1.650263
O  -1.825691     -0.000017     -0.851485
H  -1.156463     -0.000010     -1.543538

```

eq

```

=====
C  -0.308325     -1.264869     -0.181889
C  -1.023430     -0.021469      0.316905
H  -0.994474     -0.017755      1.414149
C  -0.343997      1.242399     -0.193329
C   1.129708      1.274149      0.214195
H   1.605810      2.174012     -0.177436
H   1.201311      1.324803      1.305035
C   1.167023     -1.244999      0.220046
C   1.858340      0.023990     -0.278733
H   2.899176      0.039962      0.048621
H   1.865568      0.021989     -1.373160
H  -0.428386      1.258415     -1.284322
H   1.243776     -1.289307      1.310783
H   1.669796     -2.131164     -0.169509
H  -0.868667      2.121310      0.190275
H  -0.806300     -2.152708      0.211283
H  -0.395050     -1.294246     -1.272448
O  -2.379633     -0.101502     -0.118371
H  -2.831405      0.701497      0.160526

```

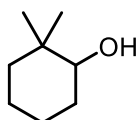
eq2

```

=====
C   0.329540      1.255597     -0.169525
C   1.027424     -0.000124      0.337452
H   1.005012     -0.000206      1.430637
C   0.330016     -1.255726     -0.169639
C  -1.151157     -1.258925      0.211708
H  -1.635943     -2.152978     -0.182731
H  -1.239746     -1.303190      1.301583
C  -1.151526      1.258974      0.211467
C  -1.853466     -0.000140     -0.296214

```

| | | | |
|---|-----------|-----------|-----------|
| H | -2.899546 | -0.000386 | 0.014204 |
| H | -1.843163 | -0.000166 | -1.390656 |
| H | 0.426707 | -1.284976 | -1.261139 |
| H | -1.240734 | 1.303644 | 1.301238 |
| H | -1.636227 | 2.152803 | -0.183618 |
| H | 0.836941 | -2.136641 | 0.227585 |
| H | 0.836971 | 2.136138 | 0.227849 |
| H | 0.426523 | 1.284737 | -1.261009 |
| O | 2.412538 | 0.000629 | -0.001558 |
| H | 2.477914 | -0.001738 | -0.962973 |



2,2-dimethylcyclohexan-1-ol

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -389.676572 | -389.434581 | -389.478199 |
| ax2 | -389.676683 | -389.43462 | -389.478202 |
| ax3 | -389.677087 | -389.434954 | -389.478348 |
| eq | -389.677641 | -389.435687 | -389.479444 |
| eq2 | -389.678184 | -389.436127 | -389.479712 |
| eq3 | -389.678073 | -389.43603 | -389.479604 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.898603 | -0.231971 | 0.051513 |
| C | 0.097081 | 1.008175 | 0.486028 |
| H | 0.636398 | 1.487003 | 1.312100 |
| C | -1.320924 | 0.664302 | 0.940305 |
| C | -2.085566 | -0.118681 | -0.126915 |
| H | -3.078491 | -0.377946 | 0.243531 |
| H | -2.227004 | 0.514746 | -1.006157 |
| C | 0.096184 | -1.026582 | -0.993725 |
| C | -1.320082 | -1.376960 | -0.534705 |
| H | -1.848249 | -1.894385 | -1.337480 |
| H | -1.280802 | -2.068597 | 0.310836 |
| H | -1.270415 | 0.084489 | 1.864209 |
| H | 0.031032 | -0.426827 | -1.905604 |
| H | 0.651095 | -1.933895 | -1.246683 |
| H | -1.843989 | 1.592919 | 1.184984 |
| C | 1.195989 | -1.097212 | 1.281117 |
| H | 1.796298 | -1.960557 | 0.987852 |
| H | 1.765486 | -0.529289 | 2.020080 |
| H | 0.295892 | -1.469289 | 1.767700 |
| C | 2.233714 | 0.202759 | -0.555172 |
| H | 2.805167 | 0.805126 | 0.155305 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.831689 | -0.674679 | -0.810277 |
| H | 2.085747 | 0.792182 | -1.458517 |
| O | 0.053284 | 1.910934 | -0.622199 |
| H | -0.546124 | 2.628535 | -0.394960 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.895615 | -0.241395 | 0.050217 |
| C | 0.111488 | 1.013319 | 0.494220 |
| H | 0.659608 | 1.483896 | 1.313512 |
| C | -1.307866 | 0.681221 | 0.956316 |
| C | -2.088656 | -0.085523 | -0.113064 |
| H | -3.082616 | -0.333152 | 0.261634 |
| H | -2.243712 | 0.551250 | -0.990728 |
| C | 0.076711 | -1.017949 | -0.997174 |
| C | -1.343174 | -1.351123 | -0.536075 |
| H | -1.881817 | -1.854903 | -1.340272 |
| H | -1.309079 | -2.048680 | 0.304347 |
| H | -1.260248 | 0.084070 | 1.868891 |
| H | 0.017468 | -0.420691 | -1.914403 |
| H | 0.618120 | -1.929699 | -1.261881 |
| H | -1.814441 | 1.613965 | 1.208905 |
| C | 1.180969 | -1.119937 | 1.273472 |
| H | 1.772278 | -1.988383 | 0.976633 |
| H | 1.755570 | -0.561967 | 2.016201 |
| H | 0.276300 | -1.484406 | 1.756934 |
| C | 2.235608 | 0.173417 | -0.557509 |
| H | 2.816623 | 0.766198 | 0.153095 |
| H | 2.820291 | -0.711806 | -0.816199 |
| H | 2.097845 | 0.767987 | -1.459538 |
| O | 0.076808 | 2.011027 | -0.527894 |
| H | -0.420826 | 1.665927 | -1.276389 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.880798 | -0.262809 | 0.054717 |
| C | 0.115716 | 1.004809 | 0.495584 |
| H | 0.663811 | 1.456544 | 1.330977 |
| C | -1.312567 | 0.705483 | 0.936261 |
| C | -2.094095 | -0.048059 | -0.140231 |
| H | -3.098417 | -0.273295 | 0.221916 |
| H | -2.204937 | 0.592631 | -1.018294 |
| C | 0.058205 | -1.026531 | -0.996558 |
| C | -1.370083 | -1.331931 | -0.543913 |
| H | -1.910675 | -1.832265 | -1.349249 |
| H | -1.356465 | -2.024180 | 0.302065 |
| H | -1.286159 | 0.115874 | 1.854331 |
| H | 0.013496 | -0.419240 | -1.905096 |
| H | 0.585012 | -1.948990 | -1.254982 |
| H | -1.801992 | 1.650560 | 1.177009 |
| C | 1.150128 | -1.138968 | 1.283134 |
| H | 1.718487 | -2.024044 | 0.990929 |
| H | 1.740278 | -0.591327 | 2.021416 |
| H | 0.237024 | -1.476660 | 1.770324 |

| | | | |
|---|----------|-----------|-----------|
| C | 2.232655 | 0.129031 | -0.546637 |
| H | 2.806421 | 0.749926 | 0.146651 |
| H | 2.821664 | -0.764954 | -0.759479 |
| H | 2.120338 | 0.671555 | -1.486975 |
| O | 0.011252 | 1.961488 | -0.560851 |
| H | 0.897560 | 2.239808 | -0.808883 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.684216 | -0.524269 | -0.015661 |
| C | 0.316852 | 0.918110 | -0.398747 |
| H | 0.235231 | 0.945940 | -1.493925 |
| C | -1.016261 | 1.372242 | 0.184680 |
| C | -2.149417 | 0.440751 | -0.242989 |
| H | -3.090670 | 0.763574 | 0.203758 |
| H | -2.273341 | 0.502016 | -1.328628 |
| C | -0.486333 | -1.434694 | -0.430718 |
| C | -1.835992 | -1.004069 | 0.142472 |
| H | -2.619256 | -1.669874 | -0.223828 |
| H | -1.828227 | -1.096782 | 1.231321 |
| H | -0.940963 | 1.399822 | 1.274400 |
| H | -0.554637 | -1.431428 | -1.523908 |
| H | -0.252312 | -2.459764 | -0.132555 |
| H | -1.215892 | 2.393621 | -0.150162 |
| C | 0.965274 | -0.651868 | 1.484800 |
| H | 1.225200 | -1.685671 | 1.721930 |
| H | 1.802807 | -0.016846 | 1.772726 |
| H | 0.108550 | -0.376172 | 2.098389 |
| C | 1.936226 | -0.948749 | -0.785441 |
| H | 2.795480 | -0.339694 | -0.504677 |
| H | 2.174762 | -1.993223 | -0.573686 |
| H | 1.783169 | -0.848594 | -1.862297 |
| O | 1.378442 | 1.778544 | 0.010361 |
| H | 1.135175 | 2.680008 | -0.222120 |

eq2

```
=====
```

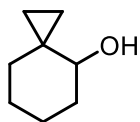
| | | | |
|---|-----------|-----------|-----------|
| C | 0.683877 | -0.522682 | -0.020367 |
| C | 0.317590 | 0.920735 | -0.424009 |
| H | 0.252963 | 0.943141 | -1.516197 |
| C | -1.020876 | 1.381424 | 0.143252 |
| C | -2.153639 | 0.432079 | -0.244305 |
| H | -3.091416 | 0.765006 | 0.202575 |
| H | -2.288409 | 0.462595 | -1.329959 |
| C | -0.490646 | -1.440053 | -0.407128 |
| C | -1.832281 | -1.000651 | 0.176222 |
| H | -2.619227 | -1.677587 | -0.160551 |
| H | -1.807302 | -1.064595 | 1.267027 |
| H | -0.947441 | 1.444000 | 1.233677 |
| H | -0.573070 | -1.449488 | -1.499428 |
| H | -0.252705 | -2.461734 | -0.100183 |
| H | -1.220486 | 2.390134 | -0.222124 |
| C | 0.978250 | -0.624702 | 1.480096 |
| H | 1.196292 | -1.661916 | 1.742066 |

| | | | |
|---|----------|-----------|-----------|
| H | 1.855128 | -0.031896 | 1.748289 |
| H | 0.144621 | -0.294966 | 2.099317 |
| C | 1.928362 | -0.962198 | -0.792207 |
| H | 2.783184 | -0.330455 | -0.549952 |
| H | 2.185547 | -1.994154 | -0.543842 |
| H | 1.757204 | -0.906711 | -1.869507 |
| O | 1.349706 | 1.850733 | -0.103058 |
| H | 1.363653 | 1.959060 | 0.853927 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.676276 | -0.522650 | -0.008009 |
| C | 0.314971 | 0.926000 | -0.396033 |
| H | 0.235193 | 0.953163 | -1.491289 |
| C | -1.014884 | 1.383254 | 0.181413 |
| C | -2.148759 | 0.453428 | -0.247256 |
| H | -3.088357 | 0.777304 | 0.202224 |
| H | -2.274431 | 0.520155 | -1.332351 |
| C | -0.492321 | -1.428299 | -0.438471 |
| C | -1.843097 | -0.995349 | 0.129862 |
| H | -2.627394 | -1.654939 | -0.245395 |
| H | -1.841823 | -1.096439 | 1.217913 |
| H | -0.942398 | 1.412297 | 1.271424 |
| H | -0.552974 | -1.416802 | -1.532163 |
| H | -0.264402 | -2.456550 | -0.146403 |
| H | -1.205745 | 2.403521 | -0.155342 |
| C | 0.942692 | -0.653349 | 1.493990 |
| H | 1.207407 | -1.685681 | 1.732232 |
| H | 1.773142 | -0.013798 | 1.793838 |
| H | 0.078348 | -0.383869 | 2.099278 |
| C | 1.933895 | -0.953777 | -0.766953 |
| H | 2.813604 | -0.384770 | -0.456620 |
| H | 2.149017 | -2.006735 | -0.574486 |
| H | 1.804425 | -0.826790 | -1.844093 |
| O | 1.298706 | 1.869608 | 0.021385 |
| H | 2.134106 | 1.647524 | -0.401107 |



spiro[2.5]octan-4-ol

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -388.445907 | -388.227106 | -388.269148 |
| ax2 | -388.447224 | -388.228351 | -388.270284 |

| | | | | | | |
|-----|--|-------------|--|-------------|--|-------------|
| ax3 | | -388.446020 | | -388.22707 | | -388.268931 |
| eq | | -388.445798 | | -388.226972 | | -388.268985 |
| eq2 | | -388.446155 | | -388.227277 | | -388.269129 |
| eq3 | | -388.446340 | | -388.227374 | | -388.269119 |

ax

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.842424 | -0.121582 | -0.064406 |
| C | -0.016271 | 1.094636 | 0.280556 |
| H | -0.589673 | 1.729517 | 0.964325 |
| C | -1.800869 | -0.600934 | 0.986164 |
| C | -2.312964 | 0.065936 | -0.267336 |
| C | 1.295969 | 0.682420 | 0.946030 |
| C | 2.062360 | -0.344071 | 0.110808 |
| H | 2.370321 | 0.113602 | -0.832729 |
| H | 2.972488 | -0.639495 | 0.634746 |
| C | -0.101231 | -1.157782 | -0.883194 |
| C | 1.195627 | -1.568818 | -0.184280 |
| H | 0.951903 | -2.072749 | 0.756382 |
| H | 1.745499 | -2.283196 | -0.798970 |
| H | -1.864672 | -0.044816 | 1.911347 |
| H | -1.940052 | -1.668888 | 1.081244 |
| H | -2.800572 | -0.556908 | -1.004380 |
| H | -2.709585 | 1.067507 | -0.174891 |
| H | 1.059181 | 0.256564 | 1.925120 |
| H | -0.746924 | -2.023058 | -1.044596 |
| H | 0.134476 | -0.738890 | -1.865414 |
| H | 1.905860 | 1.572091 | 1.123328 |
| O | 0.223266 | 1.808821 | -0.934588 |
| H | 0.844442 | 2.519323 | -0.744858 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.826406 | -0.152916 | -0.045742 |
| C | -0.036851 | 1.091240 | 0.300455 |
| H | -0.621962 | 1.697322 | 1.000753 |
| C | -1.780118 | -0.660237 | 0.993570 |
| C | -2.302812 | 0.004263 | -0.257340 |
| C | 1.299423 | 0.729511 | 0.935796 |
| C | 2.085916 | -0.269204 | 0.085465 |
| H | 2.358717 | 0.199659 | -0.863002 |
| H | 3.015297 | -0.531299 | 0.593171 |
| C | -0.060034 | -1.161937 | -0.875143 |
| C | 1.259615 | -1.525394 | -0.193302 |
| H | 1.047121 | -2.035006 | 0.751887 |
| H | 1.825169 | -2.221642 | -0.814480 |
| H | -1.862207 | -0.111133 | 1.921515 |
| H | -1.898178 | -1.731387 | 1.080312 |
| H | -2.772072 | -0.623762 | -1.001738 |
| H | -2.728439 | 0.993745 | -0.153922 |
| H | 1.096514 | 0.293265 | 1.917452 |
| H | -0.676928 | -2.048931 | -1.030679 |
| H | 0.149818 | -0.735429 | -1.860404 |

| | | | |
|---|-----------|----------|-----------|
| H | 1.875547 | 1.642177 | 1.096528 |
| O | 0.242997 | 1.862817 | -0.869031 |
| H | -0.584766 | 1.977934 | -1.347699 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.841138 | -0.126892 | -0.065072 |
| C | -0.029289 | 1.104475 | 0.281724 |
| H | -0.611673 | 1.737529 | 0.952598 |
| C | -1.792670 | -0.623645 | 0.983724 |
| C | -2.313491 | 0.037053 | -0.270056 |
| C | 1.280006 | 0.702435 | 0.960563 |
| C | 2.065525 | -0.312635 | 0.126863 |
| H | 2.389276 | 0.146464 | -0.813415 |
| H | 2.975604 | -0.597166 | 0.656280 |
| C | -0.082481 | -1.152523 | -0.882551 |
| C | 1.217737 | -1.548001 | -0.180521 |
| H | 0.976055 | -2.058816 | 0.756503 |
| H | 1.780520 | -2.251282 | -0.796046 |
| H | -1.864251 | -0.068192 | 1.908861 |
| H | -1.917577 | -1.693466 | 1.078697 |
| H | -2.790846 | -0.593684 | -1.007178 |
| H | -2.725164 | 1.032612 | -0.177883 |
| H | 1.038349 | 0.259068 | 1.930355 |
| H | -0.716473 | -2.024656 | -1.051245 |
| H | 0.150857 | -0.739236 | -1.870591 |
| H | 1.875288 | 1.597497 | 1.146777 |
| O | 0.210910 | 1.920063 | -0.867599 |
| H | 0.727564 | 1.411221 | -1.500959 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.614772 | -0.483009 | -0.177686 |
| C | -0.241160 | 0.962801 | -0.434703 |
| H | -0.044794 | 1.072004 | -1.509870 |
| C | -1.454221 | -0.805484 | 1.022636 |
| C | -2.028997 | -0.930205 | -0.370288 |
| C | 1.027105 | 1.324102 | 0.331415 |
| C | 2.176164 | 0.382069 | -0.029236 |
| H | 2.425734 | 0.507549 | -1.087352 |
| H | 3.067461 | 0.646453 | 0.541063 |
| C | 0.510196 | -1.434394 | -0.531388 |
| C | 1.789547 | -1.075028 | 0.224916 |
| H | 1.625489 | -1.222552 | 1.296542 |
| H | 2.602081 | -1.740024 | -0.071726 |
| H | -1.809453 | 0.016692 | 1.626173 |
| H | -1.226487 | -1.716602 | 1.558711 |
| H | -2.186133 | -1.925098 | -0.763718 |
| H | -2.756452 | -0.189107 | -0.666796 |
| H | 0.809375 | 1.256178 | 1.401434 |
| H | 0.202037 | -2.457403 | -0.308514 |
| H | 0.702180 | -1.382019 | -1.608438 |
| H | 1.297730 | 2.360536 | 0.114169 |
| O | -1.330079 | 1.801637 | -0.068837 |

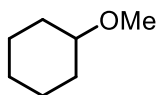
H -1.051306 2.715189 -0.184980

eq2

```
=====
C -0.606480 -0.483568 -0.175490
C -0.246988 0.973190 -0.427680
H -0.053113 1.092195 -1.501396
C -1.419762 -0.821683 1.036918
C -2.017737 -0.952492 -0.345334
C 1.017075 1.338071 0.336082
C 2.171747 0.404472 -0.027991
H 2.425113 0.542843 -1.083572
H 3.058572 0.670264 0.548626
C 0.523113 -1.421463 -0.550684
C 1.799837 -1.059394 0.208350
H 1.638012 -1.222594 1.277963
H 2.618982 -1.712052 -0.097387
H -1.775606 -0.003758 1.646491
H -1.173086 -1.730254 1.568645
H -2.164137 -1.948201 -0.740466
H -2.781439 -0.239034 -0.623573
H 0.800917 1.265546 1.406274
H 0.226136 -2.450997 -0.343089
H 0.710707 -1.349670 -1.627389
H 1.276159 2.375917 0.121528
O -1.265712 1.881321 -0.029943
H -2.006358 1.796433 -0.638129
```

eq3

```
=====
C -0.615882 -0.480471 -0.178677
C -0.237993 0.968149 -0.450354
H -0.059572 1.071871 -1.525023
C -1.472125 -0.795303 1.012753
C -2.027006 -0.926393 -0.387123
C 1.038961 1.332472 0.299150
C 2.180943 0.371915 -0.033771
H 2.435634 0.473183 -1.093192
H 3.071493 0.642809 0.534732
C 0.508389 -1.441203 -0.510637
C 1.783675 -1.076554 0.248634
H 1.610844 -1.201405 1.321845
H 2.594035 -1.752527 -0.028427
H -1.849588 0.017279 1.618419
H -1.251115 -1.702612 1.557808
H -2.183990 -1.923011 -0.775932
H -2.746849 -0.182915 -0.696990
H 0.827274 1.290810 1.374048
H 0.195487 -2.460996 -0.279384
H 0.707797 -1.400911 -1.586982
H 1.313010 2.360643 0.057286
O -1.286142 1.882480 -0.159357
H -1.329092 1.992264 0.796794
```



methoxycyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -350.350558 | -350.13737 | -350.178635 |
| ax2 | -350.341566 | -350.128174 | -350.169576 |
| eq | -350.351225 | -350.138237 | -350.180136 |
| eq2 | -350.348485 | -350.135292 | -350.1769 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.099812 | 1.009050 | 0.907124 |
| C | 0.599691 | -0.420445 | 0.694143 |
| H | 1.220718 | -0.716374 | 1.548817 |
| C | -0.572646 | -1.382877 | 0.551234 |
| C | -1.524308 | -0.952632 | -0.566518 |
| H | -1.004842 | -1.022594 | -1.524988 |
| H | -2.373770 | -1.636126 | -0.611439 |
| C | -0.828723 | 1.447301 | -0.224370 |
| C | -2.008184 | 0.483121 | -0.360272 |
| H | -2.612532 | 0.530881 | 0.551526 |
| H | -2.653106 | 0.786150 | -1.186908 |
| H | -1.110302 | -1.406373 | 1.502700 |
| H | -1.185969 | 2.462100 | -0.042670 |
| H | -0.267864 | 1.467033 | -1.163116 |
| H | -0.189262 | -2.387722 | 0.366815 |
| O | 1.380834 | -0.552676 | -0.489687 |
| C | 2.562888 | 0.214986 | -0.485339 |
| H | 3.105705 | 0.102579 | 0.459374 |
| H | 3.190189 | -0.151110 | -1.296475 |
| H | 2.364959 | 1.277304 | -0.651612 |
| H | -0.442714 | 1.029280 | 1.856423 |
| H | 0.940934 | 1.695360 | 1.013037 |

ax2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.307547 | 1.436429 | -0.460230 |
| C | -0.668354 | 0.338617 | -0.899173 |
| H | -1.019953 | 0.605813 | -1.896955 |
| C | 0.015992 | -1.028800 | -1.010229 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.982238 | -1.378740 | 0.127479 |
| H | 0.438912 | -1.581464 | 1.051516 |
| H | 1.513534 | -2.296499 | -0.131193 |
| C | 1.243965 | 1.056764 | 0.688432 |
| C | 1.977160 | -0.246594 | 0.377742 |
| H | 2.595825 | -0.104425 | -0.514466 |
| H | 2.650052 | -0.510256 | 1.195214 |
| H | 0.591243 | -1.007364 | -1.940159 |
| H | 1.960499 | 1.864540 | 0.848511 |
| H | 0.686052 | 0.945990 | 1.620378 |
| H | -0.744879 | -1.802137 | -1.133780 |
| O | -1.881985 | 0.342937 | -0.141266 |
| C | -1.922785 | -0.374815 | 1.072519 |
| H | -1.186377 | -0.021314 | 1.796807 |
| H | -2.916787 | -0.216340 | 1.488817 |
| H | -1.784619 | -1.447647 | 0.918669 |
| H | 0.925439 | 1.677949 | -1.330950 |
| H | -0.267640 | 2.332498 | -0.221523 |

eq

```
=====
```

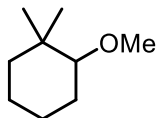
| | | | |
|---|-----------|-----------|-----------|
| C | -0.352788 | -1.347414 | -0.194596 |
| C | 0.592084 | -0.228302 | 0.212807 |
| H | 0.652662 | -0.193829 | 1.310664 |
| C | 0.088794 | 1.121814 | -0.290276 |
| C | -1.334177 | 1.391672 | 0.203470 |
| H | -1.324943 | 1.475195 | 1.294730 |
| H | -1.684776 | 2.349371 | -0.183713 |
| C | -1.775119 | -1.081905 | 0.297820 |
| C | -2.286066 | 0.268175 | -0.202943 |
| H | -2.363819 | 0.240461 | -1.294242 |
| H | -3.287387 | 0.461876 | 0.185184 |
| H | 0.106425 | 1.105665 | -1.384783 |
| H | -2.436230 | -1.886076 | -0.027888 |
| H | -1.784828 | -1.085060 | 1.392119 |
| H | 0.753420 | 1.921739 | 0.038176 |
| O | 1.876117 | -0.558985 | -0.298418 |
| C | 2.913291 | 0.269432 | 0.179794 |
| H | 2.876301 | 0.358049 | 1.270713 |
| H | 3.855749 | -0.196413 | -0.102735 |
| H | 2.876405 | 1.270856 | -0.255764 |
| H | -0.347833 | -1.416391 | -1.286752 |
| H | 0.023797 | -2.294390 | 0.195182 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.078663 | -1.279403 | 0.072158 |
| C | -0.557618 | -0.063156 | -0.595154 |
| H | -0.288309 | -0.084868 | -1.655232 |
| C | -0.013041 | 1.230857 | 0.000734 |
| C | 1.507707 | 1.286065 | -0.161108 |
| H | 1.756101 | 1.309341 | -1.226503 |
| H | 1.895515 | 2.206911 | 0.276601 |
| C | 1.600641 | -1.231621 | -0.082980 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.171606 | 0.068754 | 0.482526 |
| H | 1.998245 | 0.096356 | 1.562832 |
| H | 3.251663 | 0.103870 | 0.330884 |
| H | -0.257231 | 1.275985 | 1.065750 |
| H | 2.053650 | -2.092736 | 0.410243 |
| H | 1.855108 | -1.301959 | -1.144990 |
| H | -0.488586 | 2.085860 | -0.484277 |
| O | -1.981853 | -0.127273 | -0.609699 |
| C | -2.618976 | 0.075895 | 0.634702 |
| H | -2.542482 | 1.113766 | 0.967800 |
| H | -3.671337 | -0.162392 | 0.490069 |
| H | -2.222314 | -0.576606 | 1.416269 |
| H | -0.170647 | -1.291090 | 1.136600 |
| H | -0.328447 | -2.188598 | -0.373725 |



2-methoxy-1,1-dimethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -428.964672 | -428.69288 | -428.739858 |
| ax2 | -428.963510 | -428.691866 | -428.739651 |
| ax3 | -428.956634 | -428.684483 | -428.730627 |
| eq | -428.965357 | -428.693731 | -428.741864 |
| eq2 | -428.965357 | -428.693731 | -428.741869 |
| eq3 | -428.960734 | -428.68876 | -428.735152 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.894072 | -0.666344 | 0.040713 |
| C | -0.529607 | -0.392455 | 0.562100 |
| H | -0.730676 | -1.071450 | 1.402719 |
| C | 1.891920 | -0.573920 | 1.200681 |
| C | 0.972241 | -2.081582 | -0.534416 |
| C | -0.704886 | 1.055333 | 1.024200 |
| C | -0.382710 | 2.034222 | -0.103825 |
| H | -1.097760 | 1.888920 | -0.918318 |
| H | -0.499222 | 3.060840 | 0.246740 |
| C | 1.239242 | 0.353754 | -1.059396 |
| C | 1.035131 | 1.808135 | -0.630026 |
| H | 1.754366 | 2.073060 | 0.149322 |
| H | 1.233320 | 2.469440 | -1.475410 |
| H | 1.622327 | -1.273198 | 1.995377 |
| H | 1.949515 | 0.421664 | 1.636673 |
| H | 0.310191 | -2.199846 | -1.390189 |
| H | 0.691400 | -2.821787 | 0.219020 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.045110 | 1.234501 | 1.874965 |
| H | 2.273093 | 0.192789 | -1.376622 |
| H | 0.603745 | 0.150599 | -1.925414 |
| H | -1.721357 | 1.204960 | 1.390038 |
| O | -1.434010 | -0.710904 | -0.491001 |
| C | -2.793389 | -0.638881 | -0.127297 |
| H | -3.152632 | 0.392150 | -0.069957 |
| H | -3.361696 | -1.160216 | -0.896111 |
| H | -2.973088 | -1.127389 | 0.836373 |
| H | 1.993310 | -2.298581 | -0.854965 |
| H | 2.890265 | -0.838799 | 0.847352 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.185670 | 0.989847 | 0.052614 |
| C | 0.581580 | -0.245051 | 0.566858 |
| H | 1.195645 | 0.065573 | 1.419243 |
| C | -0.942273 | 1.644204 | 1.213593 |
| C | 0.804058 | 2.012156 | -0.506972 |
| C | -0.345944 | -1.380384 | 0.995401 |
| C | -1.290831 | -1.783230 | -0.136892 |
| H | -0.702346 | -2.192043 | -0.961963 |
| H | -1.962514 | -2.573704 | 0.201523 |
| C | -1.156599 | 0.556490 | -1.059010 |
| C | -2.089942 | -0.580913 | -0.639725 |
| H | -2.767969 | -0.239507 | 0.146747 |
| H | -2.714541 | -0.872694 | -1.485898 |
| H | -0.249223 | 1.934360 | 2.006557 |
| H | -1.695440 | 0.991634 | 1.651777 |
| H | 1.380939 | 1.591996 | -1.330721 |
| H | 1.500119 | 2.346372 | 0.266286 |
| H | -0.923523 | -1.068404 | 1.868121 |
| H | -1.734627 | 1.426300 | -1.382366 |
| H | -0.565956 | 0.226934 | -1.918702 |
| H | 0.269515 | -2.227950 | 1.303498 |
| O | 1.439059 | -0.744199 | -0.461680 |
| C | 2.808852 | -0.688107 | -0.135165 |
| H | 3.031999 | -1.284753 | 0.755430 |
| H | 3.363764 | -1.097288 | -0.978173 |
| H | 3.140431 | 0.339902 | 0.040157 |
| H | 0.268902 | 2.889542 | -0.876497 |
| H | -1.447024 | 2.547242 | 0.864213 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.927751 | 0.501945 | -0.009354 |
| C | 0.361728 | 0.451527 | 0.858244 |
| H | 0.094550 | 0.900921 | 1.817541 |
| C | -2.113131 | 0.208529 | 0.923037 |
| C | -1.109605 | 1.903622 | -0.588778 |
| C | 0.843716 | -0.977730 | 1.146752 |
| C | 0.806610 | -1.947135 | -0.038617 |
| H | 1.561795 | -1.684387 | -0.780918 |
| H | 1.050503 | -2.950076 | 0.316513 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.925964 | -0.525813 | -1.158274 |
| C | -0.564557 | -1.939502 | -0.708737 |
| H | -1.316719 | -2.316024 | -0.010456 |
| H | -0.568038 | -2.612417 | -1.567825 |
| H | -2.214321 | 0.997582 | 1.670450 |
| H | -2.001121 | -0.738105 | 1.452083 |
| H | -0.322738 | 2.144457 | -1.303959 |
| H | -1.089443 | 2.659181 | 0.199173 |
| H | 0.198926 | -1.383022 | 1.930327 |
| H | -1.916203 | -0.517010 | -1.621987 |
| H | -0.220440 | -0.212538 | -1.931367 |
| H | 1.847173 | -0.919801 | 1.573744 |
| O | 1.399941 | 1.323577 | 0.411550 |
| C | 2.209387 | 0.902476 | -0.663178 |
| H | 1.629610 | 0.646706 | -1.552158 |
| H | 2.859526 | 1.741870 | -0.907312 |
| H | 2.837868 | 0.050844 | -0.391294 |
| H | -2.071764 | 1.971562 | -1.101483 |
| H | -3.041295 | 0.164130 | 0.349962 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.283363 | 0.950130 | -0.019838 |
| C | 0.602326 | -0.293112 | -0.213947 |
| H | 0.725041 | -0.434651 | -1.297763 |
| C | -0.381263 | 1.337993 | 1.458891 |
| C | 0.320684 | 2.122506 | -0.794424 |
| C | -0.014271 | -1.562631 | 0.368625 |
| C | -1.395597 | -1.827468 | -0.229181 |
| H | -1.291233 | -2.019999 | -1.301651 |
| H | -1.830838 | -2.724374 | 0.213826 |
| C | -1.677054 | 0.640719 | -0.596758 |
| C | -2.314864 | -0.624870 | -0.025777 |
| H | -2.515097 | -0.496424 | 1.040907 |
| H | -3.278395 | -0.799690 | -0.507607 |
| H | 0.606158 | 1.567949 | 1.859200 |
| H | -0.817528 | 0.550255 | 2.071910 |
| H | 0.420788 | 1.878088 | -1.854388 |
| H | 1.307019 | 2.379618 | -0.408205 |
| H | -0.090245 | -1.453338 | 1.453147 |
| H | -2.323292 | 1.506075 | -0.428720 |
| H | -1.581924 | 0.523062 | -1.681648 |
| H | 0.647906 | -2.408140 | 0.176243 |
| O | 1.880092 | -0.035534 | 0.354670 |
| C | 2.921868 | -0.768368 | -0.250075 |
| H | 3.012914 | -0.517402 | -1.311992 |
| H | 3.846910 | -0.498563 | 0.256545 |
| H | 2.776269 | -1.848005 | -0.156479 |
| H | -0.319458 | 3.003340 | -0.710515 |
| H | -1.006530 | 2.227080 | 1.564745 |

eq2

```
=====
```

| | | | |
|---|-----------|----------|-----------|
| C | -0.283540 | 0.950122 | -0.019853 |
|---|-----------|----------|-----------|

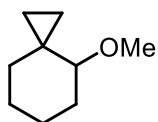
| | | | |
|---|-----------|-----------|-----------|
| C | 0.602365 | -0.292932 | -0.214144 |
| H | 0.724963 | -0.434430 | -1.297975 |
| C | -0.381361 | 1.337869 | 1.458917 |
| C | 0.320167 | 2.122681 | -0.794400 |
| C | -0.013925 | -1.562598 | 0.368470 |
| C | -1.395297 | -1.827672 | -0.229130 |
| H | -1.291045 | -2.020197 | -1.301610 |
| H | -1.830315 | -2.724653 | 0.213942 |
| C | -1.677242 | 0.640472 | -0.596642 |
| C | -2.314765 | -0.625244 | -0.025623 |
| H | -2.514924 | -0.496844 | 1.041079 |
| H | -3.278307 | -0.800243 | -0.507363 |
| H | 0.606035 | 1.568113 | 1.859117 |
| H | -0.817293 | 0.549968 | 2.071954 |
| H | 0.420216 | 1.878382 | -1.854394 |
| H | 1.306479 | 2.380008 | -0.408258 |
| H | -0.089733 | -1.453380 | 1.453008 |
| H | -2.323607 | 1.505712 | -0.428506 |
| H | -1.582202 | 0.522863 | -1.681543 |
| H | 0.648341 | -2.407992 | 0.175931 |
| O | 1.880163 | -0.034999 | 0.354252 |
| C | 2.922015 | -0.768270 | -0.249814 |
| H | 3.012421 | -0.519037 | -1.312189 |
| H | 3.847168 | -0.497129 | 0.255894 |
| H | 2.777069 | -1.847825 | -0.154344 |
| H | -0.320183 | 3.003349 | -0.710339 |
| H | -1.006893 | 2.226751 | 1.564901 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.164788 | 0.957309 | -0.008152 |
| C | 0.480493 | -0.296878 | -0.636794 |
| H | 0.229468 | -0.263539 | -1.702915 |
| C | 0.210860 | 1.126964 | 1.467584 |
| C | 0.306475 | 2.197029 | -0.770015 |
| C | -0.077832 | -1.607560 | -0.088338 |
| C | -1.594125 | -1.665848 | -0.272874 |
| H | -1.828401 | -1.664339 | -1.341817 |
| H | -1.981172 | -2.599329 | 0.137963 |
| C | -1.691746 | 0.835839 | -0.169504 |
| C | -2.266525 | -0.464562 | 0.387250 |
| H | -2.114093 | -0.510802 | 1.468837 |
| H | -3.344321 | -0.494297 | 0.218556 |
| H | 1.276192 | 1.335650 | 1.571278 |
| H | -0.024020 | 0.248979 | 2.069181 |
| H | 0.053302 | 2.122616 | -1.830019 |
| H | 1.385882 | 2.321568 | -0.684863 |
| H | 0.155617 | -1.711059 | 0.973299 |
| H | -2.162490 | 1.701115 | 0.304084 |
| H | -1.930701 | 0.890829 | -1.237035 |
| H | 0.399776 | -2.440702 | -0.607400 |
| O | 1.908716 | -0.223080 | -0.612519 |
| C | 2.587204 | -0.909671 | 0.420750 |
| H | 2.540837 | -1.993426 | 0.289732 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.629871 | -0.601287 | 0.358830 |
| H | 2.212619 | -0.660754 | 1.414706 |
| H | -0.173821 | 3.092983 | -0.370377 |
| H | -0.334371 | 1.974697 | 1.888670 |



4-methoxyspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -427.734228 | -427.48564 | -427.530967 |
| ax2 | -427.735125 | -427.486545 | -427.531358 |
| ax3 | -427.726136 | -427.477088 | -427.522176 |
| ax4 | -427.726512 | -427.477505 | -427.522638 |
| eq | -427.733542 | -427.484981 | -427.530805 |
| eq2 | -427.732911 | -427.484309 | -427.529667 |
| eq3 | -427.728421 | -427.479569 | -427.524518 |
| eq4 | -427.726496 | -427.477562 | -427.522626 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.931821 | -0.470107 | -0.069791 |
| C | -0.481103 | -0.538464 | 0.461013 |
| H | -0.554815 | -1.344688 | 1.202504 |
| C | 2.027121 | -0.853321 | 0.881035 |
| C | 1.668474 | -1.755640 | -0.275161 |
| C | -0.858630 | 0.793117 | 1.113242 |
| C | -0.670190 | 1.958605 | 0.142469 |
| H | -1.350069 | 1.834910 | -0.705194 |
| H | -0.934915 | 2.896840 | 0.632107 |
| C | 1.172880 | 0.687796 | -1.016493 |
| C | 0.770925 | 2.013836 | -0.367984 |
| H | 1.439724 | 2.218456 | 0.474003 |
| H | 0.891292 | 2.831710 | -1.080202 |
| H | 1.749909 | -1.177859 | 1.874646 |
| H | 2.954470 | -0.300700 | 0.820084 |
| H | 2.361288 | -1.809977 | -1.103485 |
| H | 1.146664 | -2.675225 | -0.049076 |
| H | -0.207869 | 0.928698 | 1.981397 |
| H | 2.224157 | 0.704007 | -1.310590 |
| H | 0.582752 | 0.535817 | -1.924397 |
| H | -1.881516 | 0.756953 | 1.489623 |
| O | -1.323667 | -0.861495 | -0.640678 |
| C | -2.678261 | -1.038678 | -0.291388 |
| H | -3.182916 | -0.087672 | -0.101753 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.167569 | -1.528798 | -1.131393 |
| H | -2.779476 | -1.673376 | 0.595497 |

ax2

```
=====
C  0.316126    0.790510   -0.004490
C  0.358982   -0.544781    0.714264
H  1.033093   -0.463207    1.577426
C  0.379962    2.015094    0.862872
C  1.540531    1.654494   -0.026984
C -1.043456   -0.930507    1.172298
C -2.032436   -0.934618    0.004126
H -1.750464   -1.720551   -0.700151
H -3.032059   -1.174791    0.369608
C -0.638454    0.804315   -1.179182
C -2.045396    0.411863   -0.722066
H -2.424766    1.182775   -0.044049
H -2.723343    0.373619   -1.576291
H  0.505344    1.875233    1.928233
H -0.234875    2.857954    0.579168
H  1.709192    2.257688   -0.908634
H  2.434661    1.278600    0.450697
H -1.366265   -0.208027    1.925846
H -0.642848    1.795271   -1.637169
H -0.289725    0.095542   -1.936698
H -1.006552   -1.910836    1.649625
O  0.812318   -1.604153   -0.120033
C  2.134959   -1.452438   -0.584760
H  2.821458   -1.229513    0.238914
H  2.425294   -2.398507   -1.038749
H  2.218399   -0.661610   -1.333989
```

ax3

```
=====
C  0.972558   -0.148041   -0.077284
C -0.194865   -0.673365    0.746491
H  0.229750   -1.155961    1.628348
C  2.273465   -0.004626    0.670205
C  2.092035   -1.104108   -0.344094
C -1.092399    0.472470    1.232568
C -1.381386    1.569398    0.200668
H -2.042698    1.200348   -0.584650
H -1.907755    2.387359    0.695618
C  0.670598    0.934610   -1.096149
C -0.093882    2.083793   -0.441214
H  0.537926    2.542727    0.325744
H -0.321194    2.856468   -1.177111
H  2.296150   -0.283116    1.714561
H  2.908084    0.828836    0.402643
H  2.616426   -1.011733   -1.285151
H  1.982608   -2.114487    0.024499
H -0.569904    0.935768    2.074046
H  1.610891    1.290256   -1.522609
H  0.081768    0.531929   -1.923738
```

| | | | |
|---|-----------|-----------|-----------|
| H | -2.018810 | 0.054507 | 1.631259 |
| O | -0.895262 | -1.751904 | 0.123800 |
| C | -1.878475 | -1.443549 | -0.839757 |
| H | -1.479102 | -0.872363 | -1.680069 |
| H | -2.248040 | -2.396006 | -1.217408 |
| H | -2.719893 | -0.898792 | -0.404988 |

ax4

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.818254 | -0.386925 | -0.010884 |
| C | -0.075776 | 0.608868 | 0.865092 |
| H | -0.641782 | 0.714216 | 1.792303 |
| C | -1.803069 | -1.269111 | 0.713413 |
| C | -2.288889 | -0.167552 | -0.191322 |
| C | 1.319069 | 0.091876 | 1.234807 |
| C | 2.106852 | -0.517857 | 0.073932 |
| H | 2.375124 | 0.251830 | -0.653004 |
| H | 3.043561 | -0.930023 | 0.453100 |
| C | -0.031482 | -1.043169 | -1.133288 |
| C | 1.291412 | -1.608932 | -0.618233 |
| H | 1.087763 | -2.412705 | 0.096341 |
| H | 1.857939 | -2.045575 | -1.442008 |
| H | -1.921712 | -1.135921 | 1.779372 |
| H | -1.901542 | -2.287011 | 0.363025 |
| H | -2.722244 | -0.449716 | -1.141025 |
| H | -2.722049 | 0.708618 | 0.271127 |
| H | 1.181013 | -0.683112 | 1.995292 |
| H | -0.642448 | -1.833903 | -1.573338 |
| H | 0.176186 | -0.324985 | -1.929100 |
| H | 1.873981 | 0.905200 | 1.704452 |
| O | -0.045204 | 1.951591 | 0.368720 |
| C | 0.111745 | 2.157361 | -1.018220 |
| H | -0.708564 | 1.717390 | -1.589818 |
| H | 0.097148 | 3.235797 | -1.170868 |
| H | 1.059610 | 1.769822 | -1.397395 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.339688 | 0.871721 | -0.168623 |
| C | 0.600127 | -0.314577 | -0.280651 |
| H | 0.690747 | -0.576374 | -1.345355 |
| C | -0.194164 | 1.791042 | 1.007771 |
| C | 0.187480 | 2.255307 | -0.379551 |
| C | 0.027613 | -1.513145 | 0.475285 |
| C | -1.379059 | -1.856969 | -0.016596 |
| H | -1.327623 | -2.166814 | -1.065103 |
| H | -1.771739 | -2.705105 | 0.545798 |
| C | -1.740907 | 0.547492 | -0.645677 |
| C | -2.313977 | -0.654550 | 0.104302 |
| H | -2.433478 | -0.395366 | 1.160560 |
| H | -3.304184 | -0.902117 | -0.281387 |
| H | 0.613745 | 1.601865 | 1.699220 |
| H | -1.099728 | 2.190742 | 1.443287 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.464526 | 2.964829 | -0.870198 |
| H | 1.241901 | 2.366837 | -0.584300 |
| H | -0.002648 | -1.256122 | 1.538391 |
| H | -2.377587 | 1.424859 | -0.518375 |
| H | -1.712899 | 0.321770 | -1.717188 |
| H | 0.686197 | -2.375152 | 0.362598 |
| O | 1.879156 | 0.053670 | 0.206433 |
| C | 2.919580 | -0.783240 | -0.249757 |
| H | 2.953220 | -0.806892 | -1.343572 |
| H | 3.854122 | -0.368729 | 0.123570 |
| H | 2.819197 | -1.806079 | 0.121571 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.081789 | 0.827268 | -0.141008 |
| C | 0.467560 | -0.589317 | -0.165946 |
| H | 0.545109 | -0.908180 | -1.213250 |
| C | 0.193987 | 1.670020 | 1.068415 |
| C | 0.850719 | 1.991967 | -0.253540 |
| C | -0.488064 | -1.532541 | 0.553744 |
| C | -1.890084 | -1.462355 | -0.054146 |
| H | -1.850262 | -1.825671 | -1.085818 |
| H | -2.564611 | -2.125182 | 0.489486 |
| C | -1.462102 | 0.916797 | -0.758794 |
| C | -2.430165 | -0.031790 | -0.050082 |
| H | -2.562323 | 0.300998 | 0.983711 |
| H | -3.410628 | 0.003192 | -0.527602 |
| H | 0.827939 | 1.253665 | 1.837878 |
| H | -0.596752 | 2.322018 | 1.413344 |
| H | 0.501285 | 2.860955 | -0.793874 |
| H | 1.909639 | 1.791952 | -0.330018 |
| H | -0.522561 | -1.245053 | 1.608770 |
| H | -1.820274 | 1.946633 | -0.706659 |
| H | -1.403456 | 0.647514 | -1.818895 |
| H | -0.093727 | -2.548871 | 0.501451 |
| O | 1.750187 | -0.665272 | 0.439031 |
| C | 2.801343 | -0.859181 | -0.484516 |
| H | 3.735478 | -0.829247 | 0.073729 |
| H | 2.715159 | -1.830760 | -0.980826 |
| H | 2.820058 | -0.076997 | -1.248436 |

eq3

```
=====
```

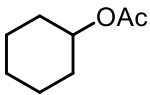
| | | | |
|---|-----------|-----------|-----------|
| C | -0.167302 | 0.902975 | -0.166916 |
| C | 0.437421 | -0.409457 | -0.646171 |
| H | 0.191236 | -0.500713 | -1.710321 |
| C | 0.465611 | 1.646105 | 0.973709 |
| C | 0.559150 | 2.182861 | -0.435240 |
| C | -0.194111 | -1.600184 | 0.072185 |
| C | -1.715138 | -1.580628 | -0.086026 |
| H | -1.971874 | -1.685978 | -1.144537 |
| H | -2.148083 | -2.436062 | 0.434017 |
| C | -1.679866 | 0.918740 | -0.274380 |
| C | -2.303923 | -0.275032 | 0.445190 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.102649 | -0.198054 | 1.518019 |
| H | -3.387567 | -0.267037 | 0.318318 |
| H | 1.376404 | 1.259812 | 1.405131 |
| H | -0.194001 | 2.151182 | 1.666017 |
| H | -0.036809 | 3.049072 | -0.687814 |
| H | 1.524849 | 2.119977 | -0.914890 |
| H | 0.049250 | -1.562282 | 1.136720 |
| H | -2.061865 | 1.860327 | 0.124216 |
| H | -1.960213 | 0.880814 | -1.332798 |
| H | 0.217667 | -2.527781 | -0.329035 |
| O | 1.863288 | -0.383273 | -0.606624 |
| C | 2.510123 | -1.032147 | 0.471263 |
| H | 2.418525 | -2.118707 | 0.406786 |
| H | 3.564036 | -0.769492 | 0.395013 |
| H | 2.143004 | -0.708299 | 1.446457 |

eq4

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.062122 | 0.854664 | -0.208584 |
| C | 0.361088 | -0.550306 | -0.616075 |
| H | 0.027114 | -0.678388 | -1.651003 |
| C | 0.524007 | 1.538505 | 0.994067 |
| C | 0.865916 | 2.009245 | -0.402267 |
| C | -0.387831 | -1.581248 | 0.226325 |
| C | -1.897113 | -1.408756 | 0.028057 |
| H | -2.146434 | -1.622740 | -1.015597 |
| H | -2.437171 | -2.132817 | 0.639494 |
| C | -1.550894 | 1.048164 | -0.428425 |
| C | -2.346835 | 0.013184 | 0.369139 |
| H | -2.191865 | 0.192766 | 1.437238 |
| H | -3.414654 | 0.126753 | 0.175677 |
| H | 1.292490 | 1.051242 | 1.572200 |
| H | -0.150917 | 2.155051 | 1.572555 |
| H | 0.449349 | 2.949761 | -0.735751 |
| H | 1.859635 | 1.784748 | -0.764388 |
| H | -0.152302 | -1.448874 | 1.284845 |
| H | -1.834860 | 2.061507 | -0.138641 |
| H | -1.778011 | 0.938806 | -1.493962 |
| H | -0.072087 | -2.585017 | -0.064805 |
| O | 1.759751 | -0.777964 | -0.715101 |
| C | 2.528721 | -0.887438 | 0.468601 |
| H | 1.953862 | -1.270800 | 1.311403 |
| H | 3.338256 | -1.586737 | 0.260233 |
| H | 2.969963 | 0.072367 | 0.746288 |



cyclohexyl acetate

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -463.717580 | -463.49268 | -463.539456 |
| ax2 | -463.704904 | -463.479797 | -463.52696 |
| eq | -463.718499 | -463.493656 | -463.540647 |
| eq2 | -463.713924 | -463.48906 | -463.535763 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 1.214500 | -0.999986 | 1.088749 |
| C | 0.123187 | 0.044182 | 0.911885 |
| H | -0.395782 | 0.215676 | 1.853050 |
| C | 0.672546 | 1.355750 | 0.362868 |
| C | 1.489473 | 1.144193 | -0.912115 |
| H | 0.831072 | 0.790224 | -1.710113 |
| H | 1.904883 | 2.097127 | -1.242462 |
| C | 2.032937 | -1.203632 | -0.186583 |
| C | 2.603932 | 0.122242 | -0.688955 |
| H | 3.307427 | 0.514835 | 0.052295 |
| H | 3.164671 | -0.033315 | -1.611912 |
| H | 1.309313 | 1.790728 | 1.137989 |
| H | 2.835292 | -1.917732 | 0.003352 |
| H | 1.395411 | -1.637566 | -0.961129 |
| H | -0.149766 | 2.050593 | 0.192045 |
| O | -0.833214 | -0.516691 | -0.022567 |
| C | -2.073802 | -0.019636 | -0.010677 |
| O | -2.441943 | 0.844676 | 0.747269 |
| C | -2.934938 | -0.674523 | -1.048741 |
| H | -2.512580 | -0.490385 | -2.036370 |
| H | -2.948389 | -1.751819 | -0.888248 |
| H | -3.942767 | -0.276012 | -0.996187 |
| H | 0.765909 | -1.937315 | 1.420555 |
| H | 1.869553 | -0.650444 | 1.890925 |

ax2

| | | | |
|---|----------|-----------|-----------|
| C | 0.845177 | -1.251456 | 0.851089 |
| C | 0.128165 | 0.053689 | 1.213212 |
| H | 0.080506 | 0.101477 | 2.298610 |
| C | 0.844443 | 1.322281 | 0.737642 |
| C | 1.584160 | 1.232333 | -0.598817 |
| H | 0.876833 | 1.226013 | -1.425667 |
| H | 2.209753 | 2.120414 | -0.706862 |
| C | 1.586430 | -1.278959 | -0.487370 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.444992 | -0.027872 | -0.663359 |
| H | 3.200004 | 0.008130 | 0.129655 |
| H | 2.981230 | -0.069780 | -1.612713 |
| H | 1.584483 | 1.548036 | 1.510672 |
| H | 2.213755 | -2.171931 | -0.515709 |
| H | 0.879765 | -1.347244 | -1.311885 |
| H | 0.131998 | 2.149078 | 0.743082 |
| O | -1.300103 | 0.040954 | 0.917281 |
| C | -1.778541 | -0.016396 | -0.323113 |
| O | -1.098227 | -0.063848 | -1.317961 |
| C | -3.280110 | -0.012066 | -0.320692 |
| H | -3.648331 | -0.850690 | 0.269008 |
| H | -3.640276 | 0.904953 | 0.144689 |
| H | -3.648864 | -0.081140 | -1.338831 |
| H | 0.133013 | -2.074914 | 0.928170 |
| H | 1.584478 | -1.408578 | 1.641660 |

eq

```
=====
```

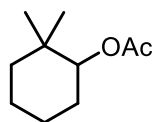
| | | | |
|---|-----------|-----------|-----------|
| C | -1.004160 | -1.389620 | 0.016890 |
| C | -0.090774 | -0.190879 | 0.195638 |
| H | 0.010210 | 0.045365 | 1.255978 |
| C | -0.607796 | 1.025105 | -0.556903 |
| C | -2.023034 | 1.372225 | -0.091755 |
| H | -1.992794 | 1.666472 | 0.961644 |
| H | -2.394596 | 2.231048 | -0.651716 |
| C | -2.420977 | -1.047961 | 0.480842 |
| C | -2.962749 | 0.177985 | -0.254047 |
| H | -3.063510 | -0.056852 | -1.318072 |
| H | -3.958411 | 0.428313 | 0.115093 |
| H | -0.618089 | 0.787658 | -1.624782 |
| H | -3.075307 | -1.906529 | 0.326586 |
| H | -2.407660 | -0.845250 | 1.555932 |
| H | 0.068251 | 1.866930 | -0.407213 |
| O | 1.210052 | -0.571520 | -0.305317 |
| C | 2.272136 | 0.098151 | 0.155575 |
| O | 2.203299 | 0.976295 | 0.980539 |
| C | 3.540700 | -0.383925 | -0.481229 |
| H | 3.641084 | -1.458669 | -0.336406 |
| H | 3.498667 | -0.194679 | -1.553747 |
| H | 4.389971 | 0.133857 | -0.047720 |
| H | -0.606805 | -2.238766 | 0.574495 |
| H | -1.017894 | -1.663591 | -1.041914 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.661184 | 1.264829 | -0.053898 |
| C | -0.129824 | -0.000051 | -0.712457 |
| H | -0.454898 | -0.000297 | -1.754628 |
| C | -0.660755 | -1.264817 | -0.053443 |
| C | -2.190434 | -1.260907 | -0.118303 |
| H | -2.508643 | -1.304778 | -1.164273 |
| H | -2.580824 | -2.153328 | 0.372029 |
| C | -2.190808 | 1.260526 | -0.118705 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.764915 | -0.000172 | 0.528529 |
| H | -2.517747 | 0.000001 | 1.594528 |
| H | -3.853222 | -0.000343 | 0.451306 |
| H | -0.338374 | -1.300228 | 0.986957 |
| H | -2.581419 | 2.152984 | 0.371394 |
| H | -2.509140 | 1.303988 | -1.164657 |
| H | -0.254183 | -2.139231 | -0.564508 |
| O | 1.313102 | 0.000252 | -0.850823 |
| C | 2.103086 | 0.000352 | 0.226411 |
| O | 1.706654 | 0.000873 | 1.366044 |
| C | 3.550431 | -0.000531 | -0.170693 |
| H | 3.763431 | -0.883155 | -0.772828 |
| H | 3.762925 | 0.877144 | -0.780204 |
| H | 4.173902 | 0.003110 | 0.717391 |
| H | -0.254791 | 2.139101 | -0.565357 |
| H | -0.338646 | 1.300659 | 0.986438 |



2,2-dimethylcyclohexyl acetate

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -542.332275 | -542.048704 | -542.102007 |
| ax2 | -542.332109 | -542.048489 | -542.100745 |
| ax3 | -542.320019 | -542.0362 | -542.088341 |
| eq | -542.333115 | -542.049649 | -542.102294 |
| eq2 | -542.332901 | -542.049305 | -542.101436 |
| eq3 | -542.325672 | -542.042075 | -542.094026 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 1.172937 | -0.874990 | 0.005139 |
| C | -0.019671 | -0.138845 | 0.635408 |
| H | -0.376381 | -0.702880 | 1.497076 |
| C | 2.224316 | -1.119241 | 1.094014 |
| C | 0.721688 | -2.234277 | -0.531547 |
| C | 0.293328 | 1.300285 | 1.031707 |
| C | 0.872938 | 2.096992 | -0.137776 |
| H | 0.110198 | 2.204164 | -0.913625 |
| H | 1.130265 | 3.103073 | 0.195875 |
| C | 1.759300 | -0.034025 | -1.142174 |
| C | 2.096672 | 1.399730 | -0.730803 |
| H | 2.907112 | 1.399643 | 0.002373 |
| H | 2.459318 | 1.953376 | -1.598351 |
| H | 1.804772 | -1.722134 | 1.902057 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.608521 | -0.198054 | 1.528286 |
| H | 0.008686 | -2.125574 | -1.347802 |
| H | 0.252037 | -2.826850 | 0.257209 |
| H | 1.002990 | 1.284502 | 1.860921 |
| H | 2.646921 | -0.540849 | -1.528880 |
| H | 1.029802 | -0.003622 | -1.956711 |
| H | -0.619515 | 1.766103 | 1.404539 |
| O | -1.081467 | -0.121293 | -0.350053 |
| H | 1.583330 | -2.791379 | -0.904014 |
| H | 3.068618 | -1.665876 | 0.670465 |
| C | -2.339940 | -0.049629 | 0.092552 |
| O | -2.640295 | -0.017774 | 1.261338 |
| C | -3.316297 | -0.014949 | -1.044858 |
| H | -3.147684 | 0.886041 | -1.634683 |
| H | -3.155894 | -0.873702 | -1.695371 |
| H | -4.330628 | -0.019760 | -0.659620 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.831617 | 0.963909 | 0.107072 |
| C | 0.025510 | -0.037585 | -0.741493 |
| H | -0.430215 | 0.484462 | -1.580661 |
| C | 1.819790 | 1.695826 | -0.808520 |
| C | -0.102875 | 2.005873 | 0.724190 |
| C | 0.853186 | -1.218902 | -1.232126 |
| C | 1.569307 | -1.932623 | -0.085760 |
| H | 0.827559 | -2.392395 | 0.572172 |
| H | 2.187292 | -2.738816 | -0.483167 |
| C | 1.573740 | 0.215092 | 1.227745 |
| C | 2.420322 | -0.954026 | 0.722834 |
| H | 3.238933 | -0.583416 | 0.100787 |
| H | 2.878295 | -1.466509 | 1.570359 |
| H | 1.287444 | 2.216306 | -1.607423 |
| H | 2.545794 | 1.028055 | -1.268973 |
| H | -0.824337 | 1.549030 | 1.403302 |
| H | -0.652507 | 2.546734 | -0.047992 |
| H | 1.584215 | -0.850588 | -1.954206 |
| H | 2.194995 | 0.930285 | 1.772632 |
| H | 0.833358 | -0.167410 | 1.936587 |
| H | 0.195005 | -1.905336 | -1.766850 |
| O | -1.037944 | -0.596139 | 0.068349 |
| H | 0.479966 | 2.729388 | 1.297335 |
| H | 2.370895 | 2.440878 | -0.231917 |
| C | -2.289198 | -0.159652 | -0.112305 |
| O | -2.613796 | 0.646503 | -0.948996 |
| C | -3.228467 | -0.802050 | 0.864599 |
| H | -3.132322 | -1.885571 | 0.815319 |
| H | -2.959461 | -0.489553 | 1.874020 |
| H | -4.248593 | -0.503632 | 0.646436 |

ax3

```
=====
```

| | | | |
|---|----------|-----------|-----------|
| C | 0.929966 | -0.952450 | -0.070129 |
| C | 0.096107 | -0.210979 | 1.005819 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.218833 | -0.776100 | 1.929025 |
| C | 2.175417 | -1.489911 | 0.655357 |
| C | 0.151080 | -2.143842 | -0.626079 |
| C | 0.551439 | 1.223910 | 1.297152 |
| C | 1.012836 | 2.058002 | 0.100900 |
| H | 0.159388 | 2.355716 | -0.504185 |
| H | 1.485698 | 2.967850 | 0.475620 |
| C | 1.378475 | -0.044053 | -1.230571 |
| C | 1.995866 | 1.274036 | -0.765777 |
| H | 2.911054 | 1.080891 | -0.198995 |
| H | 2.285513 | 1.868359 | -1.634029 |
| H | 1.892684 | -2.244455 | 1.391334 |
| H | 2.720188 | -0.702294 | 1.176670 |
| H | -0.708817 | -1.823621 | -1.216198 |
| H | -0.205891 | -2.792695 | 0.176006 |
| H | 1.392764 | 1.136184 | 1.989500 |
| H | 2.099317 | -0.604908 | -1.831365 |
| H | 0.522686 | 0.173533 | -1.867866 |
| H | -0.244087 | 1.729457 | 1.847440 |
| O | -1.348113 | -0.336794 | 0.853224 |
| H | 0.800355 | -2.733815 | -1.275931 |
| H | 2.855677 | -1.951518 | -0.062030 |
| C | -2.035184 | 0.207199 | -0.147753 |
| O | -1.555513 | 0.875791 | -1.029512 |
| C | -3.493072 | -0.137548 | -0.043314 |
| H | -3.613029 | -1.214410 | -0.165865 |
| H | -3.870941 | 0.129451 | 0.942267 |
| H | -4.049962 | 0.384212 | -0.814720 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.956326 | 0.954550 | -0.099124 |
| C | 0.049365 | -0.201404 | -0.191514 |
| H | 0.198922 | -0.440523 | -1.246090 |
| C | -1.088983 | 1.481658 | 1.333008 |
| C | -0.497176 | 2.098039 | -1.005146 |
| C | -0.386161 | -1.458742 | 0.546215 |
| C | -1.734722 | -1.943984 | 0.015424 |
| H | -1.619669 | -2.244052 | -1.030581 |
| H | -2.055180 | -2.828043 | 0.567661 |
| C | -2.307498 | 0.421797 | -0.612856 |
| C | -2.786003 | -0.839142 | 0.106192 |
| H | -2.992521 | -0.617719 | 1.156130 |
| H | -3.725273 | -1.176904 | -0.334534 |
| H | -0.139215 | 1.884559 | 1.685209 |
| H | -1.410179 | 0.714411 | 2.035998 |
| H | -0.378166 | 1.755162 | -2.035082 |
| H | 0.454995 | 2.510052 | -0.668699 |
| H | -0.458279 | -1.243609 | 1.614647 |
| H | -3.048863 | 1.219578 | -0.525707 |
| H | -2.205788 | 0.197918 | -1.679971 |
| H | 0.378204 | -2.225740 | 0.417099 |
| O | 1.310017 | 0.261504 | 0.340501 |
| H | -1.234433 | 2.903130 | -0.999081 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.826456 | 2.286185 | 1.357953 |
| C | 2.429509 | -0.291108 | -0.137975 |
| O | 2.445282 | -1.143882 | -0.991847 |
| C | 3.646591 | 0.288092 | 0.518574 |
| H | 3.661884 | 1.367607 | 0.372569 |
| H | 3.605725 | 0.097330 | 1.590653 |
| H | 4.540332 | -0.158856 | 0.095809 |

eq2

```
=====
```

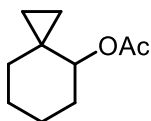
| | | | |
|---|-----------|-----------|-----------|
| C | -0.719205 | 0.926281 | 0.026715 |
| C | -0.022776 | -0.434159 | -0.140682 |
| H | 0.149683 | -0.601569 | -1.203905 |
| C | -0.836269 | 1.324642 | 1.501130 |
| C | 0.080622 | 2.002476 | -0.709084 |
| C | -0.811178 | -1.602896 | 0.427753 |
| C | -2.192881 | -1.675521 | -0.222220 |
| H | -2.074293 | -1.897043 | -1.287179 |
| H | -2.764799 | -2.495695 | 0.212988 |
| C | -2.112359 | 0.805656 | -0.619117 |
| C | -2.942683 | -0.353201 | -0.068731 |
| H | -3.171692 | -0.183497 | 0.986098 |
| H | -3.897782 | -0.401192 | -0.594090 |
| H | 0.151252 | 1.439424 | 1.948955 |
| H | -1.390550 | 0.597129 | 2.092208 |
| H | 0.196339 | 1.752958 | -1.765078 |
| H | 1.075483 | 2.124701 | -0.275824 |
| H | -0.909349 | -1.489154 | 1.509504 |
| H | -2.638853 | 1.753921 | -0.487300 |
| H | -1.981345 | 0.661933 | -1.696823 |
| H | -0.252422 | -2.522528 | 0.247190 |
| O | 1.259307 | -0.405968 | 0.524002 |
| H | -0.432627 | 2.963542 | -0.638638 |
| H | -1.355024 | 2.282044 | 1.579419 |
| C | 2.374316 | -0.329705 | -0.212360 |
| O | 2.393509 | -0.329472 | -1.418408 |
| C | 3.589281 | -0.240524 | 0.662061 |
| H | 3.544729 | 0.683217 | 1.239457 |
| H | 3.601973 | -1.072316 | 1.364863 |
| H | 4.485545 | -0.250642 | 0.050620 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.774179 | 0.971501 | 0.040282 |
| C | -0.074407 | -0.180120 | -0.701931 |
| H | -0.380424 | -0.098924 | -1.748024 |
| C | -0.388386 | 1.055009 | 1.519543 |
| C | -0.423076 | 2.300156 | -0.632125 |
| C | -0.476144 | -1.572108 | -0.229353 |
| C | -1.983164 | -1.744281 | -0.425537 |
| H | -2.225808 | -1.678008 | -1.490513 |
| H | -2.287426 | -2.735500 | -0.087503 |
| C | -2.290580 | 0.730254 | -0.111924 |
| C | -2.745014 | -0.658862 | 0.333521 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.576867 | -0.782041 | 1.406557 |
| H | -3.818454 | -0.762928 | 0.167573 |
| H | 0.661353 | 1.324670 | 1.634591 |
| H | -0.550197 | 0.118636 | 2.050501 |
| H | -0.663329 | 2.275652 | -1.697144 |
| H | 0.637489 | 2.530269 | -0.526105 |
| H | -0.226942 | -1.715721 | 0.818448 |
| H | -2.819431 | 1.506308 | 0.446114 |
| H | -2.554488 | 0.861543 | -1.166492 |
| H | 0.078911 | -2.315138 | -0.805423 |
| O | 1.357387 | 0.035009 | -0.808733 |
| H | -0.992307 | 3.111828 | -0.174808 |
| H | -0.987726 | 1.829957 | 2.002251 |
| C | 2.234926 | -0.353076 | 0.120535 |
| O | 1.956590 | -0.904109 | 1.156011 |
| C | 3.633839 | -0.007989 | -0.304969 |
| H | 3.868381 | -0.520584 | -1.237440 |
| H | 3.707072 | 1.063708 | -0.487094 |
| H | 4.335481 | -0.303839 | 0.468033 |



spiro[2.5]octan-4-yl acetate

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -541.101469 | -540.841047 | -540.891543 |
| ax2 | -541.100662 | -540.840294 | -540.891807 |
| ax3 | -541.089474 | -540.82871 | -540.879811 |
| eq | -541.100405 | -540.840034 | -540.890852 |
| eq2 | -541.100513 | -540.840117 | -540.890322 |
| eq3 | -541.092173 | -540.83174 | -540.882344 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 1.204212 | -0.741685 | -0.110568 |
| C | -0.026662 | -0.217212 | 0.582676 |
| H | -0.348961 | -0.912687 | 1.356228 |
| C | 2.138066 | -1.554281 | 0.739077 |
| C | 1.305362 | -2.218869 | -0.328534 |
| C | 0.212311 | 1.169505 | 1.169874 |
| C | 0.787045 | 2.135908 | 0.133119 |
| H | 0.045210 | 2.310020 | -0.651065 |
| H | 0.984445 | 3.099757 | 0.603738 |
| C | 1.800633 | 0.209468 | -1.127037 |
| C | 2.063666 | 1.577550 | -0.496436 |
| H | 2.831846 | 1.475379 | 0.276327 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.450298 | 2.269267 | -1.246186 |
| H | 1.865887 | -1.731832 | 1.770232 |
| H | 3.197224 | -1.440799 | 0.555073 |
| H | 1.810422 | -2.555622 | -1.222979 |
| H | 0.475976 | -2.833466 | -0.006742 |
| H | 0.919102 | 1.054788 | 1.995987 |
| H | 2.721346 | -0.219334 | -1.526274 |
| H | 1.106579 | 0.324726 | -1.964786 |
| H | -0.718892 | 1.550805 | 1.589047 |
| O | -1.073734 | -0.148811 | -0.419173 |
| C | -2.338799 | -0.160608 | 0.011529 |
| O | -2.648738 | -0.248189 | 1.174925 |
| C | -3.306284 | -0.055656 | -1.128940 |
| H | -3.147838 | 0.888345 | -1.650054 |
| H | -3.126811 | -0.862082 | -1.838779 |
| H | -4.323357 | -0.105985 | -0.754342 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.806347 | 0.862277 | 0.144689 |
| C | 0.013564 | -0.054000 | -0.756120 |
| H | -0.443775 | 0.512868 | -1.564349 |
| C | 1.462736 | 2.037015 | -0.521104 |
| C | 0.284224 | 2.243742 | 0.397428 |
| C | 0.882449 | -1.177145 | -1.306110 |
| C | 1.634026 | -1.919218 | -0.200242 |
| H | 0.916909 | -2.439579 | 0.439807 |
| H | 2.277526 | -2.680151 | -0.643422 |
| C | 1.568411 | 0.143214 | 1.238596 |
| C | 2.458733 | -0.951560 | 0.649216 |
| H | 3.229527 | -0.489801 | 0.024436 |
| H | 2.970897 | -1.490497 | 1.447542 |
| H | 1.300537 | 2.178128 | -1.580784 |
| H | 2.441173 | 2.325048 | -0.162898 |
| H | 0.477577 | 2.673558 | 1.370454 |
| H | -0.658648 | 2.515202 | -0.053675 |
| H | 1.599949 | -0.724107 | -1.994967 |
| H | 2.161349 | 0.866957 | 1.800476 |
| H | 0.857980 | -0.306438 | 1.938830 |
| H | 0.260674 | -1.860924 | -1.885356 |
| O | -1.046057 | -0.682897 | 0.010055 |
| C | -2.266058 | -0.135320 | -0.018180 |
| O | -2.556711 | 0.838000 | -0.669323 |
| C | -3.218871 | -0.893844 | 0.856787 |
| H | -3.235885 | -1.941937 | 0.561175 |
| H | -2.874410 | -0.844616 | 1.889637 |
| H | -4.212597 | -0.465501 | 0.777477 |

ax3

```
=====
```

| | | | |
|---|----------|-----------|-----------|
| C | 0.947790 | -0.820678 | -0.085584 |
| C | 0.072875 | -0.223620 | 1.001510 |
| H | 0.201361 | -0.831594 | 1.894274 |
| C | 1.948157 | -1.840035 | 0.408205 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.746534 | -2.275533 | -0.384383 |
| C | 0.452941 | 1.215159 | 1.367681 |
| C | 0.936297 | 2.106333 | 0.221430 |
| H | 0.101228 | 2.391224 | -0.415556 |
| H | 1.352557 | 3.020517 | 0.648463 |
| C | 1.433626 | 0.092434 | -1.196830 |
| C | 1.992379 | 1.393188 | -0.621801 |
| H | 2.864665 | 1.168114 | 0.000910 |
| H | 2.332847 | 2.043714 | -1.428783 |
| H | 1.964570 | -2.071953 | 1.463507 |
| H | 2.910619 | -1.857133 | -0.083017 |
| H | 0.902571 | -2.594392 | -1.405510 |
| H | -0.042576 | -2.792073 | 0.143842 |
| H | 1.270560 | 1.126918 | 2.088601 |
| H | 2.202912 | -0.435269 | -1.764088 |
| H | 0.617350 | 0.321750 | -1.879873 |
| H | -0.382249 | 1.672435 | 1.900470 |
| O | -1.360417 | -0.414278 | 0.796054 |
| C | -2.020690 | 0.110449 | -0.233066 |
| O | -1.525033 | 0.810481 | -1.081001 |
| C | -3.468999 | -0.285136 | -0.199664 |
| H | -3.550384 | -1.369937 | -0.262544 |
| H | -3.913822 | 0.027672 | 0.744227 |
| H | -3.994072 | 0.175012 | -1.030332 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.999373 | 0.862870 | -0.222243 |
| C | 0.039306 | -0.238494 | -0.236037 |
| H | 0.186047 | -0.578628 | -1.263030 |
| C | -0.961549 | 1.891493 | 0.868132 |
| C | -0.608335 | 2.267524 | -0.553222 |
| C | -0.394807 | -1.408498 | 0.636285 |
| C | -1.756262 | -1.936804 | 0.182346 |
| H | -1.665084 | -2.340215 | -0.830678 |
| H | -2.064719 | -2.760570 | 0.826786 |
| C | -2.354152 | 0.352379 | -0.671208 |
| C | -2.807784 | -0.827401 | 0.188989 |
| H | -2.963130 | -0.483551 | 1.215862 |
| H | -3.763682 | -1.209677 | -0.171783 |
| H | -0.151456 | 1.850405 | 1.581510 |
| H | -1.909441 | 2.233498 | 1.259857 |
| H | -1.319909 | 2.861002 | -1.110148 |
| H | 0.431781 | 2.470126 | -0.763983 |
| H | -0.458016 | -1.057861 | 1.670320 |
| H | -3.077654 | 1.167941 | -0.626492 |
| H | -2.289783 | 0.032872 | -1.716681 |
| H | 0.360346 | -2.193651 | 0.592975 |
| O | 1.286346 | 0.297018 | 0.242406 |
| C | 2.414582 | -0.303186 | -0.158348 |
| O | 2.438810 | -1.250764 | -0.903816 |
| C | 3.621475 | 0.353908 | 0.439300 |
| H | 3.610687 | 1.419667 | 0.215080 |
| H | 3.591873 | 0.240353 | 1.522964 |

H 4.522276 -0.104495 0.044765

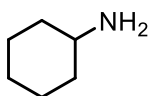
eq2

```
=====
C 0.714700 0.842211 0.103238
C 0.053500 -0.522079 0.140688
H -0.088390 -0.824182 1.178634
C 0.516526 1.707753 -1.106051
C -0.103298 2.088689 0.217927
C 0.905159 -1.552334 -0.583346
C 2.304270 -1.609072 0.032675
H 2.225815 -1.961459 1.065563
H 2.913594 -2.335158 -0.506306
C 2.096992 0.802746 0.723532
C 2.974031 -0.234764 0.021532
H 3.138544 0.078256 -1.013680
H 3.951899 -0.288093 0.502080
H -0.152369 1.357380 -1.878989
H 1.365927 2.280936 -1.450812
H 0.331075 2.916908 0.760238
H -1.176764 1.998904 0.306845
H 0.972469 -1.271424 -1.638024
H 2.547095 1.795146 0.666332
H 2.009940 0.546044 1.784450
H 0.418133 -2.526789 -0.527520
O -1.233179 -0.486406 -0.501671
C -2.327148 -0.356415 0.263314
O -2.304763 -0.301715 1.467271
C -3.564555 -0.281740 -0.578726
H -3.527172 0.625458 -1.182657
H -3.604189 -1.132409 -1.257293
H -4.443139 -0.264509 0.057645
```

eq3

```
=====
C -0.814702 0.919137 -0.157926
C -0.102208 -0.299931 -0.712010
H -0.394416 -0.387974 -1.761820
C -0.263565 1.668591 1.017870
C -0.240290 2.285957 -0.361235
C -0.539394 -1.581849 -0.011735
C -2.052282 -1.743827 -0.178374
H -2.298972 -1.840847 -1.239990
H -2.375951 -2.662589 0.311703
C -2.320525 0.755933 -0.259026
C -2.790620 -0.538398 0.404502
H -2.596414 -0.484202 1.479758
H -3.867793 -0.653661 0.275960
H 0.678555 1.353415 1.438729
H -0.977081 2.057157 1.731458
H -0.934495 3.088248 -0.569245
H 0.721152 2.366349 -0.847487
H -0.296997 -1.534286 1.046999
H -2.805299 1.623630 0.191147
```


| | | | |
|---|-----------|-----------|-----------|
| H | -2.604669 | 0.738955 | -1.316560 |
| H | -0.005854 | -2.430950 | -0.442935 |
| O | 1.327108 | -0.107031 | -0.823896 |
| C | 2.198169 | -0.373071 | 0.156355 |
| O | 1.908468 | -0.758565 | 1.260735 |
| C | 3.601632 | -0.117967 | -0.312213 |
| H | 3.821051 | -0.750050 | -1.171961 |
| H | 3.695739 | 0.920153 | -0.629776 |
| H | 4.299551 | -0.326032 | 0.492060 |



cyclohexanamine

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -291.187901 | -290.991647 | -291.029768 |
| ax2 | -291.188025 | -290.991689 | -291.029826 |
| eq | -291.190040 | -290.993874 | -291.032066 |
| eq2 | -291.189840 | -290.993727 | -291.032056 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.277597 | -1.259473 | 0.604168 |
| C | 1.135141 | -0.000015 | 0.458684 |
| H | 1.874583 | -0.000047 | 1.267608 |
| C | 0.277625 | 1.259465 | 0.604162 |
| C | -0.937104 | 1.258284 | -0.324841 |
| H | -1.537907 | 2.151432 | -0.144316 |
| H | -0.604464 | 1.301854 | -1.364545 |
| C | -0.937126 | -1.258274 | -0.324847 |
| C | -1.780167 | 0.000012 | -0.119555 |
| H | -2.634045 | 0.000022 | -0.799364 |
| H | -2.182045 | 0.000012 | 0.899255 |
| H | -0.065458 | 1.319565 | 1.641013 |
| H | -0.604488 | -1.301851 | -1.364551 |
| H | -1.537939 | -2.151414 | -0.144309 |
| H | 0.898289 | 2.140742 | 0.422831 |
| H | 0.898258 | -2.140756 | 0.422856 |
| H | -0.065485 | -1.319503 | 1.641018 |
| N | 1.792569 | 0.000001 | -0.857579 |
| H | 2.398509 | 0.810987 | -0.930476 |
| H | 2.398419 | -0.811044 | -0.930585 |

ax2

| | | | |
|---|----------|-----------|----------|
| C | 0.244971 | -1.275554 | 0.614654 |
|---|----------|-----------|----------|

| | | | |
|---|-----------|-----------|-----------|
| C | 1.149912 | -0.051828 | 0.452331 |
| H | 1.915969 | -0.085132 | 1.229330 |
| C | 0.332968 | 1.236118 | 0.633922 |
| C | -0.877133 | 1.289492 | -0.299911 |
| H | -1.448321 | 2.200680 | -0.115351 |
| H | -0.540083 | 1.338955 | -1.339916 |
| C | -0.965279 | -1.229150 | -0.320958 |
| C | -1.764835 | 0.057963 | -0.116764 |
| H | -2.610576 | 0.093086 | -0.805604 |
| H | -2.176898 | 0.063246 | 0.897616 |
| H | -0.015404 | 1.283767 | 1.670376 |
| H | -0.636430 | -1.289694 | -1.363064 |
| H | -1.597908 | -2.100904 | -0.146311 |
| H | 0.981141 | 2.100611 | 0.472424 |
| H | 0.828844 | -2.181805 | 0.445206 |
| H | -0.111778 | -1.304533 | 1.647894 |
| N | 1.862403 | -0.127082 | -0.833484 |
| H | 1.199919 | -0.084576 | -1.600951 |
| H | 2.451083 | 0.693620 | -0.936909 |

eq

```
=====
```

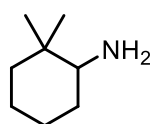
| | | | |
|---|-----------|-----------|-----------|
| C | -0.307334 | -1.252566 | -0.194649 |
| C | -1.018668 | 0.000009 | 0.306582 |
| H | -0.962185 | -0.000027 | 1.404282 |
| C | -0.307201 | 1.252612 | -0.194557 |
| C | 1.163882 | 1.260280 | 0.219836 |
| H | 1.657504 | 2.151969 | -0.169573 |
| H | 1.231544 | 1.310014 | 1.311002 |
| C | 1.163737 | -1.260321 | 0.219920 |
| C | 1.877768 | -0.000077 | -0.269277 |
| H | 2.916660 | -0.000119 | 0.064868 |
| H | 1.892694 | -0.000137 | -1.363732 |
| H | -0.383269 | 1.276146 | -1.286520 |
| H | 1.231247 | -1.309886 | 1.311114 |
| H | 1.657340 | -2.152101 | -0.169272 |
| H | -0.818264 | 2.141156 | 0.184699 |
| H | -0.818460 | -2.141170 | 0.184379 |
| H | -0.383229 | -1.275958 | -1.286633 |
| N | -2.409634 | 0.000030 | -0.161875 |
| H | -2.893707 | -0.810897 | 0.210838 |
| H | -2.893544 | 0.811184 | 0.210538 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.329526 | 1.242136 | 0.177078 |
| C | -1.023852 | -0.020792 | -0.338230 |
| H | -0.978222 | -0.012601 | -1.432317 |
| C | -0.295249 | -1.266170 | 0.157488 |
| C | 1.186581 | -1.243118 | -0.216638 |
| H | 1.684689 | -2.130436 | 0.177274 |
| H | 1.280585 | -1.283078 | -1.306358 |
| C | 1.149937 | 1.273738 | -0.207023 |
| C | 1.870585 | 0.023771 | 0.296236 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.917327 | 0.039213 | -0.012106 |
| H | 1.858745 | 0.020178 | 1.390821 |
| H | -0.395517 | -1.310295 | 1.248364 |
| H | 1.237081 | 1.322837 | -1.297041 |
| H | 1.622918 | 2.173426 | 0.189987 |
| H | -0.781478 | -2.155833 | -0.246765 |
| H | -0.846900 | 2.124020 | -0.208353 |
| H | -0.424396 | 1.262413 | 1.268778 |
| N | -2.441704 | -0.105074 | 0.033926 |
| H | -2.512377 | -0.108098 | 1.048191 |
| H | -2.921382 | 0.736374 | -0.271427 |



2,2-dimethylcyclohexan-1-amine

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -369.802433 | -369.547346 | -369.59069 |
| ax2 | -369.802471 | -369.547233 | -369.590521 |
| ax3 | -369.801475 | -369.546479 | -369.590244 |
| eq | -369.803758 | -369.548844 | -369.592656 |
| eq2 | -369.804163 | -369.549197 | -369.592894 |
| eq3 | -369.803628 | -369.548776 | -369.592573 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 1.320959 | 0.682734 | 0.926673 |
| C | -0.116974 | 0.999216 | 0.502481 |
| H | -0.649377 | 1.397984 | 1.376161 |
| C | -0.880690 | -0.271158 | 0.054203 |
| C | -0.064075 | -1.040765 | -0.998649 |
| H | -0.596254 | -1.962595 | -1.249104 |
| H | -0.020704 | -0.440631 | -1.911421 |
| C | 2.097485 | -0.074870 | -0.150823 |
| C | 1.363955 | -1.354033 | -0.551263 |
| H | 1.898993 | -1.859413 | -1.357313 |
| H | 1.348952 | -2.044746 | 0.296136 |
| H | 2.216697 | 0.560943 | -1.031223 |
| H | 3.099572 | -0.308341 | 0.213155 |
| H | 1.826904 | 1.620007 | 1.172312 |
| H | 1.302486 | 0.090319 | 1.843432 |
| N | -0.073192 | 1.993867 | -0.582349 |
| H | -0.998709 | 2.375995 | -0.740006 |
| H | 0.501273 | 2.775600 | -0.284214 |
| C | -1.148245 | -1.156361 | 1.277288 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.761323 | -0.623336 | 2.007420 |
| H | -1.691635 | -2.054484 | 0.976784 |
| H | -0.234959 | -1.473730 | 1.778097 |
| C | -2.235248 | 0.112507 | -0.546546 |
| H | -2.819471 | -0.785160 | -0.758996 |
| H | -2.811390 | 0.730312 | 0.147517 |
| H | -2.121705 | 0.660595 | -1.482479 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.305538 | 0.668569 | 0.971198 |
| C | -0.122953 | 1.000961 | 0.525682 |
| H | -0.669963 | 1.401125 | 1.384083 |
| C | -0.879854 | -0.273021 | 0.053032 |
| C | -0.051940 | -1.007094 | -1.016978 |
| H | -0.572982 | -1.926743 | -1.296538 |
| H | -0.014271 | -0.387170 | -1.919075 |
| C | 2.096409 | -0.042203 | -0.128323 |
| C | 1.379901 | -1.315576 | -0.576953 |
| H | 1.923184 | -1.786570 | -1.398055 |
| H | 1.371241 | -2.034010 | 0.246806 |
| H | 2.219721 | 0.625126 | -0.987038 |
| H | 3.100387 | -0.275705 | 0.229588 |
| H | 1.802874 | 1.595137 | 1.261416 |
| H | 1.274014 | 0.030524 | 1.856124 |
| N | -0.064053 | 2.088350 | -0.463505 |
| H | 0.330462 | 1.749571 | -1.335134 |
| H | -1.001951 | 2.400482 | -0.687327 |
| C | -1.136950 | -1.189005 | 1.255962 |
| H | -1.736674 | -0.669522 | 2.007036 |
| H | -1.691402 | -2.075456 | 0.940936 |
| H | -0.220514 | -1.525896 | 1.737053 |
| C | -2.239277 | 0.104344 | -0.538886 |
| H | -2.814089 | -0.796268 | -0.763922 |
| H | -2.819970 | 0.705366 | 0.165973 |
| H | -2.136939 | 0.669705 | -1.465795 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.323395 | 0.631404 | 0.958261 |
| C | -0.096773 | 1.010526 | 0.505828 |
| H | -0.626623 | 1.442032 | 1.359970 |
| C | -0.899744 | -0.233158 | 0.051083 |
| C | -0.099489 | -1.017099 | -1.006340 |
| H | -0.659957 | -1.917403 | -1.272059 |
| H | -0.032167 | -0.416079 | -1.919339 |
| C | 2.086631 | -0.136743 | -0.121337 |
| C | 1.314863 | -1.383060 | -0.553898 |
| H | 1.840341 | -1.890325 | -1.364914 |
| H | 1.269287 | -2.088551 | 0.279639 |
| H | 2.243690 | 0.507862 | -0.991503 |
| H | 3.077080 | -0.409516 | 0.246292 |
| H | 1.857734 | 1.546592 | 1.224106 |
| H | 1.272233 | 0.024147 | 1.864837 |

| | | | |
|---|-----------|-----------|-----------|
| N | -0.094383 | 2.046140 | -0.541775 |
| H | 0.487810 | 2.818227 | -0.232707 |
| H | 0.354154 | 1.689154 | -1.379614 |
| C | -1.186988 | -1.124130 | 1.266317 |
| H | -1.786299 | -0.581325 | 2.000668 |
| H | -1.753482 | -2.004777 | 0.956835 |
| H | -0.283555 | -1.470669 | 1.764741 |
| C | -2.246069 | 0.182316 | -0.544986 |
| H | -2.850360 | -0.703311 | -0.753496 |
| H | -2.801400 | 0.813484 | 0.153076 |
| H | -2.122751 | 0.737156 | -1.473673 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.655077 | -0.554579 | -0.009398 |
| C | 0.351714 | 0.915418 | -0.379956 |
| H | 0.249171 | 0.931789 | -1.475246 |
| C | -0.974537 | 1.401604 | 0.199628 |
| C | -2.138905 | 0.518597 | -0.243326 |
| H | -3.068379 | 0.865393 | 0.210809 |
| H | -2.261926 | 0.604933 | -1.327414 |
| C | -0.542823 | -1.411514 | -0.459373 |
| C | -1.880309 | -0.944454 | 0.112946 |
| H | -2.684964 | -1.573954 | -0.271189 |
| H | -1.882702 | -1.060451 | 1.199752 |
| H | -0.908599 | 1.416741 | 1.290671 |
| H | -0.599477 | -1.378747 | -1.552890 |
| H | -0.352167 | -2.452127 | -0.184553 |
| H | -1.138928 | 2.433578 | -0.121208 |
| N | 1.424701 | 1.814934 | 0.063905 |
| H | 2.283233 | 1.608230 | -0.435107 |
| H | 1.180577 | 2.766765 | -0.190258 |
| C | 1.898301 | -1.028240 | -0.767196 |
| H | 1.784157 | -0.871771 | -1.842397 |
| H | 2.797425 | -0.504291 | -0.437653 |
| H | 2.061557 | -2.094670 | -0.597115 |
| C | 0.904891 | -0.734395 | 1.491374 |
| H | 1.065182 | -1.792160 | 1.711886 |
| H | 1.792906 | -0.186825 | 1.805597 |
| H | 0.069569 | -0.391597 | 2.100783 |

eq2

```
=====
```

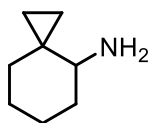
| | | | |
|---|-----------|-----------|-----------|
| C | 0.653629 | -0.550166 | -0.015725 |
| C | 0.350697 | 0.918421 | -0.420208 |
| H | 0.267758 | 0.922363 | -1.513089 |
| C | -0.980994 | 1.413588 | 0.142868 |
| C | -2.146099 | 0.507163 | -0.246618 |
| H | -3.071419 | 0.870419 | 0.203389 |
| H | -2.281547 | 0.548371 | -1.332013 |
| C | -0.551532 | -1.420812 | -0.416962 |
| C | -1.878539 | -0.938836 | 0.164495 |
| H | -2.688246 | -1.585253 | -0.178741 |
| H | -1.858906 | -1.011439 | 1.255032 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.909159 | 1.475118 | 1.233495 |
| H | -0.628507 | -1.417300 | -1.509944 |
| H | -0.354620 | -2.453935 | -0.118688 |
| H | -1.150847 | 2.429271 | -0.218472 |
| N | 1.391442 | 1.892747 | -0.072718 |
| H | 1.478105 | 1.948271 | 0.937514 |
| H | 2.294460 | 1.584749 | -0.416525 |
| C | 1.880421 | -1.053383 | -0.779963 |
| H | 1.739304 | -0.948023 | -1.858067 |
| H | 2.785111 | -0.511077 | -0.499114 |
| H | 2.053366 | -2.110052 | -0.564596 |
| C | 0.930909 | -0.679376 | 1.485562 |
| H | 1.086428 | -1.729116 | 1.743587 |
| H | 1.835314 | -0.136246 | 1.764953 |
| H | 0.112363 | -0.304943 | 2.099611 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.662847 | -0.554405 | -0.024645 |
| C | 0.356187 | 0.910725 | -0.414310 |
| H | 0.280341 | 0.928708 | -1.507063 |
| C | -0.981905 | 1.400780 | 0.150590 |
| C | -2.146997 | 0.496642 | -0.244573 |
| H | -3.075964 | 0.860305 | 0.197772 |
| H | -2.275558 | 0.531037 | -1.331182 |
| C | -0.548106 | -1.427017 | -0.405686 |
| C | -1.873864 | -0.944509 | 0.178436 |
| H | -2.682168 | -1.598141 | -0.154321 |
| H | -1.848361 | -1.005392 | 1.269706 |
| H | -0.910230 | 1.454362 | 1.241415 |
| H | -0.633268 | -1.434697 | -1.497944 |
| H | -0.346481 | -2.456489 | -0.098309 |
| H | -1.152274 | 2.420145 | -0.204046 |
| N | 1.473859 | 1.796949 | -0.057502 |
| H | 1.290142 | 2.720327 | -0.436860 |
| H | 1.490897 | 1.919365 | 0.951065 |
| C | 1.876629 | -1.058576 | -0.807934 |
| H | 1.712841 | -0.959552 | -1.883467 |
| H | 2.776821 | -0.502509 | -0.548799 |
| H | 2.054057 | -2.114308 | -0.590528 |
| C | 0.963769 | -0.683343 | 1.473100 |
| H | 1.123450 | -1.733087 | 1.728405 |
| H | 1.873209 | -0.140869 | 1.737174 |
| H | 0.154173 | -0.309626 | 2.099633 |



spiro[2.5]octan-4-amine

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -368.572634 | -368.340878 | -368.38288 |
| ax2 | -368.572914 | -368.341009 | -368.382958 |
| ax3 | -368.571943 | -368.340034 | -368.381978 |
| eq | -368.572147 | -368.34033 | -368.382264 |
| eq2 | -368.572339 | -368.340575 | -368.382529 |
| eq3 | -368.572712 | -368.340824 | -368.382688 |

ax

```

=====
C  -0.827486   -0.152769   -0.050922
C  -0.029907   1.081455    0.326673
H  -0.607416   1.635351    1.076633
C  -1.770268  -0.695579    0.982105
C  -2.304692   0.007574   -0.243888
C   1.307419   0.674375    0.951179
C   2.083752  -0.316316    0.081515
H   2.377311   0.168301   -0.852415
H   3.002705  -0.609261    0.592021
C  -0.074879  -1.148378   -0.909385
C   1.238490  -1.550318   -0.236684
H   1.015801  -2.084246    0.692701
H   1.795510  -2.236946   -0.876284
H  -1.845258  -0.175987    1.927500
H  -1.889188  -1.768897    1.036191
H  -2.783663  -0.597304   -1.001368
H  -2.727749   0.993813   -0.106477
H   1.102500   0.215508    1.922503
H  -0.703668  -2.023195   -1.086349
H   0.140638  -0.700460   -1.883197
H   1.905065   1.569588    1.139635
N   0.209835   1.896802   -0.873452
H  -0.681948   2.188110   -1.261140
H   0.695933   2.747756   -0.609351

```

ax2

```

=====
C  -0.830239  -0.150886   -0.052146
C  -0.039387   1.092045    0.334501
H  -0.627935   1.653204    1.064282
C  -1.772356  -0.708941    0.973199
C  -2.306087  -0.003457   -0.252364
C   1.283493   0.677677    0.984050

```

| | | | |
|---|-----------|-----------|-----------|
| C | 2.080871 | -0.291359 | 0.107000 |
| H | 2.390750 | 0.206360 | -0.817153 |
| H | 2.996976 | -0.582161 | 0.623230 |
| C | -0.061677 | -1.130544 | -0.915037 |
| C | 1.251338 | -1.528882 | -0.239162 |
| H | 1.026993 | -2.078225 | 0.680505 |
| H | 1.820536 | -2.199784 | -0.884526 |
| H | -1.854738 | -0.192915 | 1.920257 |
| H | -1.885701 | -1.783214 | 1.023871 |
| H | -2.776799 | -0.609088 | -1.014606 |
| H | -2.738750 | 0.978587 | -0.113416 |
| H | 1.058398 | 0.186318 | 1.934425 |
| H | -0.680385 | -2.008152 | -1.111484 |
| H | 0.157075 | -0.671860 | -1.885261 |
| H | 1.871606 | 1.569307 | 1.206836 |
| N | 0.216622 | 2.004266 | -0.790278 |
| H | 0.757669 | 1.527851 | -1.504823 |
| H | -0.667796 | 2.239991 | -1.230445 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.845438 | -0.114777 | -0.066907 |
| C | -0.011505 | 1.096321 | 0.310444 |
| H | -0.583724 | 1.694059 | 1.023366 |
| C | -1.798685 | -0.635178 | 0.969236 |
| C | -2.316011 | 0.072768 | -0.261206 |
| C | 1.287456 | 0.631236 | 0.986980 |
| C | 2.054648 | -0.376474 | 0.128467 |
| H | 2.391353 | 0.103950 | -0.795409 |
| H | 2.953357 | -0.701263 | 0.654826 |
| C | -0.109559 | -1.133451 | -0.914489 |
| C | 1.178953 | -1.580620 | -0.221393 |
| H | 0.920931 | -2.115430 | 0.697952 |
| H | 1.727393 | -2.278011 | -0.856572 |
| H | -1.861305 | -0.109122 | 1.912020 |
| H | -1.939452 | -1.705722 | 1.029843 |
| H | -2.806993 | -0.526412 | -1.015685 |
| H | -2.714188 | 1.070238 | -0.134778 |
| H | 1.032115 | 0.163328 | 1.942695 |
| H | -0.763112 | -1.986785 | -1.105298 |
| H | 0.134467 | -0.698680 | -1.889836 |
| H | 1.910226 | 1.500781 | 1.208525 |
| N | 0.205106 | 1.947823 | -0.870619 |
| H | 0.769600 | 2.747997 | -0.602166 |
| H | 0.754432 | 1.447372 | -1.561935 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.600247 | -0.502992 | -0.178626 |
| C | -0.274033 | 0.963348 | -0.436306 |
| H | -0.089064 | 1.066646 | -1.511012 |
| C | -1.450541 | -0.869033 | 1.004156 |
| C | -1.985828 | -1.021867 | -0.400989 |
| C | 1.011158 | 1.345001 | 0.308097 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.180367 | 0.423927 | -0.036906 |
| H | 2.424501 | 0.535093 | -1.098153 |
| H | 3.068119 | 0.716714 | 0.526029 |
| C | 0.555090 | -1.427824 | -0.511476 |
| C | 1.823707 | -1.034678 | 0.243463 |
| H | 1.658553 | -1.166105 | 1.317273 |
| H | 2.648718 | -1.690970 | -0.038465 |
| H | -1.872887 | -0.078719 | 1.608862 |
| H | -1.189626 | -1.767286 | 1.546980 |
| H | -2.080892 | -2.024462 | -0.795084 |
| H | -2.745532 | -0.321671 | -0.714137 |
| H | 0.807251 | 1.290681 | 1.383505 |
| H | 0.272416 | -2.457280 | -0.283208 |
| H | 0.750760 | -1.378745 | -1.588332 |
| H | 1.258886 | 2.383824 | 0.078231 |
| N | -1.400795 | 1.845103 | -0.115241 |
| H | -1.467947 | 1.947256 | 0.893355 |
| H | -1.195729 | 2.774001 | -0.467635 |

eq2

```
=====
```

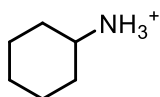
| | | | |
|---|-----------|-----------|-----------|
| C | -0.589673 | -0.509359 | -0.175836 |
| C | -0.281726 | 0.962148 | -0.420452 |
| H | -0.050666 | 1.062421 | -1.490763 |
| C | -1.365313 | -0.907681 | 1.044498 |
| C | -1.983826 | -1.034488 | -0.328900 |
| C | 0.973991 | 1.350555 | 0.358017 |
| C | 2.160594 | 0.463549 | -0.017954 |
| H | 2.414659 | 0.633079 | -1.068844 |
| H | 3.036476 | 0.743388 | 0.569221 |
| C | 0.566577 | -1.404178 | -0.575488 |
| C | 1.835338 | -1.016607 | 0.185117 |
| H | 1.683089 | -1.208688 | 1.251481 |
| H | 2.674044 | -1.636012 | -0.136907 |
| H | -1.745968 | -0.122524 | 1.680772 |
| H | -1.067101 | -1.816615 | 1.548874 |
| H | -2.099485 | -2.027438 | -0.741365 |
| H | -2.777425 | -0.343272 | -0.575460 |
| H | 0.759756 | 1.255310 | 1.427206 |
| H | 0.305677 | -2.446810 | -0.384521 |
| H | 0.745682 | -1.306917 | -1.651676 |
| H | 1.208626 | 2.400368 | 0.165229 |
| N | -1.391742 | 1.835257 | -0.031349 |
| H | -1.085836 | 2.800530 | -0.095181 |
| H | -2.155104 | 1.742745 | -0.692636 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.590796 | -0.500050 | -0.177373 |
| C | -0.272503 | 0.973587 | -0.442123 |
| H | -0.070234 | 1.066208 | -1.515033 |
| C | -1.404183 | -0.878870 | 1.025222 |
| C | -1.978162 | -1.029833 | -0.364647 |
| C | 0.999613 | 1.361037 | 0.312622 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.174437 | 0.445670 | -0.028378 |
| H | 2.430868 | 0.573624 | -1.084681 |
| H | 3.053300 | 0.736561 | 0.549088 |
| C | 0.565495 | -1.413618 | -0.536524 |
| C | 1.829728 | -1.020849 | 0.226062 |
| H | 1.663629 | -1.172934 | 1.296940 |
| H | 2.662525 | -1.663126 | -0.065050 |
| H | -1.815570 | -0.093686 | 1.644382 |
| H | -1.122077 | -1.777306 | 1.556783 |
| H | -2.078256 | -2.030029 | -0.763113 |
| H | -2.765452 | -0.346111 | -0.650040 |
| H | 0.789721 | 1.304981 | 1.386982 |
| H | 0.292213 | -2.449452 | -0.326400 |
| H | 0.757719 | -1.342337 | -1.612673 |
| H | 1.244332 | 2.399803 | 0.085081 |
| N | -1.324506 | 1.936917 | -0.123126 |
| H | -2.186878 | 1.700609 | -0.601076 |
| H | -1.526075 | 1.912335 | 0.871523 |



cyclohexanaminium

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -291.653446 | -291.440894 | -291.478459 |
| eq | -291.655130 | -291.44356 | -291.481983 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.345993 | -0.580418 | -1.267796 |
| C | -0.255405 | -1.175273 | 0.000000 |
| H | -0.146526 | -2.257146 | 0.000000 |
| C | 0.345993 | -0.580418 | 1.267796 |
| C | 0.345993 | 0.949341 | 1.258848 |
| H | -0.679730 | 1.328007 | 1.313392 |
| H | 0.853901 | 1.310266 | 2.153127 |
| C | 0.345993 | 0.949341 | -1.258848 |
| C | 1.020995 | 1.492369 | -0.000000 |
| H | 2.072991 | 1.191896 | 0.000000 |
| H | 0.997099 | 2.582476 | -0.000000 |
| H | 1.374997 | -0.940877 | 1.322564 |
| H | 0.853901 | 1.310266 | -2.153127 |
| H | -0.679730 | 1.328007 | -1.313392 |
| H | -0.177888 | -0.970016 | 2.142426 |
| N | -1.745869 | -0.945722 | -0.000000 |
| H | -2.178448 | -1.364976 | -0.826262 |
| H | -2.178448 | -1.364976 | 0.826262 |

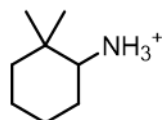
| | | | |
|---|-----------|-----------|-----------|
| H | -1.985524 | 0.048379 | -0.000000 |
| H | -0.177888 | -0.970016 | -2.142426 |
| H | 1.374997 | -0.940877 | -1.322564 |

eq

```

=====
C   0.095515   0.299968   1.262194
C  -0.571776   0.821771   0.000000
H  -1.631400   0.565404   0.000000
C   0.095515   0.299968  -1.262194
C   0.095515  -1.228833  -1.259218
H  -0.936795  -1.587123  -1.305821
H   0.602334  -1.592637  -2.152903
C   0.095515  -1.228833   1.259218
C   0.765197  -1.776946  -0.000000
H   1.821117  -1.490412  -0.000000
H   0.727077  -2.866748  -0.000000
H   1.126296   0.667901  -1.290044
H   0.602334  -1.592637   2.152903
H  -0.936795  -1.587123   1.305821
H  -0.421217   0.686783  -2.142209
N  -0.516593   2.321163   0.000000
H   0.454068   2.646414   0.000000
H  -0.974414   2.712392  -0.826794
H  -0.974414   2.712392   0.826794
H  -0.421217   0.686783   2.142209
H   1.126296   0.667901   1.290044

```



2,2-dimethylcyclohexan-1-aminium

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -370.267659 | -369.997031 | -370.04077 |
| eq | -370.268844 | -369.998268 | -370.042111 |

ax

```

=====
C  -0.885623  -0.308051   0.053088
C  -0.119122   0.920934   0.582129
H  -0.658569   1.348187   1.426502
C  -1.159180  -1.234062   1.243906
C  -2.233409   0.110099  -0.541985
C   1.327969   0.628749   0.969478
C   2.100626  -0.083436  -0.141529
H   2.224847   0.579555  -1.003965

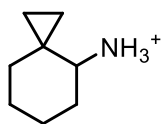
```

| | | | |
|---|-----------|-----------|-----------|
| H | 3.104182 | -0.316368 | 0.214103 |
| C | -0.053741 | -1.034384 | -1.020376 |
| C | 1.374392 | -1.353545 | -0.579812 |
| H | 1.361647 | -2.067691 | 0.246727 |
| H | 1.911259 | -1.829375 | -1.400980 |
| H | -0.247802 | -1.574544 | 1.731639 |
| H | -1.704348 | -2.113846 | 0.900248 |
| H | -2.119464 | 0.676279 | -1.469157 |
| H | -2.806657 | 0.712183 | 0.166888 |
| H | 1.311275 | 0.002750 | 1.861690 |
| H | -0.584632 | -1.946874 | -1.299303 |
| H | -0.013826 | -0.417606 | -1.924963 |
| H | 1.816608 | 1.563770 | 1.251169 |
| N | -0.113193 | 2.018400 | -0.454795 |
| H | -1.048196 | 2.399674 | -0.606083 |
| H | 0.486480 | 2.789335 | -0.152738 |
| H | 0.239483 | 1.691401 | -1.357603 |
| H | -2.818637 | -0.778769 | -0.779240 |
| H | -1.772758 | -0.724686 | 1.989247 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.607628 | -0.621733 | -0.016826 |
| C | -0.349633 | 0.842122 | -0.419981 |
| H | -0.315297 | 0.896663 | -1.509025 |
| C | -0.879348 | -0.770288 | 1.484290 |
| C | -1.799714 | -1.186759 | -0.794412 |
| C | 0.925010 | 1.441068 | 0.157893 |
| C | 2.136405 | 0.603887 | -0.245658 |
| H | 2.264077 | 0.660910 | -1.330324 |
| H | 3.035478 | 1.021802 | 0.206792 |
| C | 0.652700 | -1.412923 | -0.420951 |
| C | 1.948462 | -0.854924 | 0.163061 |
| H | 1.934196 | -0.931546 | 1.252872 |
| H | 2.791643 | -1.452771 | -0.184708 |
| H | -1.828255 | -0.309722 | 1.767940 |
| H | -0.093649 | -0.339466 | 2.102794 |
| H | -1.670717 | -1.045265 | -1.868856 |
| H | -2.745768 | -0.732056 | -0.493320 |
| H | 0.845937 | 1.484495 | 1.246939 |
| H | 0.509259 | -2.452015 | -0.118691 |
| H | 0.726539 | -1.405033 | -1.513188 |
| H | 1.029821 | 2.466271 | -0.201640 |
| N | -1.496972 | 1.729818 | -0.022228 |
| H | -1.599582 | 1.775769 | 0.994604 |
| H | -1.337360 | 2.683959 | -0.353733 |
| H | -2.385736 | 1.414198 | -0.415627 |
| H | -0.953651 | -1.830551 | 1.729698 |
| H | -1.885658 | -2.257075 | -0.601425 |



spiro[2.5]octan-4-aminium

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -369.037417 | -368.790075 | -368.832217 |
| eq | -369.034441 | -368.787147 | -368.829308 |

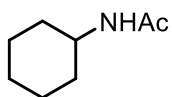
ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.834978 | -0.185668 | -0.045229 |
| C | -0.040280 | 1.012084 | 0.413532 |
| H | -0.612377 | 1.587925 | 1.138363 |
| C | -1.803541 | -0.741930 | 0.957148 |
| C | -2.309344 | -0.000818 | -0.253000 |
| C | 1.318499 | 0.622698 | 0.985418 |
| C | 2.084983 | -0.345974 | 0.081770 |
| H | 2.375675 | 0.150949 | -0.849360 |
| H | 3.010404 | -0.636366 | 0.578693 |
| C | -0.069189 | -1.159652 | -0.919061 |
| C | 1.239911 | -1.575551 | -0.248512 |
| H | 1.015709 | -2.119188 | 0.673766 |
| H | 1.795741 | -2.252050 | -0.898110 |
| H | -1.881965 | -0.248928 | 1.915735 |
| H | -1.922110 | -1.815737 | 0.977102 |
| H | -2.771469 | -0.577637 | -1.041210 |
| H | -2.723997 | 0.986006 | -0.096608 |
| H | 1.123567 | 0.140974 | 1.945504 |
| H | -0.700850 | -2.025492 | -1.120077 |
| H | 0.152696 | -0.698750 | -1.887955 |
| H | 1.902585 | 1.521827 | 1.188112 |
| N | 0.158096 | 1.953975 | -0.750510 |
| H | -0.742356 | 2.233658 | -1.146056 |
| H | 0.651938 | 2.798954 | -0.455430 |
| H | 0.703775 | 1.524891 | -1.501303 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | -0.555545 | -0.560200 | -0.176277 |
| C | -0.263800 | 0.903871 | -0.441261 |
| H | -0.109262 | 1.048994 | -1.511414 |
| C | -1.354814 | -0.984788 | 1.021180 |
| C | -1.916286 | -1.154697 | -0.370779 |
| C | 0.962328 | 1.375289 | 0.330221 |
| C | 2.175110 | 0.518129 | -0.027820 |
| H | 2.418288 | 0.667787 | -1.083552 |
| H | 3.036891 | 0.849856 | 0.550818 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.648054 | -1.411168 | -0.540177 |
| C | 1.893919 | -0.962318 | 0.221892 |
| H | 1.739544 | -1.126648 | 1.292117 |
| H | 2.752282 | -1.564236 | -0.077783 |
| H | -1.816675 | -0.239110 | 1.653832 |
| H | -1.016557 | -1.866855 | 1.546047 |
| H | -1.954478 | -2.152319 | -0.784340 |
| H | -2.748031 | -0.522949 | -0.651875 |
| H | 0.751167 | 1.293117 | 1.400778 |
| H | 0.417984 | -2.455912 | -0.328478 |
| H | 0.830721 | -1.329417 | -1.616343 |
| H | 1.151645 | 2.426535 | 0.105886 |
| N | -1.415448 | 1.793060 | -0.085872 |
| H | -1.623897 | 1.759285 | 0.915533 |
| H | -1.189421 | 2.764666 | -0.312919 |
| H | -2.265854 | 1.551082 | -0.599065 |



N-cyclohexylacetamide

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -443.851002 | -443.613224 | -443.660665 |
| ax2 | -443.839417 | -443.601308 | -443.649772 |
| eq | -443.852124 | -443.614545 | -443.662101 |
| eq2 | -443.848671 | -443.610942 | -443.658011 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 1.254584 | -0.984534 | -1.097624 |
| C | 0.152281 | 0.055377 | -0.891968 |
| H | -0.334085 | 0.261882 | -1.844851 |
| C | 0.730184 | 1.362865 | -0.336896 |
| C | 1.554209 | 1.129903 | 0.928672 |
| H | 1.971485 | 2.075490 | 1.277678 |
| H | 0.901184 | 0.759653 | 1.724923 |
| C | 2.096982 | -1.205855 | 0.161024 |
| C | 2.668647 | 0.113888 | 0.678772 |
| H | 3.241076 | -0.055411 | 1.592130 |
| H | 3.362219 | 0.519336 | -0.064791 |
| H | 1.367440 | 1.803843 | -1.108594 |
| H | 1.490828 | -1.667185 | 0.947132 |
| H | 2.900598 | -1.909809 | -0.059582 |
| H | -0.086326 | 2.060905 | -0.149467 |
| H | 0.813417 | -1.922340 | -1.439950 |
| H | 1.904178 | -0.620754 | -1.897189 |

| | | | |
|---|-----------|-----------|-----------|
| N | -0.878242 | -0.486315 | -0.009296 |
| C | -2.141223 | -0.015469 | 0.009381 |
| O | -2.515255 | 0.896729 | -0.721204 |
| C | -3.084615 | -0.681884 | 0.980513 |
| H | -2.611339 | -1.473601 | 1.557088 |
| H | -3.475397 | 0.075136 | 1.659345 |
| H | -3.923780 | -1.094011 | 0.421407 |
| H | -0.638049 | -1.228507 | 0.628176 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.955170 | 0.529727 | 1.422991 |
| C | -0.206955 | 1.221689 | 0.270233 |
| H | -0.176772 | 2.281589 | 0.519286 |
| C | -0.970428 | 1.108149 | -1.059436 |
| C | -1.541323 | -0.278010 | -1.359272 |
| H | -2.144889 | -0.223603 | -2.267546 |
| H | -0.730715 | -0.983133 | -1.539361 |
| C | -1.567454 | -0.833929 | 1.095548 |
| C | -2.391064 | -0.775589 | -0.190586 |
| H | -2.805872 | -1.759731 | -0.415692 |
| H | -3.238957 | -0.096341 | -0.048689 |
| H | -1.806527 | 1.811647 | -0.999760 |
| H | -0.779987 | -1.575619 | 0.979734 |
| H | -2.198827 | -1.143479 | 1.931081 |
| H | -0.325323 | 1.451882 | -1.869537 |
| H | -0.292938 | 0.462616 | 2.287717 |
| H | -1.770414 | 1.203885 | 1.702480 |
| N | 1.224633 | 0.889327 | 0.173263 |
| C | 1.816613 | -0.301740 | -0.050003 |
| O | 1.209209 | -1.354628 | -0.204208 |
| C | 3.327994 | -0.272199 | -0.096059 |
| H | 3.744851 | 0.725154 | 0.023034 |
| H | 3.708313 | -0.918063 | 0.694651 |
| H | 3.651087 | -0.687575 | -1.049623 |
| H | 1.847583 | 1.673925 | 0.272543 |

eq

```
=====
```

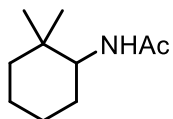
| | | | |
|---|----------|-----------|-----------|
| C | 0.673523 | 1.027975 | -0.580345 |
| C | 0.118026 | -0.176539 | 0.181680 |
| H | 0.029592 | 0.090252 | 1.236919 |
| C | 1.043768 | -1.381690 | 0.046769 |
| C | 2.458965 | -1.039863 | 0.511817 |
| H | 3.110443 | -1.904576 | 0.378769 |
| H | 2.438094 | -0.817385 | 1.582932 |
| C | 2.084166 | 1.372921 | -0.105170 |
| C | 3.015903 | 0.169073 | -0.239491 |
| H | 4.011364 | 0.416573 | 0.132446 |
| H | 3.122783 | -0.084666 | -1.298814 |
| H | 0.640980 | -2.218394 | 0.620233 |
| H | 2.471597 | 2.220932 | -0.671573 |
| H | 2.043997 | 1.681333 | 0.944129 |
| H | 1.068813 | -1.687071 | -1.005074 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.000594 | 1.876016 | -0.452607 |
| H | 0.694649 | 0.779686 | -1.646456 |
| N | -1.217649 | -0.529835 | -0.278791 |
| C | -2.334463 | 0.092707 | 0.149710 |
| O | -2.312319 | 0.977943 | 0.998848 |
| C | -3.629908 | -0.372010 | -0.468820 |
| H | -3.490490 | -1.170057 | -1.194657 |
| H | -4.289880 | -0.717056 | 0.326147 |
| H | -4.107490 | 0.478541 | -0.953776 |
| H | -1.301638 | -1.214267 | -1.014767 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.705307 | -1.263181 | -0.082305 |
| C | 0.158171 | 0.000089 | -0.750222 |
| H | 0.496997 | 0.000136 | -1.789020 |
| C | 0.705417 | 1.263241 | -0.082169 |
| C | 2.234168 | 1.258525 | -0.095022 |
| H | 2.611205 | 2.152096 | 0.404660 |
| H | 2.586665 | 1.299116 | -1.130580 |
| C | 2.234059 | -1.258598 | -0.095150 |
| C | 2.788292 | -0.000094 | 0.571657 |
| H | 3.878833 | -0.000140 | 0.531393 |
| H | 2.505491 | -0.000136 | 1.628908 |
| H | 0.319253 | 2.141805 | -0.602442 |
| H | 2.611016 | -2.152252 | 0.404442 |
| H | 2.586553 | -1.299115 | -1.130711 |
| H | 0.344002 | 1.301370 | 0.946712 |
| H | 0.319067 | -2.141658 | -0.602669 |
| H | 0.343884 | -1.301385 | 0.946573 |
| N | -1.303422 | 0.000154 | -0.831309 |
| C | -2.147252 | 0.000040 | 0.221320 |
| O | -1.769651 | -0.000090 | 1.388172 |
| C | -3.618695 | -0.000038 | -0.121864 |
| H | -3.808324 | -0.000184 | -1.192933 |
| H | -4.078061 | -0.880334 | 0.326238 |
| H | -4.078081 | 0.880376 | 0.325988 |
| H | -1.714146 | 0.000040 | -1.750248 |



N-(2,2-dimethylcyclohexyl)acetamide

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -522.465234 | -522.16885 | -522.222262 |
| ax2 | -522.465394 | -522.168931 | -522.221586 |
| eq1 | -522.467170 | -522.170884 | -522.223953 |
| eq3 | -522.461603 | -522.165077 | -522.217236 |

ax1

| ===== | | | |
|-------|-----------|-----------|-----------|
| C | 1.201418 | 0.878788 | 0.017512 |
| C | -0.008859 | 0.124102 | 0.615815 |
| H | -0.347673 | 0.665406 | 1.500196 |
| C | 0.337544 | -1.318188 | 1.011599 |
| C | 0.940607 | -2.095231 | -0.158120 |
| H | 1.200974 | -3.104948 | 0.162280 |
| H | 0.191171 | -2.198862 | -0.948815 |
| C | 1.824018 | 0.054675 | -1.125007 |
| C | 2.167935 | -1.379939 | -0.722010 |
| H | 2.554061 | -1.920256 | -1.587871 |
| H | 2.963656 | -1.377418 | 0.026976 |
| H | 1.040654 | -1.303298 | 1.846349 |
| H | 1.124539 | 0.023255 | -1.967829 |
| H | 2.714315 | 0.576190 | -1.485256 |
| H | -0.572361 | -1.801951 | 1.369265 |
| C | 2.232895 | 1.115378 | 1.127282 |
| H | 3.093822 | 1.650308 | 0.722227 |
| H | 1.800673 | 1.725984 | 1.922665 |
| H | 2.596347 | 0.192145 | 1.574293 |
| C | 0.770348 | 2.247259 | -0.514984 |
| H | 0.251074 | 2.818148 | 0.258262 |
| H | 1.647844 | 2.817778 | -0.824988 |
| H | 0.107762 | 2.162804 | -1.376608 |
| N | -1.132907 | 0.126833 | -0.317467 |
| C | -2.415444 | 0.039240 | 0.085924 |
| O | -2.735533 | -0.015380 | 1.269622 |
| C | -3.453403 | 0.021531 | -1.009658 |
| H | -3.018967 | 0.061206 | -2.006174 |
| H | -4.047413 | -0.886095 | -0.910548 |
| H | -4.119069 | 0.872770 | -0.871447 |
| H | -0.949151 | 0.136348 | -1.307805 |

ax2

```
=====
C -0.871516      0.961506      0.107839
C -0.034430     -0.053294     -0.715096
H  0.404782      0.475724     -1.560111
C -0.885130     -1.223040     -1.225416
C -1.637098     -1.929394     -0.095859
H -2.261786     -2.721450     -0.511024
H -0.927719     -2.419331      0.578748
C -1.634525      0.219238      1.218766
C -2.486796     -0.940916      0.702625
H -2.963363     -1.448850      1.542628
H -3.291472     -0.560300      0.068900
H -1.604446     -0.844560     -1.953206
H -0.908406     -0.171435      1.940230
H -2.254932      0.937988      1.760102
H -0.236230     -1.923673     -1.753015
C -1.845178      1.684604     -0.830003
H -2.424450      2.419626     -0.267725
H -1.295530      2.216614     -1.609597
H -2.548308      1.011657     -1.317302
C  0.041083      2.014925      0.736757
H  0.626805      2.529143     -0.027278
H -0.558982      2.758183      1.265578
H  0.733381      1.571446      1.453127
N  1.094343     -0.575846      0.047577
C  2.367676     -0.155747     -0.107458
O  2.701525      0.687452     -0.932886
C  3.381650     -0.788826      0.814771
H  2.965656     -1.594059      1.416265
H  4.208556     -1.169025      0.217386
H  3.774166     -0.015300      1.474971
H  0.915261     -1.255429      0.769811
```

eq1

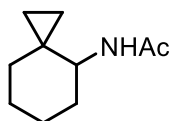
```
=====
C -0.778264      0.922251      0.049002
C -0.028731     -0.418794     -0.146620
H  0.142964     -0.541044     -1.217350
C -0.820626     -1.625152      0.361456
C -2.202003     -1.699562     -0.285346
H -2.082192     -1.879037     -1.358224
H -2.757808     -2.546204      0.120056
C -2.167752      0.789433     -0.599520
C -2.975866     -0.398962     -0.082577
H -3.933791     -0.446679     -0.603064
H -3.200459     -0.268389      0.979061
H -0.923046     -1.562076      1.448722
H -2.715357      1.722793     -0.446523
H -2.031871      0.674857     -1.680320
H -0.249190     -2.529882      0.147351
C -0.011682      2.040723     -0.657337
H -0.543833      2.988297     -0.549177
```

| | | | |
|---|-----------|-----------|-----------|
| H | 0.986725 | 2.165004 | -0.234788 |
| H | 0.095181 | 1.828412 | -1.722428 |
| C | -0.909114 | 1.281140 | 1.532827 |
| H | 0.071834 | 1.448401 | 1.981253 |
| H | -1.480548 | 2.205467 | 1.638133 |
| H | -1.416707 | 0.509977 | 2.111309 |
| N | 1.289323 | -0.405873 | 0.471560 |
| C | 2.449320 | -0.285870 | -0.207607 |
| O | 2.503795 | -0.165013 | -1.426793 |
| C | 3.704241 | -0.303491 | 0.631551 |
| H | 4.214181 | 0.651615 | 0.508339 |
| H | 3.508575 | -0.471940 | 1.688105 |
| H | 4.363523 | -1.084204 | 0.255068 |
| H | 1.339072 | -0.514453 | 1.472927 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.832986 | 0.966828 | 0.057246 |
| C | -0.092926 | -0.144387 | -0.728292 |
| H | -0.420209 | -0.041718 | -1.767517 |
| C | -0.482270 | -1.557051 | -0.288276 |
| C | -1.988239 | -1.759659 | -0.444820 |
| H | -2.260758 | -1.676157 | -1.501790 |
| H | -2.262264 | -2.765207 | -0.122150 |
| C | -2.344587 | 0.697064 | -0.066573 |
| C | -2.758883 | -0.711300 | 0.355156 |
| H | -3.833140 | -0.836741 | 0.209075 |
| H | -2.566139 | -0.855461 | 1.421392 |
| H | -0.191584 | -1.723257 | 0.746485 |
| H | -2.880918 | 1.447093 | 0.520100 |
| H | -2.634866 | 0.846469 | -1.112222 |
| H | 0.069229 | -2.277140 | -0.896130 |
| C | -0.532261 | 2.326366 | -0.576837 |
| H | -1.120752 | 3.106871 | -0.090345 |
| H | 0.521285 | 2.590525 | -0.473253 |
| H | -0.783711 | 2.327526 | -1.640057 |
| C | -0.408794 | 1.010975 | 1.527154 |
| H | 0.649809 | 1.255499 | 1.616897 |
| H | -0.979974 | 1.782914 | 2.047881 |
| H | -0.571799 | 0.063999 | 2.038854 |
| N | 1.357146 | 0.064446 | -0.786053 |
| C | 2.294991 | -0.343244 | 0.097043 |
| O | 2.053025 | -0.976996 | 1.117303 |
| C | 3.716274 | 0.038817 | -0.252705 |
| H | 4.319010 | -0.867700 | -0.286226 |
| H | 3.802449 | 0.565041 | -1.200527 |
| H | 4.107559 | 0.669273 | 0.545239 |
| H | 1.690652 | 0.606562 | -1.566334 |



N-(spiro[2.5]octan-4-yl)acetamide

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -521.234970 | -520.961945 | -521.015028 |
| ax1 | -521.223975 | -520.950404 | -521.002455 |
| ax2 | -521.234411 | -520.961109 | -521.012547 |
| eq1 | -521.235337 | -520.96219 | -521.013374 |
| eq2 | -521.229251 | -520.955808 | -521.006473 |
| eq3 | -521.235336 | -520.96219 | -521.013373 |

ax

```

=====
C  1.225860  -0.756529  -0.084882
C  -0.010489 -0.186512   0.581484
H  -0.312875 -0.841466   1.399268
C  2.141060  -1.566128   0.785593
C  1.297978  -2.240479  -0.269667
C  0.276602   1.214017   1.136405
C  0.873862   2.135473   0.073212
H  0.140001   2.296767  -0.722410
H  1.086169   3.112384   0.509412
C  1.857786   0.152373  -1.120918
C  2.143791   1.532742  -0.528401
H  2.902137   1.435938   0.254562
H  2.553237   2.192717  -1.294540
H  1.861095  -1.713319   1.819330
H  3.203386  -1.483025   0.602787
H  1.800151  -2.612413  -1.151876
H  0.454787  -2.829078   0.065144
H  0.983133   1.108275   1.964331
H  2.773645  -0.309837  -1.493247
H  1.188913   0.261819  -1.981698
H  -0.645298  1.630577   1.542845
N  -1.117791  -0.165120  -0.373056
C  -2.408300  -0.125621   0.013441
H  -0.914095  -0.191699  -1.359377
O  -2.740746  -0.100841   1.194419
C  -3.433003  -0.117943  -1.094170
H  -4.092224  -0.975230  -0.963854
H  -4.036393   0.784343  -1.001915
H  -2.986141  -0.152539  -2.085299

```

ax1

```
=====
C  1.062705    -0.775050    -0.134412
C  0.131651    -0.315388     0.981347
H  0.319399    -0.968660     1.833144
C  2.235174    -1.612539     0.302878
C  1.084796    -2.238001    -0.446028
C  0.477512     1.112605     1.440359
C  0.794379     2.113863     0.326444
H -0.116163     2.368816    -0.211241
H  1.182430     3.027750     0.780840
C  1.327069     0.221868    -1.245083
C  1.815144     1.547884    -0.661123
H  2.768824     1.383440    -0.148523
H  2.001114     2.266475    -1.461151
H  2.334778    -1.845718     1.353825
H  3.167257    -1.476855    -0.228028
H  1.251046    -2.529222    -1.473880
H  0.416172    -2.880719     0.110826
H  1.367520     1.017571     2.069301
H  2.073399    -0.196833    -1.923617
H  0.413057     0.392600    -1.814675
H -0.323554     1.484575     2.080884
N -1.296741    -0.556649     0.715828
C -2.111498     0.028553    -0.186062
H -1.706539    -1.300426     1.256146
O -1.764829     0.925487    -0.945045
C -3.531373    -0.491907    -0.207479
H -4.202755     0.333404     0.027247
H -3.758214    -0.828291    -1.218251
H -3.705318    -1.306593     0.491664
```

ax2

```
=====
C  0.874433     0.860260     0.150169
C  0.020246    -0.060164    -0.705839
H -0.427271     0.519939    -1.510958
C  1.504209     2.032099    -0.542885
C  0.359105     2.238193     0.421407
C  0.879315    -1.185774    -1.291010
C  1.682139    -1.925606    -0.218339
H  1.006789    -2.460777     0.457046
H  2.307994    -2.683397    -0.691394
C  1.677279     0.142817     1.214883
C  2.541276    -0.955711     0.593847
H  3.284719    -0.496747    -0.065032
H  3.086684    -1.492548     1.371330
H  1.301221     2.169524    -1.596174
H  2.492419     2.331611    -0.222107
H  0.587788     2.678260     1.382279
H -0.604085     2.500020     0.006425
H  1.574540    -0.733733    -2.002827
H  2.293135     0.864390     1.754510
H  0.994830    -0.304505     1.946049
```

| | | | |
|---|-----------|-----------|-----------|
| H | 0.243621 | -1.875892 | -1.847524 |
| N | -1.097748 | -0.611072 | 0.054809 |
| C | -2.357929 | -0.131369 | -0.019334 |
| H | -0.921116 | -1.367911 | 0.696500 |
| O | -2.677849 | 0.801126 | -0.748821 |
| C | -3.376081 | -0.823080 | 0.854270 |
| H | -3.800388 | -0.088315 | 1.537611 |
| H | -4.181118 | -1.194054 | 0.221364 |
| H | -2.956684 | -1.647353 | 1.426786 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.774461 | 0.841983 | -0.078782 |
| C | 0.061565 | -0.505146 | -0.148732 |
| H | -0.075907 | -0.758946 | -1.201739 |
| C | -0.008564 | 2.111652 | -0.173255 |
| C | 0.599233 | 1.693536 | 1.144946 |
| C | 0.914806 | -1.584263 | 0.518979 |
| C | 2.312692 | -1.645929 | -0.095526 |
| H | 2.907139 | -2.403994 | 0.416104 |
| H | 2.227808 | -1.957944 | -1.140887 |
| C | 2.155029 | 0.788738 | -0.700808 |
| C | 3.010903 | -0.287984 | -0.034417 |
| H | 3.179949 | -0.014857 | 1.011530 |
| H | 3.988767 | -0.344377 | -0.514934 |
| H | -1.082656 | 2.040441 | -0.268416 |
| H | 0.447646 | 2.939028 | -0.698869 |
| H | 1.463136 | 2.238395 | 1.499667 |
| H | -0.079214 | 1.356463 | 1.916454 |
| H | 0.991427 | -1.354859 | 1.587289 |
| H | 2.629721 | 1.768022 | -0.617986 |
| H | 2.059326 | 0.564201 | -1.768546 |
| H | 0.411768 | -2.548103 | 0.426051 |
| N | -1.262122 | -0.486950 | 0.447957 |
| C | -2.401427 | -0.305685 | -0.254684 |
| H | -1.336107 | -0.650354 | 1.440338 |
| O | -2.412527 | -0.113923 | -1.465229 |
| C | -3.680154 | -0.352748 | 0.545235 |
| H | -4.200174 | 0.596445 | 0.421661 |
| H | -4.315991 | -1.137233 | 0.136794 |
| H | -3.512828 | -0.537221 | 1.603889 |

eq2

```
=====
```

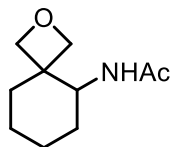
| | | | |
|---|----------|-----------|-----------|
| C | 0.869663 | 0.915367 | -0.161514 |
| C | 0.119724 | -0.277761 | -0.746586 |
| H | 0.430934 | -0.357901 | -1.792665 |
| C | 0.328016 | 2.301443 | -0.327384 |
| C | 0.310527 | 1.635276 | 1.028542 |
| C | 0.546020 | -1.575540 | -0.055599 |
| C | 2.058410 | -1.763713 | -0.174813 |
| H | 2.352717 | -2.690530 | 0.319604 |
| H | 2.334092 | -1.861355 | -1.229653 |
| C | 2.372844 | 0.728535 | -0.235432 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.805543 | -0.576333 | 0.431793 |
| H | 2.586768 | -0.523002 | 1.502512 |
| H | 3.883402 | -0.711161 | 0.328849 |
| H | -0.622255 | 2.426643 | -0.826739 |
| H | 1.043825 | 3.095008 | -0.491488 |
| H | 1.012876 | 1.987083 | 1.771807 |
| H | -0.645748 | 1.312962 | 1.412383 |
| H | 0.262658 | -1.536823 | 0.994576 |
| H | 2.866550 | 1.584451 | 0.228144 |
| H | 2.678049 | 0.710403 | -1.287405 |
| H | 0.014325 | -2.414211 | -0.509264 |
| N | -1.330220 | -0.094141 | -0.811349 |
| C | -2.252427 | -0.353516 | 0.143160 |
| H | -1.683828 | 0.279028 | -1.677323 |
| O | -1.986891 | -0.773292 | 1.262930 |
| C | -3.685495 | -0.091196 | -0.261815 |
| H | -4.238865 | -1.026867 | -0.189032 |
| H | -4.121400 | 0.609774 | 0.448643 |
| H | -3.784394 | 0.306454 | -1.269059 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.774421 | 0.841992 | -0.078757 |
| C | 0.061613 | -0.505171 | -0.148766 |
| H | -0.075825 | -0.758966 | -1.201776 |
| C | -0.008671 | 2.111622 | -0.173211 |
| C | 0.599108 | 1.693471 | 1.144991 |
| C | 0.914881 | -1.584256 | 0.518956 |
| C | 2.312771 | -1.645878 | -0.095564 |
| H | 2.907250 | -2.403924 | 0.416057 |
| H | 2.227882 | -1.957891 | -1.140923 |
| C | 2.155005 | 0.788828 | -0.700768 |
| C | 3.010922 | -0.287906 | -0.034442 |
| H | 3.179971 | -0.014810 | 1.011514 |
| H | 3.988785 | -0.344245 | -0.514967 |
| H | -1.082760 | 2.040511 | -0.268462 |
| H | 0.447647 | 2.938988 | -0.698753 |
| H | 1.462923 | 2.238389 | 1.499831 |
| H | -0.079364 | 1.356200 | 1.916391 |
| H | 0.991518 | -1.354847 | 1.587264 |
| H | 2.629678 | 1.768116 | -0.617859 |
| H | 2.059307 | 0.564383 | -1.768524 |
| H | 0.411884 | -2.548122 | 0.426053 |
| N | -1.262084 | -0.487002 | 0.447913 |
| C | -2.401402 | -0.305748 | -0.254688 |
| H | -1.336059 | -0.650763 | 1.440238 |
| O | -2.412562 | -0.113869 | -1.465227 |
| C | -3.680121 | -0.352804 | 0.545242 |
| H | -4.199526 | 0.596850 | 0.422578 |
| H | -4.316505 | -1.136467 | 0.136092 |
| H | -3.512884 | -0.538353 | 1.603721 |



N-(2-oxaspiro[3.5]nonan-5-yl)acetamide

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -596.444056 | -596.163919 | -596.217283 |
| ax2 | -596.444352 | -596.164063 | -596.217144 |
| ax3 | -596.441450 | -596.161211 | -596.213375 |
| eq1 | -596.444504 | -596.164541 | -596.217454 |
| eq2 | -596.445516 | -596.165354 | -596.218192 |

ax1

| ===== | | | |
|-------|-----------|-----------|-----------|
| C | 0.165681 | -0.041525 | 0.573392 |
| H | 0.341082 | -0.754722 | 1.378332 |
| C | 0.093115 | 1.374958 | 1.152289 |
| C | -0.290731 | 2.400539 | 0.086921 |
| H | -0.356121 | 3.391450 | 0.536438 |
| H | 0.492197 | 2.448448 | -0.675256 |
| C | -1.551251 | 0.622090 | -1.171715 |
| C | -1.616936 | 2.026495 | -0.573148 |
| H | -1.878003 | 2.749284 | -1.346306 |
| H | -2.411384 | 2.059718 | 0.178560 |
| H | -0.660403 | 1.375238 | 1.945292 |
| H | -0.839048 | 0.606694 | -2.002959 |
| H | -2.518694 | 0.329818 | -1.585520 |
| H | 1.050104 | 1.623509 | 1.611863 |
| C | -1.141495 | -0.405761 | -0.120418 |
| C | -1.276904 | -1.863035 | -0.582839 |
| C | -2.289970 | -0.764187 | 0.840435 |
| H | -0.484647 | -2.523974 | -0.227351 |
| H | -1.449956 | -2.019777 | -1.647113 |
| H | -1.986606 | -0.895220 | 1.880504 |
| H | -3.182179 | -0.141651 | 0.784895 |
| O | -2.488970 | -2.042542 | 0.190112 |
| N | 1.281283 | -0.185819 | -0.360388 |
| C | 2.542177 | -0.390146 | 0.046505 |
| H | 1.128988 | 0.000521 | -1.339987 |
| O | 2.834474 | -0.539563 | 1.240687 |
| C | 3.598383 | -0.444411 | -1.021106 |
| H | 4.330143 | 0.336960 | -0.820537 |
| H | 4.106776 | -1.405222 | -0.955780 |
| H | 3.192328 | -0.313600 | -2.020641 |

ax2

```
=====
C  0.059722   -0.199590   -0.672523
H  0.417965    0.470588   -1.451899
C -0.639414   -1.402381   -1.310431
C -1.299774   -2.306323   -0.269428
H -0.538423   -2.763727    0.369568
H -1.817219   -3.123619   -0.771915
C -1.563877   -0.332009    1.266218
C -2.273101   -1.508607    0.596810
H -2.729327   -2.150339    1.350641
H -3.082265   -1.126042   -0.033689
H  0.076751   -1.956328   -1.917386
H -2.265661    0.257650    1.858433
H -0.801900   -0.707070    1.956865
H -1.409161   -1.019546   -1.985134
C -0.911127    0.570652    0.230309
C -0.339606    1.903522    0.731020
C -1.866853    1.459918   -0.585634
H  0.727567    2.066248    0.581416
H -0.617460    2.150708    1.756725
H -1.878232    1.311550   -1.665269
H -2.887241    1.488871   -0.200012
O -1.135723    2.654880   -0.218825
N  1.240915   -0.616197    0.077337
C  2.457193   -0.067299   -0.061988
H  1.133637   -1.337041    0.775255
O  2.698608    0.838532   -0.870599
C  3.543304   -0.616777    0.820411
H  3.195556   -1.416146    1.469430
H  4.349043   -0.984535    0.186824
H  3.938070    0.198221    1.425593
```

ax3

```
=====
C  0.117595    0.204582    0.588090
H  0.551719   -0.460693    1.330993
C -0.566899    1.373927    1.301626
C -1.345183    2.263602    0.332417
H -0.657910    2.752488   -0.364578
H -1.844396    3.057899    0.887455
C -1.678650    0.293235   -1.196370
C -2.363850    1.440189   -0.454202
H -3.101763    1.026028    0.240458
H -2.905200    2.072057   -1.158363
H -1.261586    0.957055    2.035028
H -0.997438    0.698196   -1.951300
H -2.411015   -0.317121   -1.727280
H  0.180959    1.946131    1.850978
C -0.903584   -0.593120   -0.233195
C -0.333275   -1.901815   -0.793368
C -1.746439   -1.522745    0.659483
H  0.749735   -2.019969   -0.765101
H -0.712453   -2.162989   -1.782589
```

| | | | |
|---|-----------|-----------|-----------|
| H | -1.681696 | -1.370442 | 1.736545 |
| H | -2.790884 | -1.603251 | 0.353701 |
| O | -0.988698 | -2.682259 | 0.236901 |
| N | 1.207535 | 0.671621 | -0.264299 |
| C | 2.499152 | 0.308996 | -0.214410 |
| H | 0.975989 | 1.311810 | -1.013017 |
| O | 3.310540 | 0.758060 | -1.038155 |
| C | 2.941565 | -0.633590 | 0.871398 |
| H | 2.720925 | -0.214492 | 1.852794 |
| H | 2.424214 | -1.588998 | 0.790616 |
| H | 4.010728 | -0.791035 | 0.774967 |

eq1

```
=====
```

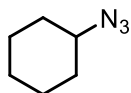
| | | | |
|---|-----------|-----------|-----------|
| C | 0.065653 | -0.423389 | -0.234920 |
| H | 0.198984 | -0.794958 | -1.254155 |
| C | -0.337574 | -1.591183 | 0.667376 |
| C | -1.652392 | -2.209577 | 0.199672 |
| H | -1.514790 | -2.635774 | -0.798339 |
| H | -1.934986 | -3.027423 | 0.862726 |
| C | -2.341612 | 0.016542 | -0.740468 |
| C | -2.754846 | -1.154475 | 0.148897 |
| H | -2.945630 | -0.784980 | 1.161556 |
| H | -3.686194 | -1.588778 | -0.214894 |
| H | 0.462597 | -2.331066 | 0.674551 |
| H | -2.214223 | -0.331955 | -1.769785 |
| H | -3.114789 | 0.786371 | -0.750721 |
| H | -0.448571 | -1.218342 | 1.689983 |
| C | -1.035189 | 0.638113 | -0.269755 |
| C | -1.113908 | 1.499448 | 1.006209 |
| C | -0.619990 | 1.953723 | -0.943717 |
| H | -0.554797 | 1.169638 | 1.882440 |
| H | -2.133428 | 1.758750 | 1.295624 |
| H | 0.306626 | 1.952536 | -1.516110 |
| H | -1.419732 | 2.417712 | -1.522405 |
| O | -0.461147 | 2.608828 | 0.339938 |
| N | 1.340892 | 0.155722 | 0.178338 |
| C | 2.520411 | -0.400231 | -0.125714 |
| H | 1.345317 | 1.023931 | 0.694212 |
| O | 2.606951 | -1.451590 | -0.775556 |
| C | 3.751653 | 0.312477 | 0.358814 |
| H | 3.522217 | 1.226896 | 0.899491 |
| H | 4.308611 | -0.363510 | 1.006200 |
| H | 4.376868 | 0.544306 | -0.502153 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.068645 | -0.678587 | 0.112810 |
| H | -0.077129 | -1.060386 | 1.123620 |
| C | 0.911776 | -1.672196 | -0.684459 |
| C | 2.298085 | -1.836996 | -0.066079 |
| H | 2.194987 | -2.282435 | 0.927485 |
| H | 2.890971 | -2.526007 | -0.667849 |
| C | 2.152449 | 0.494434 | 0.856094 |

| | | | |
|---|-----------|-----------|-----------|
| C | 3.005469 | -0.490022 | 0.059551 |
| H | 3.184360 | -0.082350 | -0.940493 |
| H | 3.979139 | -0.612748 | 0.534236 |
| H | 1.007248 | -1.305671 | -1.712052 |
| H | 2.019891 | 0.123935 | 1.877292 |
| H | 2.644024 | 1.466511 | 0.924162 |
| H | 0.391767 | -2.629340 | -0.727911 |
| C | 0.782159 | 0.674902 | 0.217842 |
| C | 0.770013 | 1.507305 | -1.079172 |
| C | -0.073535 | 1.817185 | 0.785009 |
| H | 0.344449 | 1.039973 | -1.967904 |
| H | 1.729324 | 1.962435 | -1.329591 |
| H | -1.065459 | 1.552093 | 1.148698 |
| H | 0.440266 | 2.436608 | 1.521046 |
| O | -0.137534 | 2.477006 | -0.503133 |
| N | -1.255603 | -0.556601 | -0.482052 |
| C | -2.404522 | -0.563773 | 0.209865 |
| H | -1.311031 | -0.431181 | -1.482351 |
| O | -2.445297 | -0.698383 | 1.440045 |
| C | -3.667853 | -0.402369 | -0.588545 |
| H | -4.170448 | 0.504057 | -0.253112 |
| H | -3.485108 | -0.340795 | -1.657926 |
| H | -4.321495 | -1.246779 | -0.375779 |



azidocyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -399.413929 | -399.230071 | -399.272793 |
| ax2 | -399.413929 | -399.23007 | -399.272792 |
| eq | -399.414298 | -399.230578 | -399.273312 |
| eq2 | -399.414418 | -399.230535 | -399.273207 |

ax

| | | | |
|---|-----------|-----------|----------|
| C | 1.031346 | 1.384246 | 0.436663 |
| C | -0.240904 | 0.613296 | 0.764504 |
| H | -0.729798 | 1.054480 | 1.635202 |
| C | 0.049340 | -0.863878 | 1.023019 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.825368 | -1.504783 | -0.127304 |
| H | 1.053253 | -2.542431 | 0.119182 |
| H | 0.200072 | -1.520818 | -1.024785 |
| C | 1.809670 | 0.741011 | -0.710923 |
| C | 2.110142 | -0.729192 | -0.418927 |
| H | 2.640234 | -1.180067 | -1.259127 |
| H | 2.771696 | -0.794497 | 0.450752 |
| H | 0.639454 | -0.919592 | 1.941411 |
| H | 1.223348 | 0.813714 | -1.630791 |
| H | 2.735333 | 1.292957 | -0.878759 |
| H | -0.881407 | -1.402343 | 1.215904 |
| H | 0.777588 | 2.419112 | 0.203260 |
| H | 1.648755 | 1.393570 | 1.338153 |
| N | -1.164240 | 0.799722 | -0.404536 |
| N | -2.191999 | 0.141049 | -0.350726 |
| N | -3.156375 | -0.434810 | -0.375108 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.032211 | 1.384222 | 0.435910 |
| C | -0.240411 | 0.614374 | 0.764776 |
| H | -0.728719 | 1.056486 | 1.635325 |
| C | 0.048964 | -0.862800 | 1.024057 |
| C | 0.823826 | -1.504889 | -0.126395 |
| H | 1.051054 | -2.542602 | 0.120440 |
| H | 0.198015 | -1.520907 | -1.023527 |
| C | 1.809455 | 0.739838 | -0.711777 |
| C | 2.109009 | -0.730428 | -0.419157 |
| H | 2.638294 | -1.182145 | -1.259415 |
| H | 2.771001 | -0.795764 | 0.450184 |
| H | 0.639598 | -0.918357 | 1.942119 |
| H | 1.222654 | 0.812441 | -1.631349 |
| H | 2.735409 | 1.291045 | -0.880412 |
| H | -0.882017 | -1.400517 | 1.217876 |
| H | 0.779063 | 2.419141 | 0.202098 |
| H | 1.650116 | 1.393589 | 1.337070 |
| N | -1.164046 | 0.800758 | -0.404129 |
| N | -2.191258 | 0.141248 | -0.350780 |
| N | -3.155095 | -0.435479 | -0.375791 |

eq

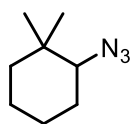
```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.723600 | -1.374177 | 0.166996 |
| C | 0.308253 | -0.321115 | -0.201720 |
| H | 0.403481 | -0.271627 | -1.291277 |
| C | -0.079979 | 1.051922 | 0.336288 |
| C | -1.460118 | 1.457365 | -0.182900 |
| H | -1.734857 | 2.430220 | 0.226176 |
| H | -1.417449 | 1.567807 | -1.270503 |
| C | -2.106195 | -0.971040 | -0.345494 |
| C | -2.510554 | 0.407328 | 0.176430 |
| H | -3.482602 | 0.692937 | -0.228128 |
| H | -2.615194 | 0.362941 | 1.264726 |
| H | -0.094759 | 1.001690 | 1.428871 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.092175 | -0.951296 | -1.439375 |
| H | -2.839653 | -1.721956 | -0.049912 |
| H | 0.669798 | 1.792240 | 0.048780 |
| H | -0.423381 | -2.339927 | -0.241469 |
| H | -0.744633 | -1.468484 | 1.256711 |
| N | 1.619648 | -0.770488 | 0.358216 |
| N | 2.572424 | -0.087795 | 0.004769 |
| N | 3.494296 | 0.487392 | -0.277586 |

eq2

```
=====
C -0.237742 -1.261150 -0.100727
C 0.258553 0.000423 -0.799078
H -0.087750 0.000590 -1.831910
C -0.238025 1.261356 -0.100007
C -1.765133 1.258668 -0.012880
H -2.104175 2.152627 0.511721
H -2.180606 1.303546 -1.023970
C -1.764783 -1.258920 -0.013750
C -2.276254 -0.000443 0.685685
H -3.366890 -0.000578 0.710539
H -1.930398 -0.000771 1.723875
H 0.182210 1.294517 0.911035
H -2.180158 -1.303187 -1.024911
H -2.103720 -2.153323 0.510173
H 0.119678 2.141776 -0.635290
H 0.120388 -2.141029 -0.636626
H 0.182416 -1.294806 0.910317
N 1.748134 0.000934 -0.931115
N 2.348284 0.000025 0.136176
N 2.973483 -0.000811 1.069165
```



2-azido-1,1-dimethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -478.028464 | -477.78597 | -477.834084 |
| ax2 | -478.025567 | -477.782713 | -477.82988 |
| ax3 | -478.028783 | -477.786209 | -477.83345 |
| eq | -478.029438 | -477.786923 | -477.834564 |
| eq2 | -478.029333 | -477.786976 | -477.83525 |
| eq3 | -478.029550 | -477.786886 | -477.834313 |

ax

```
=====
C  1.088132    0.693576    0.036642
C -0.313948    0.380183    0.591259
H -0.514651    1.045802    1.435677
C -0.473878   -1.078123    1.022586
C -0.114597   -2.046467   -0.104098
H -0.194950   -3.072787    0.255890
H -0.835985   -1.937198   -0.918937
C  1.442329   -0.315047   -1.069745
C  1.292330   -1.773926   -0.635594
H  1.506573   -2.430066   -1.480601
H  2.024731   -2.011925    0.139712
H  0.169453   -1.252925    1.886286
H  0.786367   -0.132721   -1.926121
H  2.463730   -0.119416   -1.405225
H -1.497393   -1.246516    1.365546
C  2.098281    0.618233    1.188169
H  3.092927    0.870564    0.817019
H  1.839574    1.335178    1.970169
H  2.154418   -0.368741    1.643220
C  1.128924    2.112927   -0.531191
H  0.817925    2.841650    0.221141
H  2.146713    2.358972   -0.839250
H  0.477067    2.217463   -1.397484
N -1.306494    0.716274   -0.484535
N -2.467471    0.478371   -0.193963
N -3.557739    0.284573   -0.000819
```

ax2

```
=====
C -0.836735   -0.759277   -0.059114
C  0.010084   -0.189211    1.104976
H -0.301909   -0.695382    2.017508
C -0.158159    1.320824    1.295380
C  0.054736    2.100628   -0.000814
H -0.111063    3.162780    0.183496
H  1.092154    2.002905   -0.334223
C -0.692156    0.097655   -1.333105
C -0.885015    1.595596   -1.094098
H -0.709374    2.137422   -2.024440
H -1.918057    1.798681   -0.800737
H -1.168561    1.506574    1.665720
H  0.293518   -0.063445   -1.775686
H -1.416464   -0.265381   -2.066472
H  0.531946    1.652842    2.071458
C -2.302271   -0.768228    0.397171
H -2.931965   -1.162935   -0.401849
H -2.425568   -1.408434    1.272669
H -2.669339    0.224802    0.651841
C -0.429700   -2.202961   -0.360324
H -0.466207   -2.813956    0.544101
H -1.118216   -2.634757   -1.088885
H  0.575949   -2.271385   -0.777358
```

| | | | |
|---|----------|-----------|-----------|
| N | 1.462508 | -0.538407 | 1.043364 |
| N | 2.084521 | -0.371366 | 0.007432 |
| N | 2.764179 | -0.281725 | -0.884735 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.295741 | 0.974299 | 0.060831 |
| C | -0.295183 | -0.315736 | 0.675505 |
| H | -0.861483 | -0.048898 | 1.571783 |
| C | 0.770432 | -1.352716 | 1.021418 |
| C | 1.658206 | -1.679153 | -0.178602 |
| H | 2.427543 | -2.392755 | 0.119006 |
| H | 1.056401 | -2.162585 | -0.952866 |
| C | 1.221324 | 0.614953 | -1.113690 |
| C | 2.293389 | -0.413346 | -0.751985 |
| H | 2.879794 | -0.656643 | -1.639331 |
| H | 2.988651 | 0.008593 | -0.021951 |
| H | 1.381457 | -0.960421 | 1.836066 |
| H | 0.608324 | 0.211610 | -1.925311 |
| H | 1.680568 | 1.533002 | -1.488510 |
| H | 0.277628 | -2.250863 | 1.394999 |
| C | 1.064928 | 1.726013 | 1.154160 |
| H | 1.467141 | 2.654814 | 0.745780 |
| H | 0.399775 | 1.982833 | 1.981295 |
| H | 1.897109 | 1.152647 | 1.558149 |
| C | -0.827300 | 1.885242 | -0.437944 |
| H | -1.546150 | 2.096692 | 0.357787 |
| H | -0.410742 | 2.836070 | -0.774553 |
| H | -1.362199 | 1.443923 | -1.280038 |
| N | -1.236482 | -0.979425 | -0.286373 |
| N | -2.404342 | -0.642900 | -0.171076 |
| N | -3.498181 | -0.389869 | -0.122617 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.255855 | 0.888831 | 0.038851 |
| C | -0.270883 | -0.555008 | -0.102315 |
| H | -0.469510 | -0.733809 | -1.164179 |
| C | 0.710780 | -1.608996 | 0.391954 |
| C | 2.039675 | -1.492259 | -0.353481 |
| H | 2.745640 | -2.228325 | 0.032746 |
| H | 1.875874 | -1.728740 | -1.409244 |
| C | 1.599535 | 0.957630 | -0.711601 |
| C | 2.616230 | -0.082024 | -0.242326 |
| H | 3.525169 | -0.001063 | -0.840403 |
| H | 2.902749 | 0.115186 | 0.793302 |
| H | 0.865706 | -1.485744 | 1.466188 |
| H | 1.406334 | 0.804961 | -1.778748 |
| H | 2.004065 | 1.966806 | -0.603546 |
| H | 0.272306 | -2.596087 | 0.240852 |
| C | 0.433251 | 1.288267 | 1.506340 |
| H | 0.805384 | 2.313084 | 1.561215 |
| H | -0.519465 | 1.247455 | 2.035416 |
| H | 1.138872 | 0.649643 | 2.035370 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.730491 | 1.857430 | -0.616442 |
| H | -1.675313 | 1.897483 | -0.070540 |
| H | -0.314393 | 2.866522 | -0.624979 |
| H | -0.939965 | 1.568610 | -1.648892 |
| N | -1.551180 | -0.737719 | 0.648640 |
| N | -2.562241 | -0.566953 | -0.015606 |
| N | -3.536174 | -0.435215 | -0.560239 |

eq2

```
=====
```

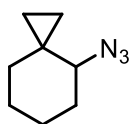
| | | | |
|---|-----------|-----------|-----------|
| C | -0.733036 | -0.909615 | -0.033820 |
| C | 0.427489 | 0.075021 | -0.252665 |
| H | 0.570128 | 0.185579 | -1.333507 |
| C | 0.183547 | 1.454924 | 0.351934 |
| C | -1.096672 | 2.068678 | -0.213280 |
| H | -1.275434 | 3.040827 | 0.247417 |
| H | -0.967479 | 2.240352 | -1.286125 |
| C | -2.008708 | -0.242729 | -0.584588 |
| C | -2.287937 | 1.138452 | 0.005634 |
| H | -3.182834 | 1.559049 | -0.455541 |
| H | -2.493861 | 1.055566 | 1.075477 |
| H | 0.112149 | 1.366670 | 1.438101 |
| H | -1.904120 | -0.144804 | -1.670238 |
| H | -2.851540 | -0.914532 | -0.406556 |
| H | 1.039334 | 2.098148 | 0.134478 |
| C | -0.903318 | -1.263763 | 1.446462 |
| H | -1.748339 | -1.945147 | 1.561543 |
| H | -0.013573 | -1.764593 | 1.829124 |
| H | -1.092535 | -0.390991 | 2.069760 |
| C | -0.469489 | -2.193921 | -0.820794 |
| H | 0.414268 | -2.712205 | -0.446901 |
| H | -1.321454 | -2.870565 | -0.731750 |
| H | -0.317223 | -1.977556 | -1.880318 |
| N | 1.672929 | -0.534395 | 0.310851 |
| N | 2.697904 | 0.053640 | 0.000286 |
| N | 3.680777 | 0.539600 | -0.245175 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.470276 | 0.958093 | 0.010156 |
| C | -0.240711 | -0.146301 | -0.802514 |
| H | 0.110721 | -0.070846 | -1.832608 |
| C | 0.037230 | -1.558979 | -0.297814 |
| C | 1.539041 | -1.837893 | -0.272146 |
| H | 1.720209 | -2.840567 | 0.116508 |
| H | 1.925816 | -1.814208 | -1.295229 |
| C | 1.971332 | 0.612308 | 0.042982 |
| C | 2.270214 | -0.791207 | 0.565000 |
| H | 3.345842 | -0.971636 | 0.537547 |
| H | 1.961272 | -0.878346 | 1.609839 |
| H | -0.368920 | -1.684279 | 0.709552 |
| H | 2.364791 | 0.696853 | -0.975429 |
| H | 2.484667 | 1.365989 | 0.644650 |
| H | -0.477297 | -2.271630 | -0.944835 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.096586 | 1.064632 | 1.429855 |
| H | 0.491129 | 1.783591 | 2.003525 |
| H | -1.126402 | 1.426392 | 1.413297 |
| H | -0.078756 | 0.117144 | 1.967660 |
| C | 0.294791 | 2.305648 | -0.690756 |
| H | -0.755361 | 2.596484 | -0.732724 |
| H | 0.839848 | 3.082755 | -0.151326 |
| H | 0.681330 | 2.266949 | -1.711221 |
| N | -1.707856 | 0.124362 | -0.917738 |
| N | -2.402084 | -0.329702 | -0.019811 |
| N | -3.117548 | -0.715010 | 0.756438 |



4-azidospiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -476.798515 | -476.5792 | -476.625529 |
| ax2 | -476.797628 | -476.578347 | -476.625004 |
| ax3 | -476.798516 | -476.5792 | -476.625532 |
| eq | -476.796558 | -476.577154 | -476.623098 |
| eq2 | -476.796667 | -476.577378 | -476.623794 |
| eq3 | -476.796291 | -476.576861 | -476.622742 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.021504 | 0.859967 | -0.053817 |
| C | -0.095996 | -0.355220 | -0.950794 |
| H | -0.538855 | -0.077406 | -1.909861 |
| C | 0.209036 | 2.175905 | -0.738186 |
| C | -1.131975 | 1.867095 | -0.124842 |
| C | 1.286290 | -0.962593 | -1.164303 |
| C | 1.996414 | -1.237041 | 0.161702 |
| H | 1.454371 | -2.014296 | 0.707081 |
| H | 2.996939 | -1.624157 | -0.034456 |
| C | 0.680059 | 0.607232 | 1.264680 |
| C | 2.073570 | 0.023815 | 1.023595 |
| H | 2.688903 | 0.771751 | 0.514298 |
| H | 2.557900 | -0.198517 | 1.975347 |
| H | 0.277001 | 2.182150 | -1.817215 |
| H | 0.844273 | 2.888582 | -0.231428 |
| H | -1.399667 | 2.375039 | 0.791094 |
| H | -1.953942 | 1.670059 | -0.799455 |
| H | 1.867922 | -0.249079 | -1.752853 |
| H | 0.740741 | 1.540983 | 1.825899 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.091573 | -0.092775 | 1.867306 |
| H | 1.193186 | -1.876257 | -1.752669 |
| N | -0.950228 | -1.441485 | -0.364103 |
| N | -1.966054 | -1.063599 | 0.201725 |
| N | -2.911676 | -0.805064 | 0.749335 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.102118 | -0.543499 | -0.074865 |
| C | -0.284881 | -0.483383 | 0.517073 |
| H | -0.397962 | -1.267099 | 1.269715 |
| C | 2.191803 | -1.019693 | 0.840568 |
| C | 1.710788 | -1.892594 | -0.292758 |
| C | -0.559435 | 0.887266 | 1.134194 |
| C | -0.278836 | 2.023018 | 0.149962 |
| H | -0.984799 | 1.966083 | -0.683810 |
| H | -0.445748 | 2.981278 | 0.642878 |
| C | 1.410012 | 0.582131 | -1.039542 |
| C | 1.149916 | 1.941635 | -0.388966 |
| H | 1.853393 | 2.084649 | 0.436980 |
| H | 1.329076 | 2.742427 | -1.107612 |
| H | 1.922153 | -1.310853 | 1.846266 |
| H | 3.160908 | -0.551486 | 0.740242 |
| H | 2.362659 | -2.012826 | -1.146574 |
| H | 1.116560 | -2.759550 | -0.038684 |
| H | 0.094626 | 0.983520 | 2.004469 |
| H | 2.447245 | 0.500907 | -1.368676 |
| H | 0.779007 | 0.478718 | -1.927509 |
| H | -1.585779 | 0.934196 | 1.504844 |
| N | -1.242375 | -0.792247 | -0.599178 |
| N | -2.420970 | -0.643719 | -0.311836 |
| N | -3.522404 | -0.526783 | -0.124202 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.021774 | -0.859991 | 0.053871 |
| C | -0.095712 | 0.355026 | 0.951132 |
| H | -0.538231 | 0.077075 | 1.910331 |
| C | 0.208342 | -2.176161 | 0.737947 |
| C | -1.132675 | -1.866645 | 0.124964 |
| C | 1.286757 | 0.962218 | 1.164287 |
| C | 1.996617 | 1.236574 | -0.161875 |
| H | 1.454563 | 2.013954 | -0.707067 |
| H | 2.997270 | 1.623504 | 0.034022 |
| C | 0.679531 | -0.607167 | -1.264731 |
| C | 2.073278 | -0.024229 | -1.023889 |
| H | 2.688539 | -0.772381 | -0.514821 |
| H | 2.557422 | 0.198088 | -1.975733 |
| H | 0.276580 | -2.182607 | 1.816953 |
| H | 0.843098 | -2.889017 | 0.230839 |
| H | -1.400824 | -2.374374 | -0.790958 |
| H | -1.954412 | -1.669288 | 0.799771 |
| H | 1.868405 | 0.248645 | 1.752744 |
| H | 0.739739 | -1.540802 | -1.826211 |

| | | | |
|---|-----------|----------|-----------|
| H | 0.091128 | 0.093171 | -1.867076 |
| H | 1.193889 | 1.875915 | 1.752643 |
| N | -0.949982 | 1.441543 | 0.365075 |
| N | -1.965426 | 1.064028 | -0.201674 |
| N | -2.910785 | 0.805909 | -0.749924 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.297297 | 0.820930 | -0.110670 |
| C | 0.265789 | -0.591596 | -0.108846 |
| H | 0.428367 | -0.904044 | -1.145437 |
| C | -0.107339 | 1.684678 | 1.100023 |
| C | 0.612735 | 2.006096 | -0.188964 |
| C | -0.711310 | -1.553094 | 0.557157 |
| C | -2.074690 | -1.501298 | -0.132749 |
| H | -1.969136 | -1.863793 | -1.159753 |
| H | -2.766452 | -2.175482 | 0.373344 |
| C | -1.640596 | 0.881077 | -0.811055 |
| C | -2.634568 | -0.079491 | -0.158355 |
| H | -2.830539 | 0.250651 | 0.865956 |
| H | -3.585415 | -0.057646 | -0.692546 |
| H | 0.490533 | 1.299314 | 1.913423 |
| H | -0.932766 | 2.319774 | 1.389828 |
| H | 0.268604 | 2.855328 | -0.762460 |
| H | 1.681697 | 1.845930 | -0.209664 |
| H | -0.811265 | -1.266569 | 1.607994 |
| H | -2.015050 | 1.905656 | -0.784206 |
| H | -1.511556 | 0.609646 | -1.864037 |
| H | -0.301311 | -2.563121 | 0.527091 |
| N | 1.561406 | -0.675877 | 0.621979 |
| N | 2.552865 | -0.574835 | -0.088181 |
| N | 3.511149 | -0.500639 | -0.667910 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.756001 | 0.819485 | -0.181647 |
| C | 0.425635 | -0.121440 | -0.303229 |
| H | 0.571838 | -0.361761 | -1.362274 |
| C | -0.834905 | 1.746304 | 0.994614 |
| C | -0.580018 | 2.289203 | -0.392855 |
| C | 0.170770 | -1.410745 | 0.475495 |
| C | -1.115887 | -2.083296 | -0.003563 |
| H | -0.995383 | -2.386544 | -1.047859 |
| H | -1.292389 | -2.990953 | 0.574480 |
| C | -2.039572 | 0.163675 | -0.652338 |
| C | -2.307496 | -1.133498 | 0.110819 |
| H | -2.482989 | -0.900113 | 1.165069 |
| H | -3.210934 | -1.612726 | -0.268703 |
| H | -0.007175 | 1.762163 | 1.689047 |
| H | -1.810422 | 1.910503 | 1.430754 |
| H | -1.385377 | 2.817085 | -0.884215 |
| H | 0.413743 | 2.658460 | -0.601243 |
| H | 0.088808 | -1.159759 | 1.536664 |
| H | -2.866058 | 0.865106 | -0.528167 |

```

H -1.959209 -0.056646 -1.721988
H 1.021466 -2.085618 0.358237
N 1.653095 0.565626 0.189477
N 2.687906 -0.040756 -0.047811
N 3.678845 -0.535917 -0.230748

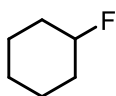
```

eq3

```

=====
C -0.528256 0.904561 -0.177859
C 0.240653 -0.251741 -0.799348
H -0.074048 -0.346761 -1.840230
C 0.067934 1.648614 0.980574
C -0.064701 2.313220 -0.370160
C -0.058989 -1.557274 -0.069155
C -1.562340 -1.835436 -0.062573
H -1.905515 -1.979425 -1.091247
H -1.759090 -2.764221 0.473730
C -2.020264 0.633338 -0.152798
C -2.332405 -0.676787 0.568975
H -2.047490 -0.585116 1.621241
H -3.404600 -0.875341 0.540515
H 1.065761 1.394972 1.310583
H -0.604612 1.960808 1.767252
H -0.826553 3.071416 -0.485570
H 0.845515 2.479373 -0.927639
H 0.294366 -1.479189 0.963991
H -2.529195 1.472073 0.324832
H -2.389157 0.574227 -1.182181
H 0.484700 -2.374763 -0.546174
N 1.700293 0.036618 -0.894949
N 2.391610 -0.385185 0.022089
N 3.108118 -0.739864 0.810712

```



fluorocyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -335.086737 | -334.915951 | -334.953331 |
| eq | -335.087173 | -334.916381 | -334.953819 |

ax

```

=====
C 0.959090 1.456544 -0.000000
C 0.282135 0.912809 -1.257890
C 0.282135 -0.616113 -1.264236
C -0.329603 -1.185503 0.000000
C 0.282135 -0.616113 1.264236

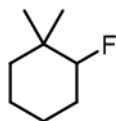
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.282135 | 0.912809 | 1.257890 |
| H | -0.255567 | -1.007764 | -2.128860 |
| H | -0.748518 | 1.275026 | -1.296647 |
| H | 0.782547 | 1.282636 | -2.153496 |
| H | 2.012160 | 1.157612 | -0.000000 |
| H | 0.935478 | 2.547222 | -0.000000 |
| H | -0.286593 | -2.274211 | 0.000000 |
| H | -0.255567 | -1.007764 | 2.128860 |
| H | 1.308901 | -0.986897 | 1.324460 |
| H | -0.748518 | 1.275026 | 1.296647 |
| H | 0.782547 | 1.282636 | 2.153496 |
| H | 1.308901 | -0.986897 | -1.324460 |
| F | -1.709325 | -0.860358 | 0.000000 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.840621 | 0.000001 | -0.285856 |
| C | 1.134721 | 1.259645 | 0.215737 |
| C | -0.343348 | 1.256855 | -0.182644 |
| C | -1.012150 | -0.000001 | 0.327776 |
| C | -0.343347 | -1.256857 | -0.182644 |
| C | 1.134722 | -1.259643 | 0.215735 |
| H | -0.857316 | 2.133528 | 0.213389 |
| H | 1.213531 | 1.305971 | 1.305923 |
| H | 1.618997 | 2.153897 | -0.177059 |
| H | 1.841050 | 0.000003 | -1.380001 |
| H | 2.882869 | -0.000003 | 0.036257 |
| H | -1.042635 | -0.000002 | 1.419879 |
| H | -0.857309 | -2.133530 | 0.213396 |
| H | -0.433989 | -1.275636 | -1.272445 |
| H | 1.213530 | -1.305970 | 1.305922 |
| H | 1.619003 | -2.153894 | -0.177059 |
| H | -0.433985 | 1.275632 | -1.272446 |
| F | -2.359007 | 0.000001 | -0.096042 |



2-fluoro-1,1-dimethylcyclohexane

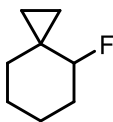
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -413.702000 | -413.472499 | -413.515448 |
| eq | -413.702292 | -413.472845 | -413.515917 |

ax

```
=====
C -1.342456 -1.354618 -0.509886
C -2.087066 -0.076493 -0.126436
C -1.315418 0.713125 0.931276
C 0.105737 0.999939 0.486491
C 0.895698 -0.236704 0.051664
C 0.077571 -1.034523 -0.978749
H -1.808065 1.662093 1.148195
H -2.214952 0.545034 -1.016397
H -3.085394 -0.310062 0.245065
H -1.312211 -2.030369 0.348434
H -1.879490 -1.877918 -1.302432
H 0.658951 1.541592 1.256328
H 0.018816 -0.449429 -1.901281
H 0.619417 -1.952345 -1.219494
H -1.276672 0.151990 1.867043
C 2.223849 0.198292 -0.569171
H 2.808761 0.790872 0.137963
H 2.812162 -0.679935 -0.841203
H 2.067562 0.793367 -1.468276
C 1.197218 -1.085089 1.292132
H 1.810040 -1.941787 1.006903
H 1.755606 -0.503412 2.028594
H 0.298215 -1.463986 1.775371
F 0.021829 1.886747 -0.614304
```

eq

```
=====
C -1.802392 -1.042472 0.154816
C -2.154207 0.389674 -0.245916
C -1.047304 1.360898 0.168683
C 0.276142 0.913752 -0.414199
C 0.702078 -0.498811 -0.014314
C -0.444119 -1.446191 -0.418353
H -1.264338 2.370036 -0.183990
H -2.282229 0.436187 -1.331473
H -3.100688 0.694916 0.200749
H -1.790379 -1.124133 1.244190
H -2.569318 -1.730540 -0.203959
H 0.238941 0.975724 -1.505403
H -0.514367 -1.456179 -1.511110
H -0.178959 -2.459801 -0.108918
H -0.968301 1.401192 1.257123
C 1.967204 -0.881228 -0.783686
H 2.800842 -0.228722 -0.520898
H 2.255413 -1.907527 -0.548813
H 1.803797 -0.812602 -1.861019
C 0.987975 -0.590902 1.487476
H 1.293474 -1.608605 1.737162
H 1.799942 0.081162 1.766936
H 0.120998 -0.344288 2.098280
F 1.271434 1.831651 -0.015100
```



4-fluorospiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -412.470798 | -412.264529 | -412.305956 |
| eq | -412.469375 | -412.263069 | -412.304281 |

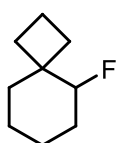
ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.837525 | -0.136615 | -0.059061 |
| C | -0.034057 | 1.087625 | 0.272020 |
| H | -0.612509 | 1.773884 | 0.891320 |
| C | -1.807097 | -0.587262 | 0.995676 |
| C | -2.308881 | 0.035062 | -0.281506 |
| C | 1.299089 | 0.753097 | 0.912021 |
| C | 2.075696 | -0.283155 | 0.098540 |
| H | 2.357116 | 0.149214 | -0.865260 |
| H | 3.001307 | -0.534745 | 0.617137 |
| C | -0.074510 | -1.184398 | -0.842700 |
| C | 1.235714 | -1.538555 | -0.138350 |
| H | 1.011695 | -2.010238 | 0.823391 |
| H | 1.796534 | -2.262853 | -0.730471 |
| H | -1.882817 | -0.003187 | 1.902281 |
| H | -1.932665 | -1.653301 | 1.122445 |
| H | -2.777195 | -0.614857 | -1.007137 |
| H | -2.714646 | 1.035560 | -0.225861 |
| H | 1.090464 | 0.359632 | 1.910404 |
| H | -0.702103 | -2.067940 | -0.969836 |
| H | 0.146136 | -0.797923 | -1.842208 |
| H | 1.874753 | 1.671157 | 1.036497 |
| F | 0.228151 | 1.786756 | -0.933615 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | -0.627292 | -0.464998 | -0.178879 |
| C | -0.203658 | 0.957924 | -0.446903 |
| H | -0.055942 | 1.104769 | -1.520280 |
| C | -1.483625 | -0.739756 | 1.020341 |
| C | -2.055564 | -0.859470 | -0.374084 |
| C | 1.053534 | 1.319343 | 0.315817 |
| C | 2.179029 | 0.342220 | -0.033114 |
| H | 2.432253 | 0.448995 | -1.092132 |
| H | 3.073620 | 0.596241 | 0.535657 |
| C | 0.476823 | -1.446023 | -0.518543 |
| C | 1.759654 | -1.102687 | 0.239637 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.588259 | -1.232769 | 1.312115 |
| H | 2.559263 | -1.787474 | -0.045776 |
| H | -1.811538 | 0.100036 | 1.615838 |
| H | -1.291622 | -1.651558 | 1.568485 |
| H | -2.248112 | -1.851625 | -0.757699 |
| H | -2.754876 | -0.096755 | -0.685329 |
| H | 0.831607 | 1.266261 | 1.385210 |
| H | 0.142533 | -2.457843 | -0.284225 |
| H | 0.673157 | -1.410474 | -1.595200 |
| H | 1.339624 | 2.345009 | 0.079996 |
| F | -1.230181 | 1.843097 | -0.073588 |



5-fluorospiro[3.5]nonane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -451.775798 | -451.539227 | -451.582671 |
| ax2 | -451.775750 | -451.539127 | -451.582518 |
| eq | -451.776194 | -451.539679 | -451.583074 |
| eq2 | -451.775613 | -451.539132 | -451.582544 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.601651 | 0.063356 | -0.062163 |
| C | -0.412920 | 1.082088 | 0.409101 |
| H | 0.051556 | 1.787021 | 1.100358 |
| C | 1.926973 | 0.636389 | -0.619735 |
| C | 1.421836 | -0.602776 | 1.075793 |
| C | -1.653609 | 0.456004 | 1.011835 |
| C | -2.292156 | -0.554322 | 0.058758 |
| H | -3.150717 | -1.022928 | 0.540815 |
| H | -2.667211 | -0.031344 | -0.824676 |
| C | -0.046219 | -0.953696 | -1.001796 |
| C | -1.274760 | -1.609923 | -0.371718 |
| H | -1.727428 | -2.308171 | -1.077072 |
| H | -0.970142 | -2.192697 | 0.502571 |
| H | 2.096633 | 1.655638 | -0.271120 |
| H | 1.430063 | 0.013566 | 1.975578 |
| H | -1.351397 | -0.044945 | 1.936094 |
| H | -0.341508 | -0.440464 | -1.921944 |
| H | 0.693790 | -1.707410 | -1.280916 |
| H | -2.356284 | 1.244316 | 1.285182 |
| C | 2.699422 | -0.397521 | 0.230565 |
| H | 3.587463 | -0.048586 | 0.752156 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.056014 | 0.600265 | -1.700775 |
| H | 2.953375 | -1.287085 | -0.342628 |
| H | 1.150799 | -1.622670 | 1.344344 |
| F | -0.808479 | 1.854212 | -0.711313 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.338916 | -1.073143 | -1.017134 |
| H | -0.213136 | -1.963508 | -1.324860 |
| C | 1.592775 | -1.456845 | -0.232007 |
| C | 2.348824 | -0.206501 | 0.214367 |
| H | 3.231556 | -0.476098 | 0.795110 |
| H | 2.699158 | 0.336264 | -0.667388 |
| C | 0.158724 | 1.038662 | 0.315823 |
| C | 1.444762 | 0.702908 | 1.045889 |
| H | 1.952000 | 1.631559 | 1.311068 |
| H | 1.177090 | 0.203234 | 1.979966 |
| H | 1.303005 | -2.037829 | 0.649780 |
| H | -0.494290 | 1.655816 | 0.935825 |
| H | 2.236708 | -2.095390 | -0.838163 |
| C | -0.584638 | -0.183274 | -0.196083 |
| C | -1.945115 | 0.200066 | -0.828949 |
| C | -1.368922 | -0.857375 | 0.964925 |
| C | -2.634316 | -0.087971 | 0.523723 |
| H | -2.232741 | -0.523513 | -1.591634 |
| H | -2.031025 | 1.205352 | -1.238759 |
| H | -1.461782 | -1.929428 | 0.791648 |
| H | -1.007783 | -0.690948 | 1.979062 |
| H | -3.567370 | -0.645611 | 0.495600 |
| H | -2.783528 | 0.818375 | 1.107578 |
| H | 0.628460 | -0.543248 | -1.930200 |
| F | 0.495291 | 1.843980 | -0.799774 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.510653 | -0.136696 | -0.224779 |
| C | -0.390882 | 1.063256 | -0.417880 |
| H | -0.617594 | 1.185580 | -1.481032 |
| C | 1.908322 | -0.073938 | -0.885912 |
| C | 1.212299 | -0.269598 | 1.154510 |
| C | -1.664934 | 0.969694 | 0.393076 |
| C | -2.441168 | -0.287813 | -0.002169 |
| H | -3.348231 | -0.366448 | 0.597373 |
| H | -2.753339 | -0.203497 | -1.047322 |
| C | -0.266602 | -1.395891 | -0.616295 |
| C | -1.571987 | -1.533278 | 0.166421 |
| H | -2.112908 | -2.420803 | -0.164682 |
| H | -1.348586 | -1.673765 | 1.227597 |
| H | 2.225703 | 0.954142 | -1.055506 |
| H | 1.300161 | 0.694747 | 1.653396 |
| H | -1.398127 | 0.925879 | 1.453192 |
| H | -0.489732 | -1.348616 | -1.687499 |

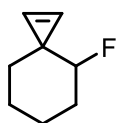
| | | | |
|---|-----------|-----------|-----------|
| H | 0.369867 | -2.270202 | -0.462243 |
| H | -2.263378 | 1.867667 | 0.235562 |
| C | 2.514618 | -0.650553 | 0.413924 |
| H | 3.436437 | -0.198285 | 0.771980 |
| H | 2.035602 | -0.649333 | -1.802495 |
| H | 2.648693 | -1.729051 | 0.356971 |
| H | 0.797400 | -0.998033 | 1.849619 |
| F | 0.295124 | 2.235436 | -0.036698 |

eq2

```

=====
C  0.603135   -1.443674   -0.553733
H  0.840706   -1.393373   -1.622221
C  1.881807   -1.253737    0.260767
C  2.472789    0.134174    0.018724
H  3.364288    0.287218    0.627208
H  2.780024    0.216883   -1.027997
C  0.179683    0.984916   -0.470619
C  1.441846    1.220190    0.330650
H  1.833645    2.212144    0.102510
H  1.190256    1.197678    1.394194
H  1.651624   -1.367256    1.324779
H  0.375221    1.106497   -1.539953
H  2.608661   -2.026226    0.006391
C -0.439024   -0.378016   -0.226502
C -1.822779   -0.543981   -0.903424
C -1.135075   -0.498775    1.159192
C -2.508504   -0.338821    0.467231
H -1.956396   -1.553150   -1.292497
H -2.064618    0.174684   -1.685941
H -0.992674   -1.490346    1.588580
H -0.876410    0.250432    1.905687
H -3.273949   -1.062510    0.738237
H -2.911605    0.664798    0.580598
H  0.167318   -2.427287   -0.368618
F -0.753262    1.990683   -0.136074

```



4-fluorospiro[2.5]oct-1-ene

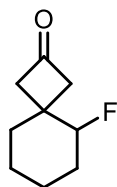
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -411.200533 | -411.019743 | -411.061205 |
| eq | -411.200139 | -411.0193 | -411.060592 |

ax

```
=====
C  -0.900475    -0.141906    -0.049807
C  -0.079143     1.081468     0.283417
H  -0.655789     1.773958     0.895904
C  -1.972039    -0.561274     0.919840
C  -2.392452    -0.020022    -0.171405
C   1.249423     0.741969     0.930670
C   2.030951    -0.290779     0.118769
H   2.322847     0.146851    -0.839477
H   2.951099    -0.548931     0.644116
C  -0.117693    -1.178307    -0.844196
C   1.188688    -1.540645    -0.134080
H   0.957232    -2.019610     0.822444
H   1.751952    -2.262409    -0.727356
H  -2.172579    -1.038441     1.863377
H  -3.205075     0.286708    -0.806593
H   1.032089     0.344093     1.925727
H  -0.738843    -2.062080    -0.992150
H   0.116003    -0.775146    -1.834677
H   1.825926     1.658469     1.065056
F   0.196842     1.772612    -0.926180
```

eq

```
=====
C  -0.665565    -0.509289    -0.177547
C  -0.260516     0.930656    -0.443803
H  -0.098120     1.079362    -1.515185
C  -1.617264    -0.815545     0.940152
C  -2.099370    -0.925506    -0.253080
C   0.979979     1.315322     0.336663
C   2.132960     0.369041    -0.004662
H   2.396985     0.490360    -1.059450
H   3.014301     0.639471     0.577385
C   0.476675    -1.454437    -0.524070
C   1.744209    -1.086941     0.251050
H   1.563577    -1.229730     1.320624
H   2.563816    -1.750366    -0.028917
H  -1.755315    -0.890026     2.005063
H  -2.929139    -1.158160    -0.898288
H   0.745745     1.247585     1.403041
H   0.171246    -2.479008    -0.310107
H   0.685763    -1.392839    -1.597767
H   1.245139     2.349913     0.114775
F  -1.305627     1.794848    -0.084377
```



5-fluorospiro[3.5]nonan-2-one

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -525.803450 | -525.586057 | -525.631901 |
| ax2 | -525.803208 | -525.585831 | -525.631918 |
| eq | -525.803740 | -525.586367 | -525.632054 |
| eq2 | -525.803554 | -525.586207 | -525.631918 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.304976 | 0.116336 | -0.113498 |
| C | -0.739528 | 1.056326 | 0.449745 |
| H | -0.282547 | 1.751293 | 1.156011 |
| C | 1.559309 | 0.816420 | -0.709926 |
| C | 1.196610 | -0.545797 | 0.981972 |
| C | -1.916988 | 0.331752 | 1.069279 |
| C | -2.531528 | -0.677236 | 0.099216 |
| H | -3.340526 | -1.214773 | 0.594378 |
| H | -2.972085 | -0.144236 | -0.747089 |
| C | -0.316038 | -0.900746 | -1.067841 |
| C | -1.473119 | -1.653289 | -0.412776 |
| H | -1.912873 | -2.351840 | -1.125440 |
| H | -1.094382 | -2.246846 | 0.424864 |
| H | 1.649662 | 1.860381 | -0.402149 |
| H | 1.152321 | -0.028483 | 1.942982 |
| H | -1.552460 | -0.184434 | 1.961726 |
| H | -0.678304 | -0.371857 | -1.953762 |
| H | 0.459023 | -1.594062 | -1.404365 |
| H | -2.652635 | 1.066941 | 1.397578 |
| H | 1.724995 | 0.730516 | -1.782841 |
| H | 1.099922 | -1.619265 | 1.136326 |
| F | -1.220219 | 1.851029 | -0.615601 |
| C | 2.399554 | -0.082994 | 0.177997 |
| O | 3.560297 | -0.384654 | 0.187146 |

ax2

| | | | |
|---|-----------|-----------|-----------|
| C | -0.651542 | -1.018024 | 1.071296 |
| H | -0.087319 | -1.870932 | 1.453762 |
| C | -1.834693 | -1.482057 | 0.223537 |
| C | -2.599100 | -0.283021 | -0.335729 |
| H | -3.429262 | -0.613979 | -0.960179 |
| H | -3.027964 | 0.289042 | 0.490918 |
| C | -0.456653 | 1.042703 | -0.351131 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.672341 | 0.618426 | -1.150931 |
| H | -2.192085 | 1.511457 | -1.499853 |
| H | -1.318358 | 0.083112 | -2.035402 |
| H | -1.467336 | -2.095482 | -0.605606 |
| H | 0.221359 | 1.650301 | -0.954622 |
| H | -2.496634 | -2.111837 | 0.818917 |
| C | 0.288061 | -0.124630 | 0.272298 |
| C | 1.576083 | 0.339888 | 1.011461 |
| C | 1.164008 | -0.847619 | -0.799407 |
| H | 1.781478 | -0.244052 | 1.910690 |
| H | 1.678354 | 1.401676 | 1.231796 |
| H | 1.191583 | -1.929660 | -0.658921 |
| H | 0.988371 | -0.619110 | -1.850240 |
| H | -1.018808 | -0.459694 | 1.937221 |
| F | -0.894527 | 1.882110 | 0.697416 |
| C | 2.373065 | -0.175622 | -0.172408 |
| O | 3.513254 | -0.043763 | -0.521143 |

eq

```
=====
```

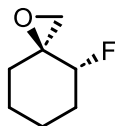
| | | | |
|---|-----------|-----------|-----------|
| C | -0.228099 | -0.043014 | 0.303702 |
| C | 0.808062 | 1.058141 | 0.385590 |
| H | 1.114381 | 1.193562 | 1.426126 |
| C | -1.556954 | 0.219212 | 1.067669 |
| C | -1.019205 | -0.127384 | -1.039177 |
| C | 2.007502 | 0.788743 | -0.495706 |
| C | 2.656592 | -0.538933 | -0.100468 |
| H | 3.507953 | -0.740561 | -0.750470 |
| H | 3.042587 | -0.460816 | 0.920017 |
| C | 0.418705 | -1.373221 | 0.689956 |
| C | 1.642617 | -1.680041 | -0.171108 |
| H | 2.099832 | -2.614985 | 0.154517 |
| H | 1.331232 | -1.820686 | -1.210072 |
| H | -1.723231 | 1.277994 | 1.274524 |
| H | -0.987557 | 0.803181 | -1.608892 |
| H | 1.670447 | 0.745243 | -1.535505 |
| H | 0.714799 | -1.323743 | 1.742398 |
| H | -0.326124 | -2.168564 | 0.604751 |
| H | 2.714059 | 1.614408 | -0.406570 |
| H | -1.755841 | -0.373982 | 1.959029 |
| H | -0.828020 | -0.973847 | -1.696617 |
| F | 0.222966 | 2.277017 | -0.007275 |
| C | -2.282247 | -0.193680 | -0.199923 |
| O | -3.407882 | -0.538663 | -0.431372 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.895992 | -1.451186 | 0.548919 |
| H | -1.208491 | -1.409955 | 1.597277 |
| C | -2.113975 | -1.263756 | -0.353932 |
| C | -2.729022 | 0.120800 | -0.152483 |
| H | -3.576625 | 0.267107 | -0.821904 |
| H | -3.109208 | 0.200727 | 0.870033 |
| C | -0.488186 | 0.993959 | 0.499298 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.688818 | 1.216972 | -0.392443 |
| H | -2.105406 | 2.205244 | -0.195493 |
| H | -1.359198 | 1.194597 | -1.434476 |
| H | -1.808965 | -1.375077 | -1.399079 |
| H | -0.757607 | 1.121738 | 1.550699 |
| H | -2.852348 | -2.040156 | -0.150968 |
| C | 0.149240 | -0.369239 | 0.304432 |
| C | 1.482836 | -0.514011 | 1.092266 |
| C | 0.935824 | -0.471490 | -1.040937 |
| H | 1.626711 | -1.524159 | 1.480585 |
| H | 1.702808 | 0.217753 | 1.868359 |
| H | 0.862613 | -1.464590 | -1.488439 |
| H | 0.772583 | 0.289307 | -1.802191 |
| H | -0.436050 | -2.427962 | 0.387580 |
| F | 0.475653 | 1.986255 | 0.222318 |
| C | 2.210392 | -0.331763 | -0.227739 |
| O | 3.349315 | -0.089073 | -0.515892 |



(3*S*,4*R*)-4-fluoro-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -448.376830 | -448.194543 | -448.235731 |
| eq | -448.377355 | -448.194976 | -448.235964 |

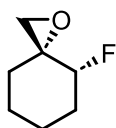
ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.853822 | -0.125843 | -0.093232 |
| C | -0.052470 | 1.110604 | 0.236375 |
| H | -0.649648 | 1.794817 | 0.838210 |
| C | -2.313493 | -0.036873 | -0.122690 |
| C | 1.260670 | 0.764759 | 0.906488 |
| C | 2.043219 | -0.282392 | 0.112477 |
| H | 2.340143 | 0.138089 | -0.851720 |
| H | 2.959274 | -0.533846 | 0.647060 |
| C | -0.099806 | -1.188991 | -0.848603 |
| C | 1.199749 | -1.536470 | -0.118766 |
| H | 0.958832 | -1.993279 | 0.845243 |
| H | 1.761352 | -2.273290 | -0.693272 |
| H | -2.868996 | -0.762597 | -0.704178 |
| H | -2.794888 | 0.919274 | 0.044897 |
| H | 1.023246 | 0.375242 | 1.900116 |
| H | -0.741145 | -2.062855 | -0.964047 |
| H | 0.130176 | -0.808373 | -1.847054 |
| H | 1.839501 | 1.678734 | 1.043953 |

```
F  0.221306    1.767654   -0.978777
O -1.631735   -0.576195    1.014686
```

eq

```
=====
C  -0.612334   -0.479004   -0.136564
C  -0.236797    0.952186   -0.428118
H  -0.116941    1.080353   -1.506941
C  -1.603225   -0.782014    0.897480
C   1.028864    1.338810    0.310696
C   2.166368    0.375579   -0.033217
H   2.405944    0.463111   -1.096685
H   3.061468    0.656928    0.521201
C   0.493084   -1.452193   -0.463859
C   1.774302   -1.068468    0.278571
H   1.611699   -1.174938    1.354729
H   2.579740   -1.749302    0.003220
H  -2.091714    0.023684    1.429518
H  -1.547078   -1.736085    1.407708
H   0.819657    1.299189    1.383304
H   0.165558   -2.459482   -0.207124
H   0.673154   -1.424763   -1.542758
H   1.291383    2.365576    0.055640
F  -1.274675    1.805539   -0.041760
O  -1.930296   -0.862937   -0.496987
```



(3*R*,4*R*)-4-fluoro-1-oxaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -448.377929 | -448.1956 | -448.236644 |
| eq | -448.376920 | -448.194522 | -448.235436 |

ax

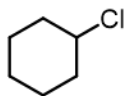
```
=====
C  -0.835590   -0.145488   -0.028326
C  -0.041188    1.095744    0.265729
H  -0.631422    1.801249    0.849268
C  -1.895629   -0.518641    0.911649
C   1.278587    0.757727    0.929908
C   2.056578   -0.288558    0.129474
H   2.351866    0.137283   -0.832535
H   2.973552   -0.544055    0.660600
C  -0.096663   -1.192591   -0.820009
C   1.214016   -1.541902   -0.109122
```

| | | | |
|---|-----------|-----------|-----------|
| H | 0.985112 | -2.012248 | 0.851685 |
| H | 1.772495 | -2.268067 | -0.699784 |
| H | -2.101308 | 0.108841 | 1.770739 |
| H | -2.158900 | -1.565298 | 1.005233 |
| H | 1.052622 | 0.372165 | 1.927539 |
| H | -0.733143 | -2.069159 | -0.939007 |
| H | 0.118323 | -0.796334 | -1.815851 |
| H | 1.856614 | 1.673726 | 1.054805 |
| F | 0.229192 | 1.731496 | -0.964529 |
| O | -2.203652 | 0.072585 | -0.353469 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.616984 | -0.496980 | -0.219104 |
| C | -0.267774 | 0.951066 | -0.463915 |
| H | -0.099512 | 1.101677 | -1.532498 |
| C | -2.008006 | -0.942191 | -0.181224 |
| C | 0.955898 | 1.348808 | 0.335181 |
| C | 2.129167 | 0.429946 | -0.016774 |
| H | 2.393194 | 0.569600 | -1.069101 |
| H | 3.001819 | 0.711276 | 0.572289 |
| C | 0.518155 | -1.431000 | -0.559612 |
| C | 1.772136 | -1.037032 | 0.224838 |
| H | 1.588454 | -1.193105 | 1.291150 |
| H | 2.604431 | -1.682009 | -0.057448 |
| H | -2.230483 | -1.976336 | -0.415774 |
| H | -2.805491 | -0.228037 | -0.340414 |
| H | 0.714910 | 1.258008 | 1.397517 |
| H | 0.213414 | -2.453371 | -0.336261 |
| H | 0.717683 | -1.366814 | -1.632580 |
| H | 1.197794 | 2.391746 | 0.130286 |
| F | -1.343944 | 1.767001 | -0.104583 |
| O | -1.262034 | -0.746418 | 1.027219 |



chlorocyclohexane

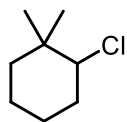
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -695.447724 | -695.277987 | -695.316442 |
| eq | -695.448482 | -695.278753 | -695.317453 |

ax

| | | | |
|----|-----------|-----------|-----------|
| C | 1.279217 | -1.582207 | 0.000000 |
| C | 0.609094 | -1.035047 | 1.260452 |
| C | 0.609094 | 0.492546 | 1.263834 |
| C | 0.002919 | 1.080431 | -0.000000 |
| C | 0.609094 | 0.492546 | -1.263834 |
| C | 0.609094 | -1.035047 | -1.260452 |
| H | 0.098370 | 0.888082 | 2.141413 |
| H | -0.419997 | -1.399489 | 1.311923 |
| H | 1.120442 | -1.398088 | 2.152629 |
| H | 2.334308 | -1.290952 | 0.000000 |
| H | 1.247990 | -2.672639 | 0.000000 |
| H | 0.078820 | 2.163330 | -0.000000 |
| H | 0.098370 | 0.888082 | -2.141413 |
| H | 1.642327 | 0.852722 | -1.300259 |
| H | -0.419997 | -1.399489 | -1.311923 |
| H | 1.120442 | -1.398088 | -2.152629 |
| H | 1.642327 | 0.852722 | 1.300259 |
| Cl | -1.814969 | 0.790263 | -0.000000 |

eq

| | | | |
|----|-----------|-----------|-----------|
| C | 0.837354 | -2.100682 | 0.000000 |
| C | 0.167765 | -1.550426 | 1.258110 |
| C | 0.167765 | -0.018488 | 1.260308 |
| C | -0.505080 | 0.492038 | -0.000000 |
| C | 0.167765 | -0.018488 | -1.260308 |
| C | 0.167765 | -1.550426 | -1.258110 |
| H | -0.345553 | 0.366691 | 2.141166 |
| H | -0.864310 | -1.909823 | 1.305226 |
| H | 0.673774 | -1.912667 | 2.153565 |
| H | 1.893140 | -1.813653 | 0.000000 |
| H | 0.800677 | -3.190897 | 0.000000 |
| H | -1.562093 | 0.231932 | -0.000000 |
| H | -0.345553 | 0.366691 | -2.141166 |
| H | 1.196699 | 0.350139 | -1.283657 |
| H | -0.864310 | -1.909823 | -1.305226 |
| H | 0.673774 | -1.912667 | -2.153565 |
| H | 1.196699 | 0.350139 | 1.283657 |
| Cl | -0.498409 | 2.321339 | -0.000000 |



2-chloro-1,1-dimethylcyclohexane

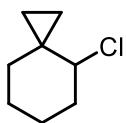
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -774.061730 | -773.833265 | -773.877184 |
| eq | -774.063144 | -773.834771 | -773.879034 |

ax

```
=====  
C  1.729420    -1.001340    -0.777546  
C  0.768349    -1.979060    -0.101591  
C  0.084867    -1.339241     1.105822  
C -0.596764    -0.022443     0.758597  
C  0.321083     0.979508     0.038057  
C  1.016588     0.298934    -1.152174  
H -0.644224    -2.017206     1.548582  
H  0.009352    -2.294955    -0.821559  
H  1.298868    -2.877222     0.216415  
H  2.566114    -0.789969    -0.107351  
H  2.153600    -1.455613    -1.674220  
H -1.024128     0.441196     1.644880  
H  0.264274     0.083185    -1.916350  
H  1.721257     1.008364    -1.592358  
H  0.828071    -1.127144     1.877970  
C -0.456332     2.203820    -0.444869  
H -1.032339     2.646056     0.371263  
H  0.240809     2.957678    -0.814421  
H -1.142955     1.953460    -1.251918  
C  1.356039     1.467463     1.066095  
H  2.021685     2.189169     0.590245  
H  0.858334     1.966775     1.899751  
H  1.968988     0.665139     1.471176  
C1 -2.083953    -0.411457    -0.258615
```

eq

```
=====  
C  2.367755    -0.030908     0.160081  
C  1.871449    -1.417521    -0.241198  
C  0.409083    -1.615309     0.163574  
C -0.445256    -0.505324    -0.425038  
C -0.022969     0.913015    -0.013780  
C  1.461338     1.050653    -0.423219  
H  0.042187    -2.577191    -0.193965  
H  1.959665    -1.530785    -1.325678  
H  2.483727    -2.196744     0.213870  
H  2.394689     0.047742     1.249473  
H  3.389221     0.119572    -0.192364  
H -0.432550    -0.570143    -1.512520  
H  1.521660     1.009338    -1.515607  
H  1.802583     2.043821    -0.123191  
H  0.316593    -1.613753     1.251256  
C -0.833466     1.953424    -0.786441  
H -1.884711     1.932917    -0.498886  
H -0.446595     2.953051    -0.580673  
H -0.767739     1.778687    -1.862325  
C -0.189087     1.163785     1.486857  
H  0.199419     2.153865     1.731779  
H -1.241284     1.137242     1.770174  
H  0.342878     0.436354     2.098144  
C1 -2.199578    -0.834992    -0.002030
```



4-chlorospiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -772.832315 | -772.627086 | -772.669498 |
| eq | -772.829456 | -772.624259 | -772.666609 |

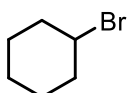
ax

| C | 0.948546 | -0.001076 | -0.040919 |
|----|-----------|-----------|-----------|
| C | -0.203553 | -0.640255 | 0.681131 |
| H | 0.149393 | -1.283771 | 1.482054 |
| C | 2.146401 | 0.307558 | 0.819436 |
| C | 2.204665 | -0.795226 | -0.206257 |
| C | -1.202642 | 0.385608 | 1.193387 |
| C | -1.621994 | 1.384341 | 0.116063 |
| H | -2.197999 | 0.867685 | -0.655920 |
| H | -2.280034 | 2.133778 | 0.556782 |
| C | 0.551222 | 1.006033 | -1.098587 |
| C | -0.403096 | 2.052457 | -0.521181 |
| H | 0.124172 | 2.638744 | 0.237472 |
| H | -0.718236 | 2.744830 | -1.302776 |
| H | 2.111535 | 0.020619 | 1.860973 |
| H | 2.675898 | 1.226208 | 0.609613 |
| H | 2.783818 | -0.620711 | -1.101974 |
| H | 2.204205 | -1.814261 | 0.155099 |
| H | -0.697814 | 0.920387 | 2.004192 |
| H | 1.449718 | 1.478157 | -1.498635 |
| H | 0.062394 | 0.486258 | -1.927846 |
| H | -2.065785 | -0.119259 | 1.625911 |
| Cl | -1.065798 | -1.816194 | -0.453140 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | -0.009834 | 0.846920 | -0.175037 |
| C | 0.407070 | -0.585492 | -0.438700 |
| H | 0.343359 | -0.790324 | -1.506706 |
| C | 0.498732 | 1.583896 | 1.026567 |
| C | 0.926486 | 1.996595 | -0.363684 |
| C | -0.456266 | -1.567137 | 0.337731 |
| C | -1.930378 | -1.368506 | -0.025299 |
| H | -2.075946 | -1.617985 | -1.080347 |
| H | -2.541215 | -2.060752 | 0.554926 |
| C | -1.470846 | 1.044368 | -0.546242 |
| C | -2.370337 | 0.073766 | 0.217181 |
| H | -2.312102 | 0.295609 | 1.286622 |
| H | -3.409641 | 0.208266 | -0.085334 |

| | | | |
|----|-----------|-----------|-----------|
| H | 1.241366 | 1.104202 | 1.647472 |
| H | -0.203338 | 2.217540 | 1.549993 |
| H | 0.507843 | 2.906115 | -0.770939 |
| H | 1.947586 | 1.788760 | -0.647007 |
| H | -0.309398 | -1.392228 | 1.406609 |
| H | -1.750342 | 2.078520 | -0.340072 |
| H | -1.593064 | 0.882855 | -1.622109 |
| H | -0.141813 | -2.587112 | 0.118296 |
| Cl | 2.160526 | -0.892937 | -0.041560 |



bromocyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|--------------|-------------------|
| ax | -2809.415613 | -2809.246216 | -2809.28596 |
| eq | -2809.416334 | -2809.246907 | -2809.286926 |

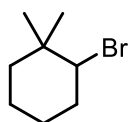
ax

| | | | |
|----|-----------|-----------|-----------|
| C | 1.743103 | -1.763947 | 0.000000 |
| C | 1.074971 | -1.215882 | 1.261018 |
| C | 1.074971 | 0.311310 | 1.264123 |
| C | 0.476327 | 0.904107 | 0.000000 |
| C | 1.074971 | 0.311310 | -1.264123 |
| C | 1.074971 | -1.215882 | -1.261018 |
| H | 0.570134 | 0.707115 | 2.144452 |
| H | 0.045818 | -1.579711 | 1.315161 |
| H | 1.588653 | -1.578254 | 2.152106 |
| H | 2.798978 | -1.475731 | 0.000000 |
| H | 1.709224 | -2.854264 | 0.000000 |
| H | 0.550889 | 1.986199 | -0.000000 |
| H | 0.570134 | 0.707115 | -2.144452 |
| H | 2.110236 | 0.668487 | -1.298413 |
| H | 0.045818 | -1.579711 | -1.315161 |
| H | 1.588653 | -1.578254 | -2.152106 |
| H | 2.110236 | 0.668487 | 1.298413 |
| Br | -1.508704 | 0.626355 | -0.000000 |

eq

| | | | |
|---|-----------|----------|-----------|
| C | -0.954470 | 2.677305 | 0.000000 |
| C | -0.283620 | 2.128010 | 1.257530 |
| C | -0.283620 | 0.594871 | 1.261298 |
| C | 0.388638 | 0.087511 | -0.000000 |
| C | -0.283620 | 0.594871 | -1.261298 |
| C | -0.283620 | 2.128010 | -1.257530 |

| | | | |
|----|-----------|-----------|-----------|
| H | 0.228897 | 0.213151 | 2.143665 |
| H | 0.748428 | 2.487429 | 1.303864 |
| H | -0.789221 | 2.489193 | 2.153780 |
| H | -2.009704 | 2.388226 | 0.000000 |
| H | -0.919951 | 3.767604 | 0.000000 |
| H | 1.446900 | 0.339208 | -0.000000 |
| H | 0.228897 | 0.213151 | -2.143665 |
| H | -1.313061 | 0.228822 | -1.288333 |
| H | 0.748428 | 2.487429 | -1.303864 |
| H | -0.789221 | 2.489193 | -2.153780 |
| H | -1.313061 | 0.228822 | 1.288333 |
| Br | 0.398130 | -1.902734 | -0.000000 |



2-bromo-1,1-dimethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|--------------|-------------------|
| ax | -2888.029178 | -2887.801028 | -2887.846182 |
| eq | -2888.030753 | -2887.802674 | -2887.84812 |

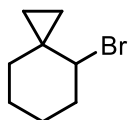
ax

| | | | |
|----|-----------|-----------|-----------|
| C | 1.895148 | -1.310237 | -0.852878 |
| C | 0.819608 | -2.088275 | -0.095207 |
| C | 0.358158 | -1.330166 | 1.148008 |
| C | -0.080635 | 0.094373 | 0.837784 |
| C | 0.950477 | 0.902492 | 0.033818 |
| C | 1.417067 | 0.102166 | -1.192880 |
| H | -0.447596 | -1.860298 | 1.653976 |
| H | -0.036259 | -2.256683 | -0.753368 |
| H | 1.194460 | -3.069365 | 0.198485 |
| H | 2.804397 | -1.262202 | -0.248901 |
| H | 2.157565 | -1.836727 | -1.771715 |
| H | -0.349725 | 0.630271 | 1.744229 |
| H | 0.584651 | 0.034659 | -1.899214 |
| H | 2.210697 | 0.664469 | -1.690388 |
| H | 1.184668 | -1.263331 | 1.860529 |
| Br | -1.850224 | -0.007107 | -0.110746 |
| C | 0.398857 | 2.257421 | -0.408889 |
| H | -0.030982 | 2.799109 | 0.436703 |
| H | 1.206701 | 2.862647 | -0.823532 |
| H | -0.370558 | 2.149819 | -1.171420 |

| | | | |
|---|----------|----------|----------|
| C | 2.133113 | 1.180998 | 0.980522 |
| H | 2.890221 | 1.756617 | 0.445944 |
| H | 1.803264 | 1.771045 | 1.837687 |
| H | 2.605573 | 0.276084 | 1.355430 |

eq

| | | | |
|----|-----------|-----------|-----------|
| C | 2.790668 | -0.470768 | 0.162220 |
| C | 2.011055 | -1.718847 | -0.240922 |
| C | 0.537837 | -1.600026 | 0.160639 |
| C | -0.054441 | -0.331675 | -0.429894 |
| C | 0.655623 | 0.963707 | -0.013602 |
| C | 2.136926 | 0.777977 | -0.423465 |
| H | -0.021983 | -2.462959 | -0.197865 |
| H | 2.075553 | -1.849095 | -1.325145 |
| H | 2.439885 | -2.611401 | 0.216121 |
| H | 2.830310 | -0.398731 | 1.251694 |
| H | 3.821787 | -0.541465 | -0.187243 |
| H | -0.059859 | -0.396439 | -1.516677 |
| H | 2.186496 | 0.723256 | -1.515713 |
| H | 2.681703 | 1.676047 | -0.124452 |
| H | 0.447080 | -1.581613 | 1.248080 |
| Br | -2.006967 | -0.287585 | -0.000610 |
| C | 0.097645 | 2.159289 | -0.784672 |
| H | -0.930123 | 2.375950 | -0.494116 |
| H | 0.701413 | 3.045406 | -0.580866 |
| H | 0.118399 | 1.974198 | -1.860679 |
| C | 0.552750 | 1.242175 | 1.487441 |
| H | 1.155097 | 2.118369 | 1.733765 |
| H | -0.478129 | 1.451402 | 1.772418 |
| H | 0.907850 | 0.411576 | 2.095546 |



4-bromospiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|--------------|-------------------|
| ax | -2886.800366 | -2886.59545 | -2886.639124 |
| eq | -2886.796914 | -2886.591992 | -2886.63557 |

ax

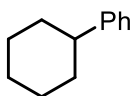
| | | | |
|---|-----------|-----------|-----------|
| C | 0.982268 | -0.747805 | -0.036073 |
| C | -0.095320 | -0.148847 | 0.817595 |
| H | -0.330493 | -0.790656 | 1.660963 |
| C | 2.015681 | -1.544315 | 0.723146 |
| C | 1.027746 | -2.234242 | -0.180100 |

| | | | |
|----|-----------|-----------|-----------|
| C | 0.235736 | 1.265832 | 1.263975 |
| C | 0.688596 | 2.159060 | 0.110672 |
| H | -0.150706 | 2.331275 | -0.567895 |
| H | 0.986127 | 3.131416 | 0.504408 |
| C | 1.458224 | 0.131835 | -1.171988 |
| C | 1.844154 | 1.520751 | -0.661061 |
| H | 2.712282 | 1.431625 | -0.000968 |
| H | 2.137756 | 2.158655 | -1.495659 |
| H | 1.885757 | -1.660204 | 1.789936 |
| H | 3.040042 | -1.459170 | 0.388444 |
| H | 1.390908 | -2.627501 | -1.119081 |
| H | 0.237619 | -2.806177 | 0.286632 |
| H | 1.056833 | 1.165531 | 1.982283 |
| H | 2.303971 | -0.348695 | -1.666011 |
| H | 0.659684 | 0.225244 | -1.913887 |
| H | -0.607975 | 1.701500 | 1.797378 |
| Br | -1.836123 | -0.139041 | -0.195530 |

eq

```
=====
```

| | | | |
|----|-----------|-----------|-----------|
| C | -0.696231 | 0.893465 | -0.174117 |
| C | 0.041339 | -0.403277 | -0.434456 |
| H | 0.036819 | -0.617339 | -1.501799 |
| C | -0.388743 | 1.734644 | 1.027060 |
| C | -0.066401 | 2.235585 | -0.362272 |
| C | -0.568377 | -1.559906 | 0.341531 |
| C | -2.048241 | -1.710639 | -0.025726 |
| H | -2.128437 | -1.988930 | -1.080579 |
| H | -2.480633 | -2.526150 | 0.555060 |
| C | -2.162558 | 0.739628 | -0.552292 |
| C | -2.812928 | -0.411062 | 0.212815 |
| H | -2.809954 | -0.179047 | 1.281759 |
| H | -3.854440 | -0.523049 | -0.091399 |
| H | 0.444105 | 1.450916 | 1.653787 |
| H | -1.227013 | 2.180074 | 1.544121 |
| H | -0.691304 | 3.015347 | -0.774443 |
| H | 0.975747 | 2.281553 | -0.640618 |
| H | -0.471074 | -1.357781 | 1.411042 |
| H | -2.676984 | 1.680717 | -0.352287 |
| H | -2.238063 | 0.549827 | -1.627810 |
| H | -0.027562 | -2.480270 | 0.124608 |
| Br | 1.981761 | -0.302757 | -0.019906 |



cyclohexylbenzene

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -466.861333 | -466.597314 | -466.643741 |
| eq | -466.865604 | -466.601955 | -466.649452 |

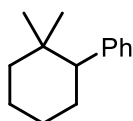
ax

| C | 1.424780 | 1.485266 | 0.262044 |
|---|-----------|-----------|-----------|
| C | 0.676241 | 0.385412 | 1.041260 |
| H | 0.507991 | 0.767612 | 2.052246 |
| C | 1.579786 | -0.850712 | 1.162549 |
| C | 2.144821 | -1.333715 | -0.177297 |
| H | 2.830017 | -2.165045 | -0.001643 |
| H | 1.343255 | -1.714892 | -0.813448 |
| C | 1.928198 | 0.994068 | -1.093709 |
| C | 2.858075 | -0.205280 | -0.920363 |
| H | 3.213086 | -0.558418 | -1.890011 |
| H | 3.738721 | 0.106478 | -0.349598 |
| H | 2.420247 | -0.574630 | 1.805414 |
| H | 1.077077 | 0.705362 | -1.719069 |
| H | 2.443351 | 1.804422 | -1.612129 |
| H | 1.055358 | -1.660009 | 1.673304 |
| H | 0.791724 | 2.363646 | 0.138967 |
| H | 2.283804 | 1.797486 | 0.863050 |
| C | -0.710383 | 0.115941 | 0.466130 |
| C | -1.605887 | 1.183003 | 0.329192 |
| C | -1.164566 | -1.154670 | 0.113039 |
| C | -2.892262 | 0.993695 | -0.155130 |
| H | -1.296662 | 2.178921 | 0.620519 |
| C | -2.454000 | -1.350550 | -0.376460 |
| H | -0.519452 | -2.014436 | 0.221416 |
| C | -3.322780 | -0.278640 | -0.518022 |
| H | -3.561521 | 1.839285 | -0.244786 |
| H | -2.775342 | -2.348371 | -0.644999 |
| H | -4.323795 | -0.430321 | -0.898622 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | -1.257099 | 0.110323 | -1.258725 |
| C | -0.579854 | -0.452046 | 0.000110 |
| H | -0.731044 | -1.536238 | 0.000377 |
| C | -1.257095 | 0.110941 | 1.258670 |
| C | -2.757957 | -0.177323 | 1.259210 |
| H | -2.914310 | -1.259676 | 1.305318 |
| H | -3.219158 | 0.249392 | 2.151518 |
| C | -2.757960 | -0.177945 | -1.259118 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.426827 | 0.372067 | -0.000089 |
| H | -4.490880 | 0.129704 | -0.000028 |
| H | -3.347004 | 1.463853 | -0.000359 |
| H | -1.097404 | 1.193209 | 1.293377 |
| H | -3.219165 | 0.248330 | -2.151636 |
| H | -2.914312 | -1.260321 | -1.304692 |
| H | -0.786381 | -0.311760 | 2.148706 |
| H | -1.097412 | 1.192574 | -1.293964 |
| H | -0.786388 | -0.312815 | -2.148554 |
| C | 0.910899 | -0.202454 | 0.000047 |
| C | 1.811820 | -1.266475 | 0.000303 |
| C | 1.424529 | 1.097284 | -0.000265 |
| C | 3.185510 | -1.045317 | 0.000250 |
| H | 1.432063 | -2.281058 | 0.000548 |
| C | 2.794871 | 1.323446 | -0.000319 |
| H | 0.746266 | 1.941811 | -0.000468 |
| C | 3.682195 | 0.251593 | -0.000062 |
| H | 3.865571 | -1.887023 | 0.000454 |
| H | 3.171945 | 2.337746 | -0.000563 |
| H | 4.749430 | 0.427704 | -0.000104 |



(2,2-dimethylcyclohexyl)benzene

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -545.473208 | -545.150506 | -545.202886 |
| eq | -545.479336 | -545.156937 | -545.208878 |

ax

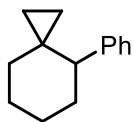
| | | | |
|---|-----------|-----------|-----------|
| C | 1.053279 | -0.927914 | -1.492464 |
| C | 0.436408 | 0.311392 | -0.805872 |
| H | 0.356274 | 1.081687 | -1.577105 |
| C | 1.390966 | 0.908371 | 0.274726 |
| C | 1.940527 | -0.182166 | 1.210963 |
| H | 2.671845 | 0.278297 | 1.880918 |
| H | 1.132949 | -0.550416 | 1.847909 |
| C | 1.599156 | -1.980058 | -0.527069 |
| C | 2.575725 | -1.359856 | 0.471187 |
| H | 2.905680 | -2.110863 | 1.191061 |
| H | 3.469301 | -1.023355 | -0.061011 |
| H | 0.781865 | -2.463303 | 0.011147 |
| H | 2.096798 | -2.765577 | -1.098827 |
| H | 0.309920 | -1.371926 | -2.157252 |
| H | 1.874471 | -0.590014 | -2.128749 |
| C | -0.994239 | 0.071831 | -0.350147 |
| C | -2.015428 | 0.804954 | -0.961209 |
| C | -1.366886 | -0.845803 | 0.638646 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.349977 | 0.635825 | -0.610403 |
| H | -1.757814 | 1.524724 | -1.728591 |
| C | -2.700075 | -1.018391 | 0.994543 |
| H | -0.622139 | -1.433762 | 1.152058 |
| C | -3.699762 | -0.280304 | 0.372661 |
| H | -4.113478 | 1.221005 | -1.105964 |
| H | -2.956115 | -1.734319 | 1.764564 |
| H | -4.735790 | -0.417305 | 0.651570 |
| C | 2.556248 | 1.603153 | -0.445327 |
| H | 2.188017 | 2.444980 | -1.035148 |
| H | 3.270930 | 1.990361 | 0.283919 |
| H | 3.094838 | 0.936493 | -1.117249 |
| C | 0.667868 | 1.968263 | 1.107618 |
| H | 0.219638 | 2.730500 | 0.465389 |
| H | -0.124295 | 1.532472 | 1.717559 |
| H | 1.374250 | 2.464537 | 1.776684 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.193479 | 0.906229 | 0.232495 |
| C | -0.428128 | -0.217132 | -0.533115 |
| H | -0.563111 | 0.016857 | -1.594926 |
| C | -1.055238 | -1.600398 | -0.301773 |
| C | -2.528459 | -1.620584 | -0.702605 |
| H | -2.608783 | -1.440921 | -1.779388 |
| H | -2.955585 | -2.606288 | -0.510399 |
| C | -2.676576 | 0.829297 | -0.178283 |
| C | -3.310545 | -0.542079 | 0.042684 |
| H | -4.348566 | -0.525833 | -0.294277 |
| H | -3.329998 | -0.778106 | 1.109986 |
| H | -0.966133 | -1.886250 | 0.748616 |
| H | -3.230138 | 1.597758 | 0.367582 |
| H | -2.749886 | 1.080691 | -1.241911 |
| H | -0.496876 | -2.342144 | -0.876692 |
| C | 1.065271 | -0.216501 | -0.280115 |
| C | 1.926851 | 0.407568 | -1.184445 |
| C | 1.628459 | -0.828733 | 0.842233 |
| C | 3.300969 | 0.430203 | -0.976444 |
| H | 1.511417 | 0.881232 | -2.065855 |
| C | 3.002110 | -0.808936 | 1.056267 |
| H | 0.991228 | -1.327051 | 1.560840 |
| C | 3.844878 | -0.178071 | 0.148517 |
| H | 3.945979 | 0.919337 | -1.694519 |
| H | 3.414623 | -1.289931 | 1.933459 |
| H | 4.913784 | -0.165325 | 0.313805 |
| C | -1.060104 | 0.776312 | 1.753412 |
| H | -0.033082 | 0.954764 | 2.073613 |
| H | -1.692109 | 1.523038 | 2.239344 |
| H | -1.361731 | -0.203599 | 2.122532 |
| C | -0.658514 | 2.278903 | -0.179702 |
| H | -0.702970 | 2.408616 | -1.263472 |
| H | -1.258815 | 3.067664 | 0.279241 |
| H | 0.375783 | 2.419022 | 0.137675 |



4-phenylspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -544.243268 | -543.943695 | -543.994695 |
| ax2 | -544.243269 | -543.943696 | -543.994702 |
| ax3 | -544.246064 | -543.946765 | -543.997341 |
| eq1 | -544.247500 | -543.948328 | -543.998962 |

ax1

```

=====
C  -1.366714    0.808823   -0.277866
C  -0.436642    0.291772    0.819574
H  -0.361528    1.090271    1.560321
C  -2.308055    1.914409    0.114716
C  -1.133389    2.194495   -0.792428
C  -1.088511   -0.911423    1.532793
C  -1.668208   -1.974104    0.596076
H  -0.868671   -2.513564    0.085883
H  -2.204615   -2.714885    1.191833
C  -1.918494   -0.240286   -1.221296
C  -2.610945   -1.355639   -0.436715
H  -3.480215   -0.935844    0.079233
H  -2.981907   -2.123240   -1.117660
H  -2.258846    2.289492    1.127608
H  -3.294805    1.913458   -0.327759
H  -1.338732    2.387591   -1.836345
H  -0.303597    2.751103   -0.377521
H  -1.909010   -0.515358    2.138602
H  -2.620707    0.234188   -1.909728
H  -1.115612   -0.660030   -1.832784
H  -0.372297   -1.360304    2.223281
C   0.988408    0.057336    0.346714
C   1.363771   -0.937023   -0.562971
C   1.995494    0.891785    0.840539
C   2.689348   -1.086801   -0.956359
H   0.628445   -1.608180   -0.978804
C   3.321545    0.746647    0.449948
H   1.733351    1.669345    1.547610
C   3.675379   -0.246972   -0.453428
H   2.949934   -1.865739   -1.660842
H   4.075604    1.409915    0.852858
H   4.705285   -0.366326   -0.761570

```

ax2

```
=====
C -1.366877    0.808764   -0.277956
C -0.436644    0.291864    0.819455
H -0.361569    1.090415    1.560143
C -2.308352    1.914188    0.114744
C -1.133769    2.194498   -0.792466
C -1.088353   -0.911311    1.532850
C -1.667967   -1.974110    0.596232
H -0.868375   -2.513474    0.086036
H -2.204198   -2.714948    1.192064
C -1.918587   -0.240479   -1.221250
C -2.610889   -1.355852   -0.436551
H -3.480154   -0.936144    0.079466
H -2.981825   -2.123551   -1.117411
H -2.259151    2.289175    1.127667
H -3.295092    1.913143   -0.327747
H -1.339329    2.387656   -1.836332
H -0.304045    2.751231   -0.377601
H -1.908859   -0.515318    2.138686
H -2.620803    0.233859   -1.909767
H -1.115687   -0.660292   -1.832682
H -0.372067   -1.360065    2.223370
C  0.988441    0.057481    0.346578
C  1.363832   -0.936783   -0.563200
C  1.995580    0.891789    0.840561
C  2.689432   -1.086604   -0.956501
H  0.628509   -1.607796   -0.979247
C  3.321660    0.746611    0.450060
H  1.733494    1.669304    1.547691
C  3.675497   -0.246922   -0.453379
H  2.950005   -1.865463   -1.661070
H  4.075714    1.409792    0.853129
H  4.705420   -0.366333   -0.761445
```

ax3

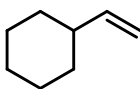
```
=====
C  1.487228    0.725733   -0.165220
C  0.463162   -0.140180   -0.885609
H  0.445642    0.177856   -1.932722
C  2.606746    1.272551   -1.007859
C  1.531618    2.189503   -0.480116
C  0.947327   -1.603562   -0.853545
C  1.245548   -2.079061    0.567815
H  0.328625   -2.047487    1.165316
H  1.575667   -3.118776    0.546570
C  1.856966    0.263807    1.232866
C  2.307047   -1.197158    1.223971
H  3.242459   -1.285073    0.662689
H  2.508683   -1.533666    2.242137
H  2.601279    1.049192   -2.065846
H  3.587187    1.336666   -0.556537
H  1.795343    2.869281    0.318721
H  0.808198    2.571859   -1.187622
```

| | | | |
|---|-----------|-----------|-----------|
| H | 1.864590 | -1.665230 | -1.445969 |
| H | 2.645023 | 0.908975 | 1.626411 |
| H | 0.999013 | 0.361157 | 1.903227 |
| H | 0.218644 | -2.258352 | -1.330103 |
| C | -0.967145 | 0.010046 | -0.374783 |
| C | -1.979460 | -0.774434 | -0.938034 |
| C | -1.334316 | 0.936762 | 0.601113 |
| C | -3.300847 | -0.652644 | -0.530935 |
| H | -1.734667 | -1.484744 | -1.717506 |
| C | -2.658211 | 1.061229 | 1.014843 |
| H | -0.586970 | 1.580040 | 1.042450 |
| C | -3.647198 | 0.264704 | 0.455761 |
| H | -4.061666 | -1.272168 | -0.987309 |
| H | -2.912489 | 1.786504 | 1.776623 |
| H | -4.675342 | 0.360183 | 0.777861 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.226057 | 0.879446 | -0.017721 |
| C | 0.460099 | -0.353163 | -0.514540 |
| H | 0.595581 | -0.374535 | -1.601614 |
| C | 0.578589 | 2.228193 | 0.049421 |
| C | 0.902613 | 1.477823 | 1.320360 |
| C | 1.128270 | -1.615519 | 0.050552 |
| C | 2.602936 | -1.685318 | -0.344665 |
| H | 2.679218 | -1.762353 | -1.433771 |
| H | 3.057314 | -2.585902 | 0.071488 |
| C | 2.692953 | 0.827237 | -0.401408 |
| C | 3.358315 | -0.443410 | 0.125704 |
| H | 4.399575 | -0.485697 | -0.197936 |
| H | 3.361599 | -0.417824 | 1.219735 |
| H | -0.464695 | 2.316092 | -0.218302 |
| H | 1.190238 | 3.084587 | -0.199293 |
| H | 1.730166 | 1.832503 | 1.919426 |
| H | 0.070615 | 1.076249 | 1.881260 |
| H | 1.055018 | -1.607985 | 1.141406 |
| H | 2.776941 | 0.851955 | -1.493194 |
| H | 3.200882 | 1.714443 | -0.018393 |
| H | 0.596178 | -2.500834 | -0.303209 |
| C | -1.031791 | -0.301026 | -0.267562 |
| C | -1.611003 | -0.751757 | 0.919536 |
| C | -1.873867 | 0.224340 | -1.249931 |
| C | -2.985428 | -0.672901 | 1.119860 |
| H | -0.989900 | -1.170446 | 1.700092 |
| C | -3.246971 | 0.305237 | -1.055713 |
| H | -1.442336 | 0.574462 | -2.180177 |
| C | -3.808939 | -0.143487 | 0.134168 |
| H | -3.412100 | -1.028987 | 2.048270 |
| H | -3.877496 | 0.715021 | -1.833693 |
| H | -4.877789 | -0.084925 | 0.289535 |



vinylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -313.217508 | -313.004442 | -313.045632 |
| ax2 | -313.217766 | -313.004702 | -313.044951 |
| eq | -313.220192 | -313.007328 | -313.048322 |
| eq2 | -313.220027 | -313.007132 | -313.047834 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.189626 | -1.259307 | 0.701170 |
| C | -0.697749 | -0.000405 | 0.675791 |
| H | -1.319198 | -0.000549 | 1.574308 |
| C | 0.189146 | 1.258967 | 0.701484 |
| C | 1.245172 | 1.259927 | -0.405233 |
| H | 0.759442 | 1.314004 | -1.383520 |
| H | 1.868434 | 2.151226 | -0.315443 |
| C | 1.245764 | -1.259516 | -0.405504 |
| C | 2.108901 | 0.000389 | -0.340641 |
| H | 2.669700 | 0.000464 | 0.599714 |
| H | 2.841288 | 0.000638 | -1.149696 |
| H | 0.697364 | 1.295170 | 1.669828 |
| H | 1.869397 | -2.150562 | -0.315847 |
| H | 0.760110 | -1.313587 | -1.383827 |
| H | -0.436679 | 2.150909 | 0.633973 |
| C | -1.625815 | -0.000287 | -0.507294 |
| C | -2.950610 | 0.000096 | -0.417346 |
| H | -1.170589 | -0.000299 | -1.493509 |
| H | -3.578721 | 0.000444 | -1.299243 |
| H | -3.449309 | 0.000188 | 0.545900 |
| H | -0.435667 | -2.151600 | 0.633286 |
| H | 0.697827 | -1.295627 | 1.669520 |

ax2

| | | | |
|---|-----------|-----------|-----------|
| C | -0.519452 | 1.433502 | 0.459198 |
| C | 0.621464 | 0.467409 | 0.826556 |
| H | 1.044842 | 0.818560 | 1.773813 |
| C | 0.068277 | -0.945806 | 1.046055 |
| C | -0.777982 | -1.444337 | -0.129092 |
| H | -0.149260 | -1.578124 | -1.012144 |
| H | -1.197309 | -2.422676 | 0.112677 |
| C | -1.328594 | 0.935191 | -0.737328 |
| C | -1.896231 | -0.457421 | -0.464766 |
| H | -2.592475 | -0.399787 | 0.378311 |
| H | -2.465614 | -0.811842 | -1.325779 |
| H | -0.561536 | -0.922004 | 1.939876 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.133660 | 1.637586 | -0.959762 |
| H | -0.686408 | 0.895331 | -1.622882 |
| H | 0.881324 | -1.643127 | 1.256222 |
| C | 1.738299 | 0.558654 | -0.182960 |
| C | 2.389523 | -0.442618 | -0.762206 |
| H | 2.035751 | 1.575471 | -0.430771 |
| H | 3.198696 | -0.250030 | -1.455279 |
| H | 2.148592 | -1.480558 | -0.568630 |
| H | -0.109800 | 2.425995 | 0.259733 |
| H | -1.184969 | 1.527759 | 1.321867 |

eq

```
=====
```

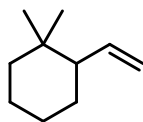
| | | | |
|---|-----------|-----------|-----------|
| C | 0.100120 | -1.257880 | 0.257718 |
| C | -0.665910 | 0.000538 | -0.177743 |
| H | -0.736211 | 0.000421 | -1.270766 |
| C | 0.100712 | 1.258332 | 0.257632 |
| C | 1.533970 | 1.258112 | -0.272322 |
| H | 1.511204 | 1.302477 | -1.365696 |
| H | 2.058563 | 2.151181 | 0.071539 |
| C | 1.533385 | -1.258676 | -0.271931 |
| C | 2.283857 | -0.000382 | 0.161597 |
| H | 2.383172 | -0.000222 | 1.251762 |
| H | 3.294103 | -0.000657 | -0.251145 |
| H | 0.118571 | 1.294382 | 1.352419 |
| H | 2.057386 | -2.151876 | 0.072501 |
| H | 1.510877 | -1.303560 | -1.365293 |
| H | -0.432202 | 2.148256 | -0.083013 |
| C | -2.053714 | 0.000430 | 0.388675 |
| C | -3.172430 | -0.000324 | -0.325824 |
| H | -2.116409 | 0.000986 | 1.475340 |
| H | -4.146695 | -0.000490 | 0.146166 |
| H | -3.146498 | -0.000701 | -1.410017 |
| H | -0.433432 | -2.147279 | -0.083061 |
| H | 0.117628 | -1.293827 | 1.352450 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.218830 | -1.325593 | -0.205278 |
| C | 0.618668 | -0.221051 | 0.460649 |
| H | 0.440357 | -0.296533 | 1.541406 |
| C | 0.144026 | 1.155869 | -0.000375 |
| C | -1.348620 | 1.348113 | 0.269263 |
| H | -1.523316 | 1.328368 | 1.349600 |
| H | -1.668083 | 2.329147 | -0.086280 |
| C | -1.711347 | -1.134753 | 0.059596 |
| C | -2.178266 | 0.248300 | -0.391916 |
| H | -2.071701 | 0.324492 | -1.478730 |
| H | -3.237004 | 0.383928 | -0.164528 |
| H | 0.331218 | 1.254792 | -1.074899 |
| H | -2.283228 | -1.913552 | -0.447822 |
| H | -1.900895 | -1.245458 | 1.131889 |
| H | 0.721529 | 1.938019 | 0.496840 |
| C | 2.081406 | -0.479538 | 0.234053 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.951017 | 0.338821 | -0.346993 |
| H | 2.431349 | -1.450396 | 0.577142 |
| H | 3.986575 | 0.049942 | -0.473779 |
| H | 2.667415 | 1.318005 | -0.712207 |
| H | 0.110647 | -2.303652 | 0.151683 |
| H | -0.033190 | -1.298114 | -1.284310 |



1,1-dimethyl-2-vinylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -391.832190 | -391.560485 | -391.606669 |
| ax2 | -391.830248 | -391.558314 | -391.603891 |
| ax3 | -391.826775 | -391.554838 | -391.600655 |
| eq | -391.834282 | -391.562742 | -391.609318 |
| eq2 | -391.833558 | -391.561943 | -391.60823 |
| eq3 | -391.828133 | -391.556322 | -391.602741 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.219936 | 0.977420 | 0.040667 |
| C | 0.656849 | -0.188629 | 0.583929 |
| H | 1.175998 | 0.182619 | 1.473019 |
| C | -0.209222 | -1.396685 | 0.999205 |
| C | -1.132762 | -1.871246 | -0.123339 |
| H | -0.537372 | -2.255904 | -0.956080 |
| H | -1.747052 | -2.700088 | 0.232442 |
| C | -1.168064 | 0.464373 | -1.058234 |
| C | -2.017212 | -0.730246 | -0.623769 |
| H | -2.706114 | -0.430502 | 0.170201 |
| H | -2.631225 | -1.068048 | -1.460462 |
| H | -0.815319 | -1.121842 | 1.865107 |
| H | -1.808738 | 1.290128 | -1.379472 |
| H | -0.574008 | 0.173742 | -1.930267 |
| H | 0.446121 | -2.208432 | 1.320433 |
| C | 1.713904 | -0.625332 | -0.394111 |
| C | 3.015899 | -0.628748 | -0.134991 |
| H | 1.375214 | -0.974043 | -1.365813 |
| H | 3.738510 | -0.972319 | -0.864511 |
| H | 3.400232 | -0.286331 | 0.819857 |
| C | -1.024295 | 1.586841 | 1.195406 |
| H | -0.350328 | 2.001143 | 1.948402 |
| H | -1.653841 | 2.399001 | 0.825477 |
| H | -1.671933 | 0.864510 | 1.689468 |
| C | 0.666764 | 2.080459 | -0.539983 |
| H | 1.201972 | 1.741942 | -1.427924 |
| H | 0.059298 | 2.943379 | -0.821220 |
| H | 1.407034 | 2.411803 | 0.192664 |

ax2

```
=====
C  0.993053    -0.462690    0.014826
C -0.391949    -0.536308    0.731969
H -0.211811    -1.090257    1.662037
C -0.903891     0.862908    1.107295
C -0.923983     1.837950   -0.073546
H -1.659046     1.515163   -0.813795
H -1.236126     2.824426    0.274188
C  0.918326     0.526630   -1.160246
C  0.443565     1.919282   -0.749710
H  1.166051     2.376007   -0.068458
H  0.389508     2.564643   -1.628257
H -0.262204     1.275109    1.887766
H  1.900943     0.581011   -1.636695
H  0.224962     0.125931   -1.907539
H -1.899442     0.780356    1.546770
C -1.404565    -1.361310   -0.026068
C -2.651672    -1.027695   -0.339586
H -1.075613    -2.359357   -0.296019
H -3.296469    -1.732222   -0.849877
H -3.079648    -0.062485   -0.101679
C  2.058673    -0.015797    1.024684
H  2.174825    -0.769288    1.806848
H  3.022626     0.099904    0.524695
H  1.820276     0.930095    1.507014
C  1.425422    -1.831003   -0.519688
H  0.820881    -2.150459   -1.368676
H  2.463652    -1.782679   -0.854150
H  1.358751    -2.597702    0.256247
```

ax3

```
=====
C  0.256902     0.969210   -0.044892
C -0.534995    -0.052728   -0.906048
H -0.684422     0.423713   -1.880821
C  0.288332    -1.339804   -1.155778
C  0.784643    -1.960955    0.148079
H -0.071445    -2.270330    0.755098
H  1.362565    -2.860955   -0.068564
C  0.836085     0.313898    1.223336
C  1.627739    -0.963848    0.941105
H  2.533949    -0.727356    0.377300
H  1.952149    -1.408380    1.883619
H  1.144541    -1.106147   -1.791122
H  1.469708     1.046430    1.731138
H  0.025242     0.073585    1.913763
H -0.324571    -2.054791   -1.708498
C -1.914748    -0.476809   -0.457215
C -2.481969    -0.469678    0.743726
H -2.498702    -0.902634   -1.270500
H -3.483137    -0.862896    0.871617
```

| | | | |
|---|-----------|-----------|-----------|
| H | -1.999384 | -0.084463 | 1.630315 |
| C | 1.409509 | 1.520800 | -0.900463 |
| H | 1.015343 | 2.052464 | -1.769213 |
| H | 2.002046 | 2.226789 | -0.315226 |
| H | 2.081273 | 0.744144 | -1.261440 |
| C | -0.612908 | 2.169359 | 0.341260 |
| H | -1.387378 | 1.912539 | 1.060348 |
| H | 0.009720 | 2.949406 | 0.785052 |
| H | -1.099038 | 2.592218 | -0.541528 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.045162 | 0.899671 | -0.001415 |
| C | 0.554008 | -0.519899 | -0.222768 |
| H | 0.635250 | -0.653328 | -1.307629 |
| C | -0.366151 | -1.628245 | 0.316263 |
| C | -1.771401 | -1.546082 | -0.274551 |
| H | -1.717558 | -1.734102 | -1.351543 |
| H | -2.403880 | -2.325303 | 0.154238 |
| C | -1.466601 | 0.922888 | -0.591855 |
| C | -2.382750 | -0.167203 | -0.040595 |
| H | -2.543572 | -0.015720 | 1.030135 |
| H | -3.362033 | -0.101313 | -0.517984 |
| H | -0.421299 | -1.557197 | 1.406324 |
| H | -1.901357 | 1.910891 | -0.418702 |
| H | -1.388614 | 0.796420 | -1.677224 |
| H | 0.082362 | -2.597639 | 0.089448 |
| C | 1.927640 | -0.674672 | 0.363417 |
| C | 3.040846 | -0.840185 | -0.340511 |
| H | 1.988018 | -0.670784 | 1.449173 |
| H | 4.002725 | -0.964827 | 0.140784 |
| H | 3.023378 | -0.855119 | -1.424982 |
| C | -0.080247 | 1.281965 | 1.482985 |
| H | 0.928617 | 1.396436 | 1.881944 |
| H | -0.592939 | 2.238674 | 1.604588 |
| H | -0.600903 | 0.546360 | 2.095426 |
| C | 0.797902 | 1.935131 | -0.747530 |
| H | 0.871091 | 1.686973 | -1.808938 |
| H | 0.342992 | 2.924593 | -0.662535 |
| H | 1.809217 | 1.994770 | -0.343169 |

eq2

```
=====
```

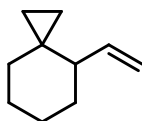
| | | | |
|---|-----------|-----------|-----------|
| C | -0.195594 | 0.949778 | 0.007932 |
| C | 0.578315 | -0.279350 | -0.562134 |
| H | 0.381400 | -0.264762 | -1.642646 |
| C | 0.036143 | -1.605167 | -0.022342 |
| C | -1.457790 | -1.757322 | -0.298808 |
| H | -1.618907 | -1.797650 | -1.380821 |
| H | -1.821065 | -2.700438 | 0.112957 |
| C | -1.698325 | 0.739764 | -0.255569 |
| C | -2.243219 | -0.582718 | 0.278075 |
| H | -2.177673 | -0.601590 | 1.369170 |
| H | -3.301238 | -0.673114 | 0.025560 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.214403 | -1.672120 | 1.054216 |
| H | -2.248458 | 1.580246 | 0.175699 |
| H | -1.863019 | 0.774627 | -1.338094 |
| H | 0.586590 | -2.429361 | -0.480523 |
| C | 2.067979 | -0.136363 | -0.399350 |
| C | 2.870804 | -0.953296 | 0.273457 |
| H | 2.513080 | 0.723141 | -0.891372 |
| H | 3.935184 | -0.762699 | 0.328503 |
| H | 2.504948 | -1.832933 | 0.788088 |
| C | 0.061646 | 1.128813 | 1.507419 |
| H | 1.115082 | 1.338046 | 1.699297 |
| H | -0.520827 | 1.972510 | 1.884131 |
| H | -0.214017 | 0.249360 | 2.088500 |
| C | 0.232742 | 2.230804 | -0.713311 |
| H | 0.155732 | 2.114970 | -1.796841 |
| H | -0.415008 | 3.058693 | -0.416730 |
| H | 1.257582 | 2.513414 | -0.471309 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.115043 | 0.832451 | -0.051282 |
| C | 0.404185 | -0.633855 | -0.463293 |
| H | 0.211329 | -0.677470 | -1.544673 |
| C | -0.591363 | -1.623144 | 0.175928 |
| C | -2.038994 | -1.273929 | -0.157332 |
| H | -2.192477 | -1.395136 | -1.234346 |
| H | -2.717378 | -1.967596 | 0.342385 |
| C | -1.359067 | 1.127166 | -0.406413 |
| C | -2.359707 | 0.166696 | 0.231016 |
| H | -2.334906 | 0.266944 | 1.319098 |
| H | -3.371628 | 0.427121 | -0.084523 |
| H | -0.449191 | -1.631554 | 1.260053 |
| H | -1.584298 | 2.156971 | -0.117837 |
| H | -1.466203 | 1.072039 | -1.495224 |
| H | -0.361226 | -2.630632 | -0.176345 |
| C | 1.795270 | -1.191082 | -0.288633 |
| C | 2.893606 | -0.672110 | 0.249373 |
| H | 1.876879 | -2.206376 | -0.672167 |
| H | 3.803205 | -1.259145 | 0.283553 |
| H | 2.950078 | 0.323356 | 0.663073 |
| C | 0.328191 | 1.096708 | 1.445575 |
| H | 1.376438 | 1.035855 | 1.729968 |
| H | -0.019615 | 2.103685 | 1.687877 |
| H | -0.224420 | 0.399199 | 2.073667 |
| C | 0.972850 | 1.804716 | -0.867601 |
| H | 0.853796 | 1.616228 | -1.937043 |
| H | 0.657384 | 2.832260 | -0.672339 |
| H | 2.032154 | 1.732548 | -0.629202 |



4-vinylspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -390.602152 | -390.353623 | -390.398496 |
| ax2 | -390.602155 | -390.353734 | -390.397852 |
| ax3 | -390.601998 | -390.353429 | -390.397494 |
| eq | -390.602353 | -390.353998 | -390.398994 |
| eq2 | -390.595500 | -390.346494 | -390.390333 |
| eq3 | -390.601806 | -390.353289 | -390.397875 |

ax1

```

=====
C  -0.174992    0.891436   -0.052093
C   0.687485   -0.219234    0.542810
H   1.270213    0.207907    1.362961
C  -0.577318    2.005547    0.870979
C   0.442655    2.243364   -0.218856
C  -0.224885   -1.324395    1.107346
C  -1.247420   -1.822182    0.083409
H  -0.733818   -2.315370   -0.746513
H  -1.889805   -2.573629    0.545205
C  -1.199820    0.418514   -1.063328
C  -2.090639   -0.668606   -0.460856
H  -2.678049   -0.236973    0.355502
H  -2.797288   -1.034155   -1.207615
H  -0.220917    1.973679    1.891441
H  -1.560556    2.436662    0.740265
H   0.139965    2.838206   -1.069630
H   1.475730    2.360896    0.080650
H  -0.761035   -0.912324    1.967321
H  -1.798416    1.268567   -1.396410
H  -0.690890    0.020372   -1.946769
H   0.384621   -2.152621    1.473410
C   1.660567   -0.755070   -0.471028
C   2.980225   -0.667201   -0.354241
H   1.242568   -1.234462   -1.351533
H   3.644255   -1.063500   -1.112050
H   3.438269   -0.196289    0.508910

```

ax2

```

=====
C  -0.631921   -0.595905    0.023469
C  -0.179250    0.599852    0.844908
H  -0.741354    0.596117    1.785761
C  -1.149299   -1.782773    0.788733
C  -2.092951   -0.922795   -0.015874

```

| | | | |
|---|-----------|-----------|-----------|
| C | 1.312185 | 0.449027 | 1.198497 |
| C | 2.170368 | 0.209570 | -0.043687 |
| H | 2.112570 | 1.081710 | -0.702536 |
| H | 3.216547 | 0.098260 | 0.245610 |
| C | 0.222223 | -0.889271 | -1.195629 |
| C | 1.694731 | -1.027929 | -0.805163 |
| H | 1.817582 | -1.909540 | -0.168244 |
| H | 2.305755 | -1.186062 | -1.695292 |
| H | -1.198630 | -1.709692 | 1.866520 |
| H | -0.916469 | -2.766472 | 0.404871 |
| H | -2.493462 | -1.335366 | -0.931930 |
| H | -2.766497 | -0.274650 | 0.528314 |
| H | 1.421876 | -0.402369 | 1.875791 |
| H | -0.137040 | -1.801518 | -1.676101 |
| H | 0.123264 | -0.080683 | -1.924662 |
| H | 1.653435 | 1.335786 | 1.736304 |
| C | -0.442555 | 1.940366 | 0.203140 |
| C | -1.151180 | 2.183749 | -0.892419 |
| H | -0.004284 | 2.783569 | 0.732477 |
| H | -1.291569 | 3.196724 | -1.247977 |
| H | -1.615844 | 1.390832 | -1.464751 |

ax3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.975055 | -0.296041 | -0.071830 |
| C | -0.323058 | -0.672149 | 0.635694 |
| H | -0.051847 | -1.330685 | 1.468551 |
| C | 2.229208 | -0.266108 | 0.752092 |
| C | 2.009918 | -1.359395 | -0.268003 |
| C | -0.981417 | 0.589615 | 1.207357 |
| C | -1.150364 | 1.694572 | 0.159906 |
| H | -1.864128 | 1.377689 | -0.603881 |
| H | -1.567316 | 2.584630 | 0.634161 |
| C | 0.808969 | 0.777881 | -1.126467 |
| C | 0.180189 | 2.030704 | -0.515145 |
| H | 0.867965 | 2.448342 | 0.226836 |
| H | 0.032530 | 2.792944 | -1.281922 |
| H | 2.156894 | -0.536104 | 1.796798 |
| H | 2.963862 | 0.493603 | 0.522973 |
| H | 2.601828 | -1.328973 | -1.172420 |
| H | 1.791224 | -2.351163 | 0.104491 |
| H | -0.339383 | 0.965077 | 2.008985 |
| H | 1.779336 | 1.007951 | -1.570592 |
| H | 0.165114 | 0.405018 | -1.930314 |
| H | -1.941586 | 0.343470 | 1.663805 |
| C | -1.204258 | -1.489428 | -0.277428 |
| C | -2.507355 | -1.343399 | -0.483008 |
| H | -0.686864 | -2.292661 | -0.796783 |
| H | -3.041556 | -2.011934 | -1.146279 |
| H | -3.087392 | -0.564706 | -0.003415 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | -0.082805 | 0.828699 | -0.148092 |
| C | 0.535956 | -0.568322 | -0.236373 |
| H | 0.568648 | -0.837644 | -1.298310 |
| C | 0.216479 | 1.708717 | 1.032216 |
| C | 0.765949 | 2.047956 | -0.334389 |
| C | -0.376385 | -1.575449 | 0.485696 |
| C | -1.805823 | -1.539883 | -0.052124 |
| H | -1.802423 | -1.861825 | -1.098189 |
| H | -2.427293 | -2.248848 | 0.497408 |
| C | -1.499256 | 0.870573 | -0.687104 |
| C | -2.395381 | -0.133474 | 0.036250 |
| H | -2.481848 | 0.156390 | 1.088008 |
| H | -3.401293 | -0.115048 | -0.386281 |
| H | 0.916264 | 1.364135 | 1.779779 |
| H | -0.591777 | 2.317709 | 1.413407 |
| H | 0.326697 | 2.885665 | -0.858378 |
| H | 1.827327 | 1.912856 | -0.488608 |
| H | -0.381656 | -1.334102 | 1.553881 |
| H | -1.895526 | 1.883092 | -0.588187 |
| H | -1.482046 | 0.632649 | -1.756239 |
| H | 0.042037 | -2.578756 | 0.385183 |
| C | 1.932263 | -0.659053 | 0.305428 |
| C | 3.010108 | -0.913101 | -0.425867 |
| H | 2.041966 | -0.532009 | 1.379479 |
| H | 3.992632 | -0.990537 | 0.022188 |
| H | 2.941658 | -1.053701 | -1.498988 |

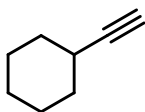
eq2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.052209 | 0.774450 | -0.209782 |
| C | 0.367915 | -0.692944 | -0.479626 |
| H | 0.112862 | -0.869005 | -1.533615 |
| C | 0.617752 | 1.504710 | 0.975095 |
| C | 1.042599 | 1.877367 | -0.428991 |
| C | -0.594200 | -1.576367 | 0.344221 |
| C | -2.057587 | -1.255574 | 0.048554 |
| H | -2.273162 | -1.511214 | -0.993576 |
| H | -2.707202 | -1.873978 | 0.670275 |
| C | -1.396811 | 1.095173 | -0.538115 |
| C | -2.355513 | 0.225213 | 0.272519 |
| H | -2.238897 | 0.460554 | 1.334844 |
| H | -3.389180 | 0.450510 | 0.004926 |
| H | 1.330606 | 1.003928 | 1.611777 |
| H | -0.045298 | 2.186083 | 1.490994 |
| H | 0.657995 | 2.803983 | -0.832876 |
| H | 2.044809 | 1.630077 | -0.742227 |
| H | -0.385129 | -1.412951 | 1.406256 |
| H | -1.583849 | 2.153178 | -0.345114 |
| H | -1.568800 | 0.925481 | -1.606545 |
| H | -0.390419 | -2.628108 | 0.134399 |
| C | 1.763703 | -1.236410 | -0.314501 |
| C | 2.872624 | -0.718927 | 0.203558 |

| | | | |
|---|----------|-----------|-----------|
| H | 1.833650 | -2.259992 | -0.676564 |
| H | 3.773403 | -1.319279 | 0.236412 |
| H | 2.952461 | 0.280593 | 0.603043 |

eq3

```
=====
C  -0.188204    0.883419   -0.179414
C   0.536791   -0.401782   -0.595497
H   0.312619   -0.546285   -1.660813
C   0.260804    1.608668    1.055950
C   0.457107    2.230051   -0.307662
C  -0.068122   -1.583766    0.168306
C  -1.575329   -1.687015   -0.064646
H  -1.759789   -1.892751   -1.123767
H  -1.981916   -2.528775    0.498286
C  -1.684515    0.800463   -0.411561
C  -2.288697   -0.393790    0.325683
H  -2.185212   -0.236916    1.403732
H  -3.356354   -0.468645    0.112738
H   1.144263    1.248059    1.564841
H  -0.502198    2.027249    1.697752
H  -0.185176    3.057302   -0.577021
H   1.467292    2.299978   -0.682813
H   0.124084   -1.453694    1.237962
H  -2.155182    1.730689   -0.087346
H  -1.875306    0.697230   -1.485135
H   0.423952   -2.509623   -0.135842
C   2.033745   -0.307008   -0.483386
C   2.805927   -1.015930    0.331324
H   2.508546    0.408686   -1.147530
H   3.880034   -0.880538    0.334283
H   2.403295   -1.751822    1.016100
```



ethynylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -311.978154 | -311.789174 | -311.829127 |
| eq | -311.978675 | -311.789716 | -311.829859 |

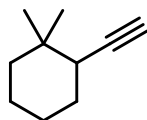
ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.581804 | 0.574052 | -1.263793 |
| C | 0.084853 | 1.150184 | -0.000000 |
| H | -0.043221 | 2.234179 | -0.000000 |
| C | -0.581804 | 0.574052 | 1.263793 |
| C | -0.581804 | -0.953324 | 1.260830 |
| H | 0.449046 | -1.316354 | 1.311414 |
| H | -1.092073 | -1.321052 | 2.152187 |
| C | -0.581804 | -0.953324 | -1.260830 |
| C | -1.249529 | -1.502670 | 0.000000 |
| H | -2.305362 | -1.213686 | 0.000000 |
| H | -1.216466 | -2.593270 | 0.000000 |
| H | -1.612909 | 0.936089 | 1.283228 |
| H | -1.092073 | -1.321052 | -2.152187 |
| H | 0.449046 | -1.316354 | -1.311414 |
| H | -0.082489 | 0.960167 | 2.152958 |
| H | -0.082489 | 0.960167 | -2.152958 |
| H | -1.612909 | 0.936089 | -1.283228 |
| C | 1.530287 | 0.885154 | -0.000000 |
| C | 2.709112 | 0.658265 | -0.000000 |
| H | 3.756858 | 0.460744 | -0.000000 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | 0.014203 | -1.264831 | -0.141007 |
| C | 0.695994 | 0.000070 | 0.407766 |
| H | 0.587456 | 0.000061 | 1.497038 |
| C | 0.014089 | 1.264904 | -0.141040 |
| C | -1.479018 | 1.259158 | 0.180033 |
| H | -1.611851 | 1.304693 | 1.265305 |
| H | -1.947585 | 2.151752 | -0.236928 |
| C | -1.478906 | -1.259255 | 0.180060 |
| C | -2.157772 | -0.000079 | -0.357087 |
| H | -2.099618 | -0.000110 | -1.449985 |
| H | -3.216282 | -0.000113 | -0.092690 |
| H | 0.158701 | 1.293215 | -1.224866 |
| H | -1.947363 | -2.151893 | -0.236919 |
| H | -1.611737 | -1.304788 | 1.265326 |
| H | 0.495143 | 2.150601 | 0.275391 |
| C | 2.128848 | 0.000236 | 0.100513 |

| | | | |
|---|----------|-----------|-----------|
| C | 3.296572 | -0.000158 | -0.177981 |
| H | 4.334933 | -0.000069 | -0.419825 |
| H | 0.495356 | -2.150463 | 0.275441 |
| H | 0.158786 | -1.293150 | -1.224834 |



2-ethynyl-1,1-dimethylcyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -390.592901 | -390.345289 | -390.39064 |
| eq | -390.594048 | -390.346536 | -390.392177 |

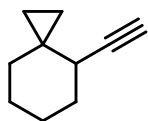
ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.575206 | -0.839304 | -0.019827 |
| C | 0.573847 | -0.177821 | -0.837507 |
| H | 0.670486 | -0.731204 | -1.775805 |
| C | 0.276567 | 1.301445 | -1.161148 |
| C | -0.022749 | 2.106053 | 0.101923 |
| H | 0.873546 | 2.140438 | 0.728350 |
| H | -0.262241 | 3.135850 | -0.166826 |
| C | -0.877546 | 0.015721 | 1.221614 |
| C | -1.168419 | 1.481975 | 0.898272 |
| H | -2.095682 | 1.562525 | 0.325524 |
| H | -1.324280 | 2.035690 | 1.825522 |
| H | -0.578495 | 1.344376 | -1.837159 |
| H | -1.719018 | -0.431298 | 1.756923 |
| H | -0.013834 | -0.031853 | 1.892736 |
| H | 1.126900 | 1.727329 | -1.694629 |
| C | 1.868411 | -0.274948 | -0.146942 |
| C | 2.928047 | -0.325447 | 0.414803 |
| H | 3.869741 | -0.377796 | 0.911900 |
| C | -1.815153 | -0.961696 | -0.912696 |
| H | -1.596293 | -1.584997 | -1.782280 |
| H | -2.624366 | -1.436089 | -0.354409 |
| H | -2.179920 | -0.001438 | -1.272060 |
| C | -0.173105 | -2.247690 | 0.417766 |
| H | -1.011409 | -2.736739 | 0.917603 |
| H | 0.108731 | -2.857483 | -0.443930 |
| H | 0.667969 | -2.227044 | 1.110986 |

eq

| | | | |
|---|----------|----------|-----------|
| C | 0.064272 | 0.883248 | -0.020282 |
|---|----------|----------|-----------|

| | | | |
|---|-----------|-----------|-----------|
| C | 0.515043 | -0.536755 | -0.469735 |
| H | 0.399732 | -0.568948 | -1.558772 |
| C | -0.361141 | -1.657284 | 0.120133 |
| C | -1.830444 | -1.444238 | -0.232103 |
| H | -1.952235 | -1.527557 | -1.316549 |
| H | -2.436460 | -2.230877 | 0.219627 |
| C | -1.428147 | 1.032037 | -0.364729 |
| C | -2.311793 | -0.067830 | 0.220751 |
| H | -2.299463 | -0.018252 | 1.312463 |
| H | -3.345964 | 0.090098 | -0.089397 |
| H | -0.234890 | -1.681928 | 1.204788 |
| H | -1.765358 | 2.014430 | -0.025213 |
| H | -1.530591 | 1.020028 | -1.455088 |
| H | -0.011523 | -2.616608 | -0.263089 |
| C | 1.929791 | -0.790898 | -0.175391 |
| C | 3.079337 | -1.018092 | 0.085451 |
| H | 4.101827 | -1.218588 | 0.311451 |
| C | 0.297491 | 1.098714 | 1.477343 |
| H | 1.361135 | 1.045291 | 1.714739 |
| H | -0.060615 | 2.088989 | 1.765427 |
| H | -0.220810 | 0.364908 | 2.093267 |
| C | 0.853247 | 1.936925 | -0.797290 |
| H | 0.499827 | 2.937423 | -0.540179 |
| H | 1.918188 | 1.886357 | -0.564501 |
| H | 0.731270 | 1.800267 | -1.873850 |



4-ethynylspiro[2.5]octane

R-Group: acetylenyl Variant: cyclopropyl

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -389.361765 | -389.137353 | -389.181301 |
| eq | -389.361407 | -389.137058 | -389.180935 |

ax

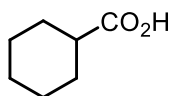
| | | | |
|---|-----------|-----------|-----------|
| C | -0.898183 | 0.238700 | -0.058938 |
| C | 0.333616 | 0.608951 | 0.761983 |
| H | 0.011994 | 1.195633 | 1.625397 |
| C | -2.184016 | 0.075889 | 0.696615 |
| C | -1.976249 | 1.262542 | -0.215841 |
| C | 1.037994 | -0.669117 | 1.256780 |
| C | 1.349694 | -1.624585 | 0.106098 |
| H | 2.072400 | -1.156335 | -0.568832 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.819756 | -2.527188 | 0.498646 |
| C | -0.610377 | -0.720495 | -1.193841 |
| C | 0.084937 | -1.980817 | -0.676269 |
| H | -0.601831 | -2.524617 | -0.020433 |
| H | 0.329143 | -2.643365 | -1.507805 |
| H | -2.173994 | 0.257536 | 1.762445 |
| H | -2.861899 | -0.699406 | 0.367449 |
| H | -2.519219 | 1.279226 | -1.150527 |
| H | -1.825405 | 2.227984 | 0.247674 |
| H | 0.364021 | -1.159196 | 1.963825 |
| H | -1.543773 | -0.972945 | -1.699808 |
| H | 0.033563 | -0.227996 | -1.929807 |
| H | 1.946253 | -0.402594 | 1.797842 |
| C | 1.248907 | 1.450741 | -0.023930 |
| C | 1.995511 | 2.128114 | -0.675214 |
| H | 2.657991 | 2.733722 | -1.250732 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.031047 | 0.813124 | -0.184590 |
| C | 0.469377 | -0.622187 | -0.481025 |
| H | 0.311461 | -0.799164 | -1.550653 |
| C | 0.591593 | 1.518153 | 1.014880 |
| C | 0.978111 | 1.954506 | -0.379386 |
| C | -0.416053 | -1.613344 | 0.299026 |
| C | -1.893121 | -1.394187 | -0.020514 |
| H | -2.066880 | -1.617822 | -1.077569 |
| H | -2.500491 | -2.091762 | 0.557836 |
| C | -1.434755 | 1.031213 | -0.501076 |
| C | -2.316738 | 0.045703 | 0.264878 |
| H | -2.225708 | 0.242660 | 1.337231 |
| H | -3.364300 | 0.192440 | -0.002098 |
| H | 1.347112 | 1.012046 | 1.599745 |
| H | -0.079219 | 2.153250 | 1.576520 |
| H | 0.564901 | 2.881871 | -0.750787 |
| H | 1.985788 | 1.734560 | -0.702892 |
| H | -0.240091 | -1.464297 | 1.367979 |
| H | -1.705965 | 2.060362 | -0.259769 |
| H | -1.592669 | 0.897433 | -1.576514 |
| H | -0.117141 | -2.633583 | 0.056757 |
| C | 1.886433 | -0.866570 | -0.200522 |
| C | 3.040208 | -1.081971 | 0.048444 |
| H | 4.066598 | -1.274646 | 0.263527 |



cyclohexanecarboxylic acid

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -424.419630 | -424.223908 | -424.266561 |
| eq | -424.420732 | -424.225036 | -424.26841 |
| eq2 | -424.419851 | -424.223994 | -424.267488 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.597651 | -1.184639 | 0.902086 |
| C | -0.385725 | -0.012669 | 0.927037 |
| H | -0.896438 | 0.015625 | 1.894682 |
| C | 0.345900 | 1.322703 | 0.722386 |
| C | 1.171635 | 1.310395 | -0.563114 |
| H | 1.690996 | 2.262720 | -0.678259 |
| H | 0.503012 | 1.207447 | -1.425092 |
| C | 1.457831 | -1.184973 | -0.363358 |
| C | 2.170657 | 0.153363 | -0.557450 |
| H | 2.884102 | 0.305128 | 0.258769 |
| H | 2.743988 | 0.142903 | -1.485750 |
| H | 1.013310 | 1.466692 | 1.575451 |
| H | 0.821896 | -1.381594 | -1.230086 |
| H | 2.184557 | -1.997070 | -0.310867 |
| H | -0.363522 | 2.148327 | 0.723159 |
| H | 1.245569 | -1.090285 | 1.776933 |
| H | 0.058048 | -2.126320 | 0.996506 |
| C | -1.501256 | -0.212008 | -0.076725 |
| O | -1.752538 | -1.236773 | -0.658652 |
| O | -2.254962 | 0.889556 | -0.238826 |
| H | -2.965664 | 0.671125 | -0.860785 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | 0.260896 | 1.184163 | 0.385519 |
| C | -0.356409 | -0.008185 | -0.370500 |
| H | -0.317043 | 0.215987 | -1.440414 |
| C | 0.413201 | -1.294347 | -0.082969 |
| C | 1.889786 | -1.133491 | -0.440906 |
| H | 2.427515 | -2.054256 | -0.210674 |
| H | 1.984107 | -0.968869 | -1.518726 |
| C | 1.739423 | 1.335583 | 0.032315 |
| C | 2.512945 | 0.046397 | 0.303813 |
| H | 3.558117 | 0.166907 | 0.014813 |
| H | 2.498615 | -0.160449 | 1.378459 |
| H | 0.317529 | -1.530081 | 0.979794 |
| H | 1.826869 | 1.591950 | -1.027851 |
| H | 2.167807 | 2.163738 | 0.598761 |

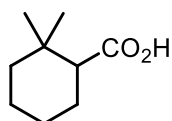
| | | | |
|---|-----------|-----------|-----------|
| H | -0.029612 | -2.123831 | -0.635924 |
| H | -0.284554 | 2.097682 | 0.148860 |
| H | 0.157222 | 1.006705 | 1.460495 |
| C | -1.808286 | -0.134447 | 0.004112 |
| O | -2.282749 | -0.979071 | 0.720866 |
| O | -2.560338 | 0.841451 | -0.534700 |
| H | -3.471213 | 0.721445 | -0.225221 |

eq2

```

=====
C  -0.313976    1.255490   -0.173099
C   0.357795    0.009722    0.426120
H   0.271128    0.051583    1.512968
C  -0.325633   -1.268020   -0.081781
C  -1.813546   -1.246824    0.264622
H  -2.292336   -2.150275   -0.115582
H  -1.929046   -1.256121    1.352606
C  -1.802329    1.272803    0.171536
C  -2.495805   -0.003243   -0.304454
H  -3.548946    0.012188   -0.019885
H  -2.459159   -0.043776   -1.397505
H  -0.204004   -1.328653   -1.165915
H  -1.917989    1.363794    1.255692
H  -2.272531    2.149985   -0.275176
H   0.157047   -2.145611    0.351977
H   0.176390    2.156977    0.198527
H  -0.189744    1.237161   -1.258736
C   1.832438    0.004040    0.132971
O   2.708574    0.094139    0.956992
O   2.104821   -0.106284   -1.178235
H   3.068370   -0.093903   -1.284511

```



2,2-dimethylcyclohexane-1-carboxylic acid

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -503.032449 | -502.777841 | -502.825876 |
| ax2 | -503.031490 | -502.776828 | -502.82471 |
| eq | -503.034693 | -502.780146 | -502.828144 |
| eq2 | -503.033947 | -502.779408 | -502.827409 |

ax

```

=====
C  -0.423890    1.025911   -0.017096
C   0.422083   -0.026623    0.760533
H   0.819051    0.466743    1.648084
C  -0.406012   -1.248702    1.201860

```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.241112 | -1.865891 | 0.080087 |
| H | -1.866214 | -2.658000 | 0.495784 |
| H | -0.581363 | -2.325798 | -0.656533 |
| C | -1.249191 | 0.343538 | -1.120596 |
| C | -2.106874 | -0.813644 | -0.610314 |
| H | -2.860997 | -0.441836 | 0.088048 |
| H | -2.647316 | -1.263646 | -1.444695 |
| H | -1.070569 | -0.923742 | 2.004579 |
| H | -0.566569 | -0.035293 | -1.885733 |
| H | -1.875617 | 1.102098 | -1.596926 |
| H | 0.261585 | -1.996002 | 1.635050 |
| C | 1.616346 | -0.462777 | -0.053421 |
| O | 1.596542 | -1.177275 | -1.025059 |
| O | 2.771053 | 0.040850 | 0.419414 |
| H | 3.485850 | -0.269481 | -0.158293 |
| C | -1.344605 | 1.735846 | 0.982074 |
| H | -0.753766 | 2.282707 | 1.719372 |
| H | -1.977776 | 2.453396 | 0.456636 |
| H | -1.994961 | 1.046824 | 1.518516 |
| C | 0.489955 | 2.078775 | -0.647678 |
| H | 1.124016 | 2.550802 | 0.105631 |
| H | 1.134568 | 1.646515 | -1.416139 |
| H | -0.110878 | 2.857523 | -1.120916 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.493996 | 1.005711 | -0.019339 |
| C | 0.428975 | 0.042737 | 0.784574 |
| H | 0.739482 | 0.571472 | 1.686034 |
| C | -0.282240 | -1.259739 | 1.208843 |
| C | -1.065315 | -1.944880 | 0.088623 |
| H | -1.616439 | -2.788116 | 0.508204 |
| H | -0.377370 | -2.349669 | -0.654755 |
| C | -1.273850 | 0.254574 | -1.112290 |
| C | -2.024490 | -0.970048 | -0.591063 |
| H | -2.797025 | -0.662588 | 0.118423 |
| H | -2.536930 | -1.464452 | -1.417866 |
| H | -0.973418 | -1.003312 | 2.013984 |
| H | -0.578220 | -0.063525 | -1.891949 |
| H | -1.970324 | 0.958486 | -1.574941 |
| H | 0.451091 | -1.945122 | 1.638461 |
| C | 1.731767 | -0.246259 | 0.078854 |
| O | 2.815749 | 0.104075 | 0.476599 |
| O | 1.602892 | -0.955237 | -1.055812 |
| H | 2.491585 | -1.086364 | -1.422122 |
| C | -1.469437 | 1.656577 | 0.969712 |
| H | -0.925292 | 2.267263 | 1.692503 |
| H | -2.164181 | 2.305573 | 0.433199 |
| H | -2.055568 | 0.924533 | 1.523777 |
| C | 0.337731 | 2.116757 | -0.663246 |
| H | 0.934199 | 2.643785 | 0.084526 |
| H | 1.013432 | 1.725242 | -1.426783 |
| H | -0.319023 | 2.843511 | -1.144995 |

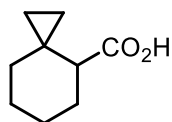
eq

```
=====
C  0.290359    0.938906    0.055224
C -0.322424   -0.412247   -0.425452
H -0.302218   -0.390621   -1.517593
C  0.474822   -1.628519    0.058013
C  1.926013   -1.544670   -0.407537
H  2.486013   -2.402056   -0.031584
H  1.954213   -1.597276   -1.500340
C  1.755784    0.963419   -0.416722
C  2.575191   -0.239456    0.046844
H  3.589072   -0.165385   -0.349718
H  2.662468   -0.235308    1.136239
H  0.431384   -1.684121    1.146581
H  1.762168    0.993140   -1.511376
H  2.213147    1.893242   -0.069813
H  0.005878   -2.537123   -0.323884
C -1.764963   -0.542089   -0.009790
O -2.151127   -0.954972    1.055243
O -2.624360   -0.147801   -0.966111
H -3.523354   -0.245013   -0.614951
C -0.447938    2.110788   -0.594037
H -0.461091    2.013818   -1.681305
H -1.479827    2.179140   -0.245772
H  0.051789    3.048194   -0.341785
C  0.216373    1.100672    1.576787
H  0.726939    2.021790    1.865118
H -0.817920    1.171435    1.914345
H  0.685926    0.277504    2.112803
```

eq2

```
=====
C  0.303284    0.948416    0.060173
C -0.321384   -0.368564   -0.495482
H -0.243411   -0.307460   -1.583474
C  0.419283   -1.625752   -0.022655
C  1.891668   -1.565122   -0.419460
H  2.409057   -2.455598   -0.059780
H  1.970844   -1.565998   -1.510979
C  1.793714    0.942682   -0.327864
C  2.550579   -0.302214    0.129815
H  3.588037   -0.241812   -0.202851
H  2.571278   -0.347667    1.221778
H  0.334147   -1.722939    1.060332
H  1.862821    1.013926   -1.418357
H  2.257555    1.843962    0.080279
H -0.056401   -2.506401   -0.458111
C -1.801391   -0.442170   -0.216871
O -2.664874   -0.046710   -0.961153
O -2.099615   -1.002994    0.967421
H -3.064624   -0.993293    1.062919
C -0.359847    2.160159   -0.596782
H -0.299059    2.098812   -1.685048
H -1.411536    2.243729   -0.319961
```

| | | | |
|---|-----------|----------|-----------|
| H | 0.144651 | 3.074801 | -0.278803 |
| C | 0.146101 | 1.071051 | 1.579390 |
| H | 0.685840 | 1.954031 | 1.927388 |
| H | -0.901824 | 1.191061 | 1.856929 |
| H | 0.536495 | 0.207568 | 2.116010 |



spiro[2.5]octane-4-carboxylic acid

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -501.802628 | -501.571481 | -501.618258 |
| ax2 | -501.802281 | -501.57125 | -501.617866 |
| eq | -501.801911 | -501.570521 | -501.617247 |
| eq2 | -501.800812 | -501.569499 | -501.616193 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.919249 | -0.592721 | -0.041025 |
| C | 0.400882 | -0.251211 | -0.701181 |
| H | 0.542629 | -0.884706 | -1.581709 |
| C | -2.007656 | -1.089365 | -0.951605 |
| C | -1.332447 | -2.027697 | 0.018903 |
| C | 0.411973 | 1.222513 | -1.146284 |
| C | 0.072764 | 2.152997 | 0.017783 |
| H | 0.845607 | 2.070458 | 0.790151 |
| H | 0.079313 | 3.188142 | -0.325685 |
| C | -1.316937 | 0.342025 | 1.084029 |
| C | -1.286699 | 1.800125 | 0.622420 |
| H | -2.063038 | 1.956726 | -0.132838 |
| H | -1.512899 | 2.462299 | 1.459394 |
| H | -1.779610 | -1.203364 | -2.002437 |
| H | -3.020234 | -0.781203 | -0.731308 |
| H | -1.895573 | -2.349386 | 0.883875 |
| H | -0.652115 | -2.763957 | -0.386605 |
| H | -0.342754 | 1.333957 | -1.928255 |
| H | -2.312443 | 0.071750 | 1.440937 |
| H | -0.625084 | 0.212885 | 1.920001 |
| H | 1.376034 | 1.476952 | -1.583556 |
| C | 1.579818 | -0.558343 | 0.199634 |
| O | 1.534541 | -1.041589 | 1.301285 |
| O | 2.751008 | -0.245885 | -0.384989 |
| H | 3.461080 | -0.480697 | 0.231624 |

ax2

| | | | |
|---|-----------|-----------|----------|
| C | 0.844598 | -0.620367 | 0.010966 |
| C | -0.387529 | -0.165902 | 0.776492 |
| H | -0.492552 | -0.789705 | 1.670407 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.012831 | -1.094037 | 0.830148 |
| C | 1.214236 | -2.067825 | -0.000041 |
| C | -0.245063 | 1.304145 | 1.182217 |
| C | 0.066371 | 2.194180 | -0.023624 |
| H | -0.792568 | 2.195918 | -0.699812 |
| H | 0.210627 | 3.222878 | 0.309634 |
| C | 1.144614 | 0.241763 | -1.197234 |
| C | 1.301512 | 1.705656 | -0.781554 |
| H | 2.181605 | 1.798536 | -0.138081 |
| H | 1.476582 | 2.330411 | -1.658693 |
| H | 1.895497 | -1.136161 | 1.904212 |
| H | 3.002500 | -0.827410 | 0.485897 |
| H | 1.670286 | -2.458075 | -0.899402 |
| H | 0.564496 | -2.756354 | 0.520655 |
| H | 0.574245 | 1.369990 | 1.901808 |
| H | 2.048538 | -0.120741 | -1.689628 |
| H | 0.325614 | 0.153828 | -1.920526 |
| H | -1.150893 | 1.642778 | 1.683039 |
| C | -1.675686 | -0.389899 | 0.004575 |
| O | -2.609806 | 0.370887 | -0.026536 |
| O | -1.713716 | -1.573900 | -0.626871 |
| H | -2.581104 | -1.648070 | -1.053917 |

eq

```
=====
```

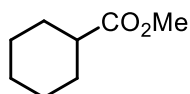
| | | | |
|---|-----------|-----------|-----------|
| C | -0.323260 | 0.871983 | -0.141893 |
| C | 0.291109 | -0.503177 | -0.415402 |
| H | 0.239924 | -0.676405 | -1.493092 |
| C | 0.027310 | 1.611101 | 1.116605 |
| C | 0.495821 | 2.122553 | -0.226398 |
| C | -0.517497 | -1.584437 | 0.309590 |
| C | -1.981359 | -1.542267 | -0.126304 |
| H | -2.044858 | -1.789340 | -1.190468 |
| H | -2.547282 | -2.303575 | 0.412202 |
| C | -1.771157 | 0.924514 | -0.587234 |
| C | -2.593694 | -0.161494 | 0.106464 |
| H | -2.620848 | 0.043987 | 1.180694 |
| H | -3.623779 | -0.139215 | -0.252111 |
| H | 0.771054 | 1.186856 | 1.775580 |
| H | -0.770973 | 2.148640 | 1.609242 |
| H | 0.013967 | 3.003341 | -0.627484 |
| H | 1.549924 | 2.040595 | -0.452103 |
| H | -0.442738 | -1.412028 | 1.385581 |
| H | -2.178208 | 1.913791 | -0.371108 |
| H | -1.819469 | 0.781557 | -1.671637 |
| H | -0.086127 | -2.565756 | 0.105759 |
| C | 1.744568 | -0.564173 | -0.022905 |
| O | 2.161404 | -0.808944 | 1.080914 |
| O | 2.569560 | -0.307995 | -1.051682 |
| H | 3.480649 | -0.344538 | -0.720042 |

eq2

```

=====
C  -0.335934    0.887862   -0.130389
C   0.287096   -0.464720   -0.487553
H   0.184844   -0.588911   -1.568596
C   0.080335    1.604358    1.121755
C   0.449337    2.157910   -0.236027
C  -0.471199   -1.594333    0.220600
C  -1.952172   -1.560581   -0.152784
H  -2.057189   -1.749133   -1.225578
H  -2.480280   -2.361739    0.365876
C  -1.807860    0.928296   -0.492166
C  -2.575509   -0.206955    0.184390
H  -2.551106   -0.059175    1.268225
H  -3.622779   -0.184971   -0.120318
H   0.873662    1.184578    1.723247
H  -0.694028    2.113088    1.679043
H  -0.078768    3.035693   -0.581567
H   1.487010    2.102668   -0.532916
H  -0.362933   -1.472419    1.300446
H  -2.220484    1.897285   -0.206071
H  -1.910691    0.838510   -1.578545
H  -0.031132   -2.556838   -0.044732
C   1.773185   -0.499488   -0.232841
O   2.612173   -0.182347   -1.038782
O   2.101739   -0.919664    0.998833
H   3.068905   -0.896635    1.071169
=====

```



methyl cyclohexanecarboxylate

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -463.708541 | -463.4829 | -463.529122 |
| eq | -463.709674 | -463.484125 | -463.531404 |
| eq2 | -463.708766 | -463.483065 | -463.530427 |

ax

```

=====
C   1.234524   -1.220319    0.746046
C   0.138937   -0.191583    1.035580
H  -0.219260   -0.321889    2.061492
C   0.679779    1.237814    0.884913
C   1.298110    1.453548   -0.495695
H   1.685573    2.470369   -0.573730
H   0.521998    1.349896   -1.262283
C   1.886154   -0.993519   -0.619610
C   2.408211    0.436428   -0.760404
=====

```

| | | | |
|---|-----------|-----------|-----------|
| H | 3.216724 | 0.598361 | -0.040389 |
| H | 2.830888 | 0.586661 | -1.755138 |
| H | 1.449016 | 1.382446 | 1.647647 |
| H | 1.150525 | -1.185770 | -1.404651 |
| H | 2.697923 | -1.708685 | -0.761469 |
| H | -0.108036 | 1.963714 | 1.077219 |
| C | -1.085661 | -0.440912 | 0.174747 |
| O | -1.305336 | -1.448329 | -0.451679 |
| O | -1.951017 | 0.578975 | 0.218280 |
| C | -3.161016 | 0.397393 | -0.524066 |
| H | -3.712280 | -0.462111 | -0.148010 |
| H | -3.736696 | 1.306115 | -0.379564 |
| H | -2.940212 | 0.254996 | -1.579981 |
| H | 1.993724 | -1.124005 | 1.526269 |
| H | 0.826710 | -2.228365 | 0.810705 |

eq

```
=====
```

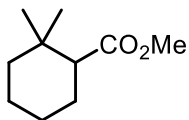
| | | | |
|---|-----------|-----------|-----------|
| C | 0.606766 | 1.143386 | 0.428377 |
| C | 0.064787 | -0.071140 | -0.348527 |
| H | 0.061222 | 0.182475 | -1.411750 |
| C | 0.941179 | -1.299345 | -0.113900 |
| C | 2.390720 | -1.012638 | -0.502731 |
| H | 3.005662 | -1.893214 | -0.311573 |
| H | 2.443432 | -0.813066 | -1.577492 |
| C | 2.058741 | 1.423820 | 0.044891 |
| C | 2.938601 | 0.193290 | 0.259526 |
| H | 3.962952 | 0.404114 | -0.051559 |
| H | 2.969543 | -0.042664 | 1.327813 |
| H | 0.891604 | -1.568329 | 0.943942 |
| H | 2.098363 | 1.715894 | -1.008885 |
| H | 2.435314 | 2.267298 | 0.625480 |
| H | 0.551193 | -2.147334 | -0.679025 |
| C | -1.363332 | -0.318995 | 0.064358 |
| O | -1.726650 | -1.144075 | 0.866368 |
| O | -2.209874 | 0.522703 | -0.541513 |
| C | -3.584229 | 0.402965 | -0.159451 |
| H | -4.118155 | 1.154250 | -0.732474 |
| H | -3.959226 | -0.590129 | -0.398468 |
| H | -3.699655 | 0.589308 | 0.906356 |
| H | -0.015877 | 2.017255 | 0.234005 |
| H | 0.546423 | 0.927060 | 1.499533 |

eq2

```
=====
```

| | | | |
|---|----------|-----------|-----------|
| C | 0.693461 | -1.261781 | -0.064282 |
| C | 0.099586 | 0.000038 | 0.578750 |
| H | 0.341003 | -0.000220 | 1.643150 |
| C | 0.693556 | 1.261828 | -0.063976 |
| C | 2.215910 | 1.260594 | 0.067211 |
| H | 2.627522 | 2.151522 | -0.409285 |
| H | 2.484626 | 1.310498 | 1.126718 |
| C | 2.215786 | -1.260694 | 0.067064 |
| C | 2.822940 | -0.000041 | -0.547782 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.905925 | -0.000086 | -0.415026 |
| H | 2.631695 | 0.000018 | -1.625411 |
| H | 0.417904 | 1.283382 | -1.121159 |
| H | 2.484402 | -1.310709 | 1.126589 |
| H | 2.627410 | -2.151604 | -0.409465 |
| H | 0.269242 | 2.152341 | 0.403538 |
| C | -1.405288 | 0.000035 | 0.502357 |
| O | -2.147086 | -0.000255 | 1.455379 |
| O | -1.851100 | 0.000313 | -0.758596 |
| C | -3.273645 | -0.000001 | -0.916779 |
| H | -3.453191 | -0.000678 | -1.987187 |
| H | -3.705733 | -0.888665 | -0.461308 |
| H | -3.705952 | 0.889142 | -0.462418 |
| H | 0.268921 | -2.152240 | 0.403108 |
| H | 0.417885 | -1.283028 | -1.121478 |



methyl 2,2-dimethylcyclohexane-1-carboxylate

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -542.321673 | -542.037245 | -542.088728 |
| ax2 | -542.320547 | -542.036014 | -542.087415 |
| eq | -542.323810 | -542.03946 | -542.091244 |
| eq2 | -542.322965 | -542.038654 | -542.090413 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.812591 | -1.014049 | -0.021844 |
| C | -0.036238 | 0.001313 | 0.800518 |
| H | -0.370403 | -0.511346 | 1.703102 |
| C | 0.763162 | 1.252856 | 1.209021 |
| C | 1.519133 | 1.907592 | 0.052595 |
| H | 2.131120 | 2.723046 | 0.442028 |
| H | 0.806810 | 2.341683 | -0.649931 |
| C | 1.557919 | -0.295317 | -1.158819 |
| C | 2.392679 | 0.892803 | -0.682624 |
| H | 3.192355 | 0.548588 | -0.021573 |
| H | 2.876249 | 1.366377 | -1.538676 |
| H | 1.478486 | 0.953183 | 1.977467 |
| H | 0.825247 | 0.059871 | -1.888185 |
| H | 2.190486 | -1.026365 | -1.669003 |
| H | 0.087521 | 1.971462 | 1.677100 |
| C | -1.286312 | 0.387251 | 0.043981 |
| O | -1.336272 | 1.116196 | -0.917515 |
| O | -2.380322 | -0.190911 | 0.559242 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.807235 | -1.693383 | 0.926380 |
| H | 1.274384 | -2.267111 | 1.687128 |
| H | 2.442415 | -2.382610 | 0.366392 |
| H | 2.455072 | -0.981998 | 1.436162 |
| C | -0.088932 | -2.098093 | -0.616916 |
| H | -0.664655 | -2.602024 | 0.162011 |
| H | -0.789357 | -1.685390 | -1.346745 |
| H | 0.517688 | -2.847519 | -1.128790 |
| C | -3.604782 | 0.079878 | -0.130507 |
| H | -3.546000 | -0.272624 | -1.158641 |
| H | -4.375318 | -0.461349 | 0.409173 |
| H | -3.818062 | 1.146745 | -0.123542 |

ax2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.997064 | -0.881793 | -0.178231 |
| C | 0.079598 | -0.279470 | 0.926706 |
| H | 0.117301 | -0.957201 | 1.780162 |
| C | 0.541615 | 1.114437 | 1.400122 |
| C | 0.867425 | 2.089448 | 0.268598 |
| H | 1.283022 | 3.003076 | 0.697082 |
| H | -0.045991 | 2.367961 | -0.258485 |
| C | 1.314427 | 0.152931 | -1.271978 |
| C | 1.852384 | 1.473442 | -0.722820 |
| H | 2.814122 | 1.310674 | -0.229266 |
| H | 2.036156 | 2.164726 | -1.546958 |
| H | 1.438010 | 0.971634 | 2.007116 |
| H | 0.406986 | 0.353480 | -1.845683 |
| H | 2.035701 | -0.293584 | -1.961382 |
| H | -0.215926 | 1.536801 | 2.063518 |
| C | -1.382109 | -0.283577 | 0.538848 |
| O | -2.225198 | -0.955050 | 1.084462 |
| O | -1.671767 | 0.537504 | -0.476900 |
| C | 2.294824 | -1.353016 | 0.490173 |
| H | 2.085768 | -2.151676 | 1.204295 |
| H | 2.981507 | -1.743906 | -0.263184 |
| H | 2.804846 | -0.551813 | 1.023455 |
| C | 0.322635 | -2.098878 | -0.814589 |
| H | 0.050537 | -2.837318 | -0.057349 |
| H | -0.581657 | -1.819418 | -1.360259 |
| H | 1.002277 | -2.575860 | -1.523312 |
| C | -3.040677 | 0.547326 | -0.896642 |
| H | -3.686146 | 0.867452 | -0.081483 |
| H | -3.093115 | 1.254112 | -1.718754 |
| H | -3.340803 | -0.443871 | -1.231132 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.682620 | 0.938605 | 0.049990 |
| C | -0.002633 | -0.398966 | -0.361726 |
| H | -0.048289 | -0.400342 | -1.453232 |
| C | 0.785106 | -1.630708 | 0.096938 |
| C | 2.205067 | -1.603928 | -0.463073 |
| H | 2.762709 | -2.470004 | -0.103713 |

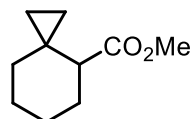
| | | | |
|---|-----------|-----------|-----------|
| H | 2.159840 | -1.682121 | -1.553786 |
| C | 2.112471 | 0.909066 | -0.520048 |
| C | 2.923718 | -0.310337 | -0.085030 |
| H | 3.910079 | -0.278285 | -0.550689 |
| H | 3.085397 | -0.285386 | 0.995547 |
| H | 0.810632 | -1.662826 | 1.187091 |
| H | 2.045937 | 0.916180 | -1.613109 |
| H | 2.621316 | 1.830371 | -0.225808 |
| H | 0.264856 | -2.531650 | -0.233724 |
| C | -1.422252 | -0.470426 | 0.143778 |
| O | -1.746253 | -0.804050 | 1.257820 |
| O | -2.315258 | -0.117679 | -0.790251 |
| C | -0.066754 | 2.119111 | -0.570312 |
| H | -0.151264 | 2.006695 | -1.652890 |
| H | -1.073593 | 2.215683 | -0.159176 |
| H | 0.467568 | 3.048827 | -0.364526 |
| C | 0.718833 | 1.131711 | 1.569583 |
| H | 1.281104 | 2.038168 | 1.803408 |
| H | -0.286678 | 1.246206 | 1.974352 |
| H | 1.193393 | 0.301431 | 2.090093 |
| C | -3.683023 | -0.115499 | -0.368087 |
| H | -4.260653 | 0.189923 | -1.234618 |
| H | -3.983018 | -1.110604 | -0.046238 |
| H | -3.826156 | 0.589783 | 0.448392 |

eq2

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.757009 | 0.932262 | 0.123846 |
| C | 0.030114 | -0.220225 | -0.634845 |
| H | 0.259258 | -0.080610 | -1.694237 |
| C | 0.517836 | -1.610876 | -0.210721 |
| C | 2.023940 | -1.744507 | -0.418843 |
| H | 2.356769 | -2.732013 | -0.095905 |
| H | 2.249618 | -1.662525 | -1.486630 |
| C | 2.270729 | 0.730043 | -0.075861 |
| C | 2.774290 | -0.651062 | 0.337342 |
| H | 3.845668 | -0.722912 | 0.143132 |
| H | 2.638069 | -0.793216 | 1.412675 |
| H | 0.275624 | -1.786033 | 0.838105 |
| H | 2.498145 | 0.882803 | -1.136113 |
| H | 2.797739 | 1.510835 | 0.478107 |
| H | -0.015241 | -2.368165 | -0.788582 |
| C | -1.471353 | -0.082267 | -0.540373 |
| O | -2.152820 | 0.533890 | -1.324835 |
| O | -1.990661 | -0.712531 | 0.519246 |
| C | 0.372027 | 2.284814 | -0.478360 |
| H | 0.571156 | 2.307243 | -1.551519 |
| H | -0.684147 | 2.508597 | -0.325222 |
| H | 0.956022 | 3.078209 | -0.007319 |
| C | 0.411025 | 0.948565 | 1.616450 |
| H | 1.013883 | 1.707271 | 2.119613 |
| H | -0.638967 | 1.200599 | 1.772631 |
| H | 0.600294 | -0.006825 | 2.103840 |
| C | -3.405383 | -0.578790 | 0.687753 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.651926 | -1.140504 | 1.583097 |
| H | -3.674816 | 0.468268 | 0.812613 |
| H | -3.930707 | -0.989642 | -0.171902 |



methyl spiro[2.5]octane-4-carboxylate

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -541.091510 | -540.830473 | -540.880691 |
| ax2 | -541.091122 | -540.83028 | -540.880968 |
| eq | -541.091327 | -540.83012 | -540.880014 |
| eq2 | -541.090110 | -540.828908 | -540.879036 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 1.220876 | -0.658773 | 0.024242 |
| C | -0.027652 | -0.193195 | 0.745758 |
| H | -0.178414 | -0.805128 | 1.639728 |
| C | 2.307666 | -1.242028 | 0.884409 |
| C | 1.501974 | -2.125063 | -0.037345 |
| C | 0.122000 | 1.277478 | 1.173260 |
| C | 0.481118 | 2.164882 | -0.018427 |
| H | -0.337114 | 2.148068 | -0.747187 |
| H | 0.588038 | 3.198897 | 0.311970 |
| C | 1.641583 | 0.225536 | -1.132812 |
| C | 1.767994 | 1.684430 | -0.690336 |
| H | 2.595074 | 1.776354 | 0.020442 |
| H | 2.007664 | 2.316201 | -1.546909 |
| H | 2.125889 | -1.325760 | 1.947063 |
| H | 3.330861 | -1.027537 | 0.608781 |
| H | 1.988378 | -2.503917 | -0.925503 |
| H | 0.781398 | -2.794342 | 0.412302 |
| H | 0.925387 | 1.325825 | 1.912315 |
| H | 2.588450 | -0.137023 | -1.537319 |
| H | 0.897134 | 0.151996 | -1.929438 |
| H | -0.789690 | 1.622808 | 1.657814 |
| C | -1.276509 | -0.399825 | -0.093169 |
| O | -1.324166 | -0.906657 | -1.185643 |
| O | -2.370283 | 0.035094 | 0.546339 |
| C | -3.607426 | -0.140470 | -0.151398 |
| H | -3.785542 | -1.195466 | -0.349593 |
| H | -4.376610 | 0.253857 | 0.504947 |
| H | -3.595042 | 0.409833 | -1.090073 |

ax2

```
=====
C  0.827353    0.885198   -0.042468
C  0.051340   -0.091878  -0.909073
H -0.135638    0.375274   -1.881801
C  1.827915    1.762867   -0.742464
C  0.564141    2.350214   -0.164932
C  0.861250   -1.378346  -1.102213
C  1.277603   -1.984461   0.240164
H  0.383438   -2.310774   0.778525
H  1.886611   -2.873090   0.068087
C  1.228841    0.303353   1.296751
C  2.042366   -0.977370   1.100437
H  2.986825   -0.725470   0.608659
H  2.290387   -1.418940   2.066854
H  1.901402    1.690089  -1.818851
H  2.759209    1.963096  -0.230857
H  0.648702    2.948447   0.731836
H -0.204414    2.665652  -0.855832
H  1.754399   -1.125438  -1.678317
H  1.800254    1.042720   1.860671
H  0.328717    0.077352   1.879843
H  0.286650   -2.097594  -1.683701
C -1.333904   -0.410094  -0.364386
O -1.874637   -1.485212  -0.453321
O -1.930680    0.649159   0.188919
C -3.260286    0.426833   0.670031
H -3.260730   -0.336960   1.445134
H -3.589867    1.376929   1.078166
H -3.913124    0.119236  -0.144269
```

eq

```
=====
C -0.706578    0.868606   -0.136344
C -0.027201   -0.486405  -0.347796
H  0.001101   -0.673720  -1.423993
C -0.471542    1.631699   1.134902
C  0.077625    2.143721  -0.176990
C -0.847136   -1.586252   0.334265
C -2.277669   -1.600529  -0.202753
H -2.257989   -1.862801  -1.265040
H -2.854608   -2.374052   0.305954
C -2.120041    0.867587  -0.683233
C -2.952007   -0.239077  -0.034280
H -3.062766   -0.021832   1.032278
H -3.954335   -0.257599  -0.464718
H  0.234693    1.237155   1.850962
H -1.319485    2.149792   1.561070
H -0.399275    3.005978  -0.621971
H  1.147646    2.090639  -0.325166
H -0.853875   -1.399184   1.410441
H -2.575050    1.844340  -0.509248
H -2.087184    0.711206  -1.766400
H -0.369859   -2.554602   0.175001
```

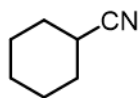

| | | | |
|---|----------|-----------|-----------|
| C | 1.399148 | -0.488128 | 0.143089 |
| O | 1.741483 | -0.693761 | 1.281778 |
| O | 2.269612 | -0.220549 | -0.836721 |
| C | 3.643692 | -0.145895 | -0.439575 |
| H | 3.970443 | -1.097175 | -0.025019 |
| H | 4.201090 | 0.083349 | -1.341945 |
| H | 3.780953 | 0.641029 | 0.299621 |

eq2

```

=====
C  0.797040    0.886688    0.091827
C  0.058040   -0.343445    0.626881
H  0.277095   -0.408960    1.695937
C  0.309230    1.572559   -1.151917
C  0.200744    2.256102    0.192330
C  0.577123   -1.608526   -0.066924
C  2.085885   -1.748270    0.127543
H  2.302425   -1.872216    1.193082
H  2.440382   -2.647826   -0.377488
C  2.297458    0.754186    0.266485
C  2.824301   -0.517719   -0.396840
H  2.678162   -0.444443   -1.478740
H  3.896873   -0.614694   -0.222396
H -0.605445    1.225211   -1.611036
H  1.056994    1.935874   -1.843237
H  0.878650    3.073331    0.396025
H -0.785364    2.361362    0.621175
H  0.350600   -1.547649   -1.133366
H  2.785979    1.637233   -0.149317
H  2.530121    0.727377    1.336183
H  0.057560   -2.483699    0.326389
C -1.443011   -0.188893    0.546442
O -2.117027    0.328177    1.404619
O -1.964139   -0.674684   -0.583509
C -3.379777   -0.515811   -0.732080
H -3.644839    0.539572   -0.718959
H -3.627386   -0.955202   -1.692923
H -3.904680   -1.034435    0.067301

```



cyclohexanecarbonitrile

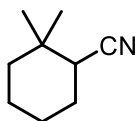
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -328.085444 | -327.907091 | -327.946788 |
| eq | -328.085581 | -327.907226 | -327.94699 |

ax

```
=====
C  0.121198    1.269077    0.790360
C -0.745340    0.000119    0.885604
H -1.296177    0.000095    1.826631
C  0.121097   -1.269008    0.790462
C  0.998534   -1.260956   -0.459213
H  1.625964   -2.152785   -0.467247
H  0.363703   -1.311072   -1.349336
C  0.998657    1.260860   -0.459331
C  1.860428   -0.000092   -0.522914
H  2.459366   -0.000175   -1.434473
H  2.557756   -0.000078    0.320505
H  0.751451   -1.286384    1.682130
H  0.363845    1.310951   -1.349465
H  1.626157    2.152638   -0.467411
H -0.513330   -2.154609    0.818318
H -0.513054    2.154815    0.818164
H  0.751613    1.286519    1.681988
C -1.757448    0.000047   -0.179318
N -2.537151   -0.000029   -1.021958
```

eq

```
=====
C -1.449660   -1.259484    0.188382
C  0.039808   -1.270339   -0.147937
H  0.175372   -1.297798   -1.232133
C  0.713462    0.000271    0.397977
C  0.039549    1.270426   -0.148052
H  0.524823    2.152968    0.268271
H  0.174845    1.297647   -1.232234
C -2.131534   -0.000156   -0.343967
C -1.449851    1.259349    0.188423
H -1.920389    2.152074   -0.224820
H -1.571311    1.304766    1.274721
H  0.639834    0.000117    1.488952
H -2.082311   -0.000124   -1.437065
H -3.187349   -0.000284   -0.070167
H -1.919988   -2.152285   -0.224952
H -1.571081   -1.305057    1.274662
H  0.525277   -2.152632    0.268706
C  2.141572    0.000155    0.074266
N  3.256029   -0.000103   -0.201214
```



2,2-dimethylcyclohexane-1-carbonitrile

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -406.700670 | -406.46376 | -406.508887 |
| eq | -406.701433 | -406.464579 | -406.509881 |

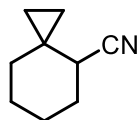
ax

| C | 0.997564 | -0.164565 | 0.026195 |
|---|-----------|-----------|-----------|
| C | -0.083525 | 0.622018 | 0.822554 |
| H | 0.366433 | 0.992067 | 1.746676 |
| C | -1.325909 | -0.229744 | 1.151814 |
| C | -1.921223 | -0.861006 | -0.104532 |
| H | -2.768526 | -1.489567 | 0.171072 |
| H | -2.309663 | -0.072044 | -0.756176 |
| C | 0.346263 | -0.818470 | -1.203196 |
| C | -0.875693 | -1.673911 | -0.866800 |
| H | -1.308380 | -2.067153 | -1.787648 |
| H | -0.576166 | -2.536338 | -0.266562 |
| H | -1.021150 | -1.007290 | 1.852586 |
| H | 0.042468 | -0.027157 | -1.896791 |
| H | 1.102034 | -1.415778 | -1.718236 |
| H | -2.063020 | 0.390789 | 1.661201 |
| C | 1.610067 | -1.219609 | 0.952755 |
| H | 2.374007 | -1.779106 | 0.410527 |
| H | 2.086872 | -0.741228 | 1.810507 |
| H | 0.878970 | -1.932787 | 1.328179 |
| C | 2.112523 | 0.779025 | -0.423921 |
| H | 2.550600 | 1.300336 | 0.429964 |
| H | 2.903345 | 0.210100 | -0.915345 |
| H | 1.747321 | 1.524545 | -1.131716 |
| C | -0.513508 | 1.814841 | 0.078561 |
| N | -0.869214 | 2.737020 | -0.505545 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | -0.131065 | 0.873982 | -0.019914 |
| C | -0.492241 | -0.570663 | -0.467028 |
| H | -0.410022 | -0.607396 | -1.557619 |
| C | 0.432562 | -1.650055 | 0.124159 |
| C | 1.884836 | -1.352362 | -0.237356 |
| H | 2.533271 | -2.104646 | 0.212847 |
| H | 2.004385 | -1.430703 | -1.322112 |
| C | 1.349824 | 1.100459 | -0.370122 |
| C | 2.291740 | 0.048545 | 0.213155 |
| H | 3.314248 | 0.260750 | -0.102107 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.281612 | 0.098311 | 1.304663 |
| H | 0.311514 | -1.677695 | 1.208543 |
| H | 1.448374 | 1.094499 | -1.460542 |
| H | 1.632723 | 2.099096 | -0.029877 |
| H | 0.132522 | -2.625009 | -0.259734 |
| C | -0.375123 | 1.072132 | 1.478127 |
| H | -0.085773 | 2.085287 | 1.762030 |
| H | -1.432517 | 0.947830 | 1.719448 |
| H | 0.194735 | 0.377244 | 2.093117 |
| C | -0.985505 | 1.873151 | -0.798780 |
| H | -2.045843 | 1.755602 | -0.566372 |
| H | -0.697336 | 2.893185 | -0.539137 |
| H | -0.853068 | 1.744944 | -1.874720 |
| C | -1.889592 | -0.885381 | -0.152739 |
| N | -2.977350 | -1.138594 | 0.113507 |



spiro[2.5]octane-4-carbonitrile

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -405.468614 | -405.254929 | -405.298581 |
| eq | -405.467693 | -405.253944 | -405.297481 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.924285 | 0.018814 | -0.053181 |
| C | 0.186456 | 0.705616 | 0.731608 |
| H | -0.244474 | 1.252229 | 1.572050 |
| C | -2.117358 | -0.422833 | 0.741367 |
| C | -2.224518 | 0.739855 | -0.215843 |
| C | 1.213237 | -0.322305 | 1.241574 |
| C | 1.730236 | -1.208498 | 0.110146 |
| H | 2.295736 | -0.597973 | -0.600887 |
| H | 2.423596 | -1.945234 | 0.516684 |
| C | -0.419838 | -0.880129 | -1.161407 |
| C | 0.580863 | -1.902767 | -0.621067 |
| H | 0.067404 | -2.575322 | 0.072454 |
| H | 0.968498 | -2.514001 | -1.436867 |
| H | -2.133273 | -0.202249 | 1.799494 |
| H | -2.583025 | -1.355733 | 0.456421 |
| H | -2.764491 | 0.585186 | -1.139208 |
| H | -2.309374 | 1.730318 | 0.209590 |
| H | 0.699116 | -0.935598 | 1.984598 |
| H | -1.268187 | -1.377884 | -1.633246 |
| H | 0.065254 | -0.270087 | -1.930922 |

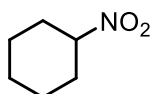
| | | | |
|---|----------|----------|-----------|
| H | 2.032196 | 0.190903 | 1.744847 |
| C | 0.846065 | 1.710337 | -0.118090 |
| N | 1.360840 | 2.483844 | -0.792235 |

eq

```

=====
C  -0.096007    0.804768   -0.184674
C  -0.440893   -0.653797   -0.479558
H  -0.307988   -0.832985   -1.551052
C  -1.114365    1.882620   -0.379246
C  -0.700435    1.472507    1.014761
C   0.488340   -1.602686    0.301252
C   1.947837   -1.295622   -0.026263
H   2.593894   -1.959078    0.549425
H   2.128633   -1.507892   -1.084215
C   1.354924    1.102154   -0.503700
C   2.289452    0.165502    0.261341
H   3.326666    0.369988   -0.006734
H   2.188338    0.355690    1.333827
H  -2.106971    1.601702   -0.703683
H  -0.760193    2.832622   -0.753560
H  -0.068690    2.146730    1.575578
H  -1.421620    0.922264    1.603728
H   0.307122   -1.462445    1.369716
H   1.517643    0.978737   -1.579340
H   1.566725    2.144389   -0.260775
H   0.244878   -2.635949    0.055228
C  -1.841208   -0.960992   -0.180256
N  -2.933472   -1.205786    0.072844

```



nitrocyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -440.344668 | -440.16108 | -440.203599 |
| eq | -440.345908 | -440.162184 | -440.205224 |

ax

```

=====
C   0.426009   -1.256043   -0.822156
C  -0.421921    0.002929   -0.930031
H  -0.999010    0.006864   -1.855811
C   0.407441    1.272870   -0.801455
C   1.266008    1.263241    0.463275
H   1.881891    2.162503    0.488578
H   0.617762    1.297985    1.344051
C   1.289475   -1.255345    0.439516

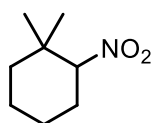
```

| | | | |
|---|-----------|-----------|-----------|
| C | 2.140578 | 0.011279 | 0.527147 |
| H | 2.725572 | 0.007748 | 1.447649 |
| H | 2.849830 | 0.026106 | -0.305964 |
| H | 1.053915 | 1.298535 | -1.681484 |
| H | 0.645801 | -1.320740 | 1.321454 |
| H | 1.922633 | -2.142924 | 0.443633 |
| H | -0.233186 | 2.150167 | -0.842788 |
| H | -0.201488 | -2.142241 | -0.875250 |
| H | 1.069649 | -1.258660 | -1.704694 |
| N | -1.525799 | -0.010621 | 0.126459 |
| O | -1.929652 | -1.084781 | 0.521397 |
| O | -1.982637 | 1.054207 | 0.488309 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.260454 | 1.233181 | 0.275718 |
| C | -0.372138 | 0.011834 | -0.387432 |
| H | -0.377505 | 0.125034 | -1.469014 |
| C | 0.312113 | -1.281986 | 0.028085 |
| C | 1.790752 | -1.208674 | -0.356948 |
| H | 2.288269 | -2.127502 | -0.046482 |
| H | 1.878616 | -1.147443 | -1.445314 |
| C | 1.740650 | 1.297822 | -0.102245 |
| C | 2.465744 | 0.007283 | 0.276347 |
| H | 3.509994 | 0.060460 | -0.033509 |
| H | 2.456799 | -0.103782 | 1.364587 |
| H | 0.216443 | -1.401106 | 1.108290 |
| H | 1.828915 | 1.461912 | -1.179808 |
| H | 2.199056 | 2.154776 | 0.391551 |
| H | -0.174736 | -2.131220 | -0.452576 |
| H | -0.261202 | 2.138060 | -0.037860 |
| H | 0.156302 | 1.135035 | 1.358423 |
| N | -1.829785 | -0.022787 | -0.012127 |
| O | -2.119086 | -0.336101 | 1.124935 |
| O | -2.643153 | 0.290917 | -0.859253 |



1,1-dimethyl-2-nitrocyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -518.958412 | -518.715926 | -518.763186 |
| eq | -518.960590 | -518.718114 | -518.76529 |

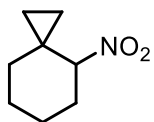
ax

```
=====
C -0.388858 -1.279705 1.155005
C 0.442829 -0.054815 0.765668
H 0.895018 0.390640 1.647655
C -0.337990 1.037637 -0.007987
C -1.235928 0.421321 -1.093674
H -1.840928 1.225032 -1.519576
H -0.607465 0.034139 -1.898795
C -1.297164 -1.818566 0.049985
C -2.131327 -0.703338 -0.576407
H -2.726710 -1.101823 -1.398879
H -2.836246 -0.312605 0.161551
H -0.698126 -2.300385 -0.722503
H -1.946690 -2.583182 0.478060
H 0.278245 -2.056743 1.531652
H -1.002516 -0.962532 2.000155
N 1.643069 -0.489001 -0.038944
O 1.463255 -1.145359 -1.046073
O 2.740607 -0.143746 0.353759
C 0.627882 2.039548 -0.642426
H 0.060391 2.856173 -1.090416
H 1.302772 2.464128 0.103098
H 1.226970 1.582319 -1.432327
C -1.186527 1.783137 1.031510
H -0.544742 2.284386 1.757619
H -1.788684 2.541055 0.528601
H -1.861176 1.123931 1.575184
```

eq

```
=====
C -0.462966 -1.622303 0.056688
C 0.311436 -0.415007 -0.452304
H 0.315449 -0.396758 -1.540893
C -0.228218 0.948182 0.050200
C -1.704639 0.993155 -0.396429
H -2.132145 1.932305 -0.039588
H -1.730897 1.023710 -1.490261
C -1.920529 -1.509831 -0.388768
C -2.535185 -0.194726 0.084440
H -3.554778 -0.100766 -0.291396
H -2.598183 -0.192096 1.175186
H -1.968455 -1.558818 -1.480387
H -2.483089 -2.360307 -0.003601
H -0.008049 -2.531012 -0.339433
H -0.404382 -1.670982 1.143088
N 1.768904 -0.549047 -0.095055
O 2.058472 -0.977107 1.004438
O 2.588355 -0.199877 -0.923295
C 0.520644 2.098321 -0.624197
H 0.045611 3.044026 -0.358387
H 1.562050 2.146889 -0.303870
H 0.500105 1.998637 -1.710667
C -0.117983 1.106763 1.569210
```

| | | | |
|---|-----------|----------|----------|
| H | 0.923073 | 1.180489 | 1.883919 |
| H | -0.620554 | 2.029997 | 1.862394 |
| H | -0.578052 | 0.286557 | 2.117100 |



4-nitrospiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -517.727026 | -517.507787 | -517.554056 |
| ax2 | -517.727702 | -517.508555 | -517.555083 |
| eq | -517.726043 | -517.506844 | -517.552514 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.409761 | -1.211101 | 1.236450 |
| C | 0.478870 | -0.073401 | 0.739350 |
| H | 1.000575 | 0.403239 | 1.564050 |
| C | -0.280492 | 0.963558 | -0.063606 |
| C | -1.244743 | 0.406156 | -1.089249 |
| H | -1.791740 | 1.235633 | -1.539722 |
| H | -0.691281 | -0.090272 | -1.891243 |
| C | -1.427598 | -1.731618 | 0.218966 |
| C | -2.202482 | -0.589032 | -0.435614 |
| H | -2.897319 | -0.984921 | -1.176992 |
| H | -2.796857 | -0.068001 | 0.321118 |
| H | -0.920304 | -2.311271 | -0.551811 |
| H | -2.113153 | -2.406689 | 0.732607 |
| H | 0.213766 | -2.019040 | 1.620749 |
| H | -0.947503 | -0.790957 | 2.090073 |
| N | 1.610278 | -0.587474 | -0.126022 |
| O | 1.370850 | -1.445459 | -0.952092 |
| O | 2.704498 | -0.081061 | 0.028276 |
| C | 0.392774 | 2.279846 | -0.308562 |
| H | 0.169717 | 2.775037 | -1.242770 |
| H | 1.403451 | 2.406356 | 0.053160 |
| C | -0.707016 | 2.178740 | 0.714114 |
| H | -0.429976 | 2.238319 | 1.756861 |
| H | -1.671421 | 2.598164 | 0.465512 |

ax2

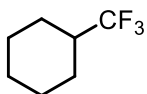
| | | | |
|---|-----------|-----------|-----------|
| C | -0.486656 | 1.214199 | 1.141423 |
| C | -0.424895 | -0.250469 | 0.706454 |
| H | -0.615312 | -0.906928 | 1.554626 |
| C | 0.874679 | -0.594516 | 0.032852 |
| C | 1.342174 | 0.377244 | -1.033641 |
| H | 2.355520 | 0.106501 | -1.334042 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.706148 | 0.282992 | -1.916119 |
| C | -0.096120 | 2.158990 | 0.006777 |
| C | 1.294756 | 1.819395 | -0.528167 |
| H | 1.569690 | 2.503978 | -1.331174 |
| H | 2.026874 | 1.948993 | 0.274500 |
| H | -0.828467 | 2.087086 | -0.804363 |
| H | -0.127842 | 3.186459 | 0.369471 |
| H | -1.475956 | 1.439210 | 1.535076 |
| H | 0.225922 | 1.315517 | 1.962645 |
| N | -1.625700 | -0.526212 | -0.195965 |
| O | -1.447395 | -0.876383 | -1.342162 |
| O | -2.723502 | -0.377547 | 0.305146 |
| C | 1.243716 | -2.040692 | -0.073660 |
| H | 1.817239 | -2.335275 | -0.940954 |
| H | 0.525528 | -2.770069 | 0.274566 |
| C | 1.915367 | -1.174252 | 0.956318 |
| H | 1.650431 | -1.326228 | 1.993135 |
| H | 2.939163 | -0.876706 | 0.780380 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -0.506882 | -1.579444 | 0.289519 |
| C | 0.277771 | -0.504365 | -0.447349 |
| H | 0.247776 | -0.665114 | -1.523924 |
| C | -0.264575 | 0.885424 | -0.136512 |
| C | -1.722463 | 0.968364 | -0.550778 |
| H | -2.098451 | 1.963841 | -0.311703 |
| H | -1.794983 | 0.843059 | -1.635559 |
| C | -1.977188 | -1.498653 | -0.126002 |
| C | -2.553191 | -0.109524 | 0.144700 |
| H | -3.588725 | -0.058719 | -0.193311 |
| H | -2.553333 | 0.077828 | 1.222191 |
| H | -2.063879 | -1.726221 | -1.192212 |
| H | -2.543474 | -2.259167 | 0.411514 |
| H | -0.091875 | -2.561198 | 0.060032 |
| H | -0.413188 | -1.413370 | 1.363226 |
| N | 1.743646 | -0.586594 | -0.116187 |
| O | 2.069132 | -0.895929 | 1.011859 |
| O | 2.532316 | -0.316365 | -1.001125 |
| C | 0.584711 | 2.111274 | -0.241712 |
| H | 0.110730 | 3.001114 | -0.631194 |
| H | 1.629862 | 2.003479 | -0.494638 |
| C | 0.141681 | 1.606345 | 1.113436 |
| H | 0.895382 | 1.166678 | 1.750304 |
| H | -0.632137 | 2.155769 | 1.630890 |



(trifluoromethyl)cyclohexane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -572.902638 | -572.716069 | -572.759863 |
| eq | -572.906179 | -572.719786 | -572.763851 |

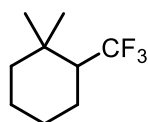
ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.636524 | -1.272071 | -0.807349 |
| C | -0.219042 | -0.000000 | -0.905956 |
| H | -0.734510 | -0.000000 | -1.868788 |
| C | 0.636524 | 1.272071 | -0.807349 |
| C | 1.627299 | 1.259660 | 0.358887 |
| H | 2.255222 | 2.149587 | 0.296647 |
| H | 1.093590 | 1.315680 | 1.309770 |
| C | 1.627300 | -1.259660 | 0.358887 |
| C | 2.491649 | 0.000000 | 0.334066 |
| H | 3.182955 | 0.000000 | 1.177949 |
| H | 3.097499 | 0.000000 | -0.577838 |
| H | 1.200749 | 1.338881 | -1.740347 |
| H | 1.093590 | -1.315680 | 1.309770 |
| H | 2.255222 | -2.149587 | 0.296648 |
| H | -0.004406 | 2.153021 | -0.763958 |
| H | -0.004406 | -2.153021 | -0.763957 |
| H | 1.200749 | -1.338882 | -1.740346 |
| C | -1.351103 | -0.000000 | 0.088465 |
| F | -0.960976 | 0.000000 | 1.375988 |
| F | -2.149021 | 1.075667 | -0.057630 |
| F | -2.149021 | -1.075667 | -0.057631 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | 0.587988 | 1.265174 | 0.138569 |
| C | -0.098211 | 0.000000 | -0.385186 |
| H | -0.068991 | -0.000000 | -1.478831 |
| C | 0.587988 | -1.265174 | 0.138569 |
| C | 2.069974 | -1.258724 | -0.234064 |
| H | 2.550744 | -2.151387 | 0.167428 |
| H | 2.164913 | -1.304674 | -1.323013 |
| C | 2.069974 | 1.258724 | -0.234064 |
| C | 2.766571 | -0.000000 | 0.279579 |
| H | 3.814843 | -0.000000 | -0.022349 |
| H | 2.746792 | -0.000000 | 1.373758 |
| H | 0.487765 | -1.297796 | 1.227000 |
| H | 2.164913 | 1.304674 | -1.323013 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.550744 | 2.151387 | 0.167428 |
| H | 0.099235 | -2.152214 | -0.264558 |
| H | 0.099235 | 2.152214 | -0.264558 |
| H | 0.487765 | 1.297796 | 1.227000 |
| C | -1.557983 | 0.000000 | -0.028938 |
| F | -1.771985 | 0.000000 | 1.300443 |
| F | -2.205994 | 1.075705 | -0.513171 |
| F | -2.205994 | -1.075705 | -0.513170 |



1,1-dimethyl-2-(trifluoromethyl)cyclohexane

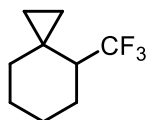
| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|------------|-------------------|
| ax | -651.514746 | -651.26945 | -651.318025 |
| eq | -651.516577 | -651.27147 | -651.32067 |

ax

| | | | |
|---|-----------|-----------|-----------|
| C | 0.844955 | 0.939397 | 0.096128 |
| C | -0.230043 | 0.032022 | 0.766615 |
| H | -0.534019 | 0.507887 | 1.702818 |
| C | 0.315595 | -1.370433 | 1.089971 |
| C | 0.963253 | -2.052810 | -0.113695 |
| H | 1.353558 | -3.024537 | 0.191407 |
| H | 0.214239 | -2.240342 | -0.887631 |
| C | 1.560054 | 0.203118 | -1.055282 |
| C | 2.082046 | -1.183598 | -0.682272 |
| H | 2.520015 | -1.655898 | -1.562828 |
| H | 2.880473 | -1.096906 | 0.059269 |
| H | 1.062374 | -1.258596 | 1.876406 |
| H | 0.874636 | 0.106738 | -1.899549 |
| H | 2.384012 | 0.836812 | -1.392416 |
| H | -0.478905 | -1.987154 | 1.506257 |
| C | -1.529614 | -0.063955 | -0.008375 |
| F | -1.378750 | -0.337552 | -1.317279 |
| F | -2.340571 | -1.025882 | 0.475995 |
| F | -2.252067 | 1.071130 | 0.054686 |
| C | 1.864205 | 1.322688 | 1.178658 |
| H | 2.642088 | 1.950471 | 0.741165 |
| H | 1.378951 | 1.890984 | 1.974451 |
| H | 2.348833 | 0.458396 | 1.629304 |
| C | 0.253180 | 2.241791 | -0.451986 |
| H | -0.421703 | 2.067275 | -1.289894 |
| H | -0.289564 | 2.788971 | 0.320479 |
| H | 1.065714 | 2.877311 | -0.808422 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | -0.433178 | -1.600728 | 0.149331 |
| C | 0.165807 | -0.301613 | -0.417223 |
| H | 0.156033 | -0.366653 | -1.509960 |
| C | -0.643426 | 0.968180 | -0.027683 |
| C | -2.107568 | 0.708346 | -0.443422 |
| H | -2.697406 | 1.578558 | -0.147765 |
| H | -2.146109 | 0.654869 | -1.536719 |
| C | -1.884500 | -1.777476 | -0.282172 |
| C | -2.715685 | -0.567673 | 0.128657 |
| H | -3.742611 | -0.673526 | -0.224263 |
| H | -2.759198 | -0.507756 | 1.219334 |
| H | -1.926160 | -1.892787 | -1.369386 |
| H | -2.287220 | -2.691954 | 0.154716 |
| H | 0.163483 | -2.448872 | -0.186236 |
| H | -0.379110 | -1.581524 | 1.239700 |
| C | 1.632769 | -0.272186 | -0.058559 |
| F | 1.861348 | -0.356090 | 1.265253 |
| F | 2.288535 | -1.315719 | -0.609993 |
| F | 2.282641 | 0.824341 | -0.483220 |
| C | -0.568517 | 1.281423 | 1.471438 |
| H | 0.432264 | 1.607030 | 1.756195 |
| H | -1.259181 | 2.095136 | 1.700981 |
| H | -0.836371 | 0.429780 | 2.095478 |
| C | -0.176886 | 2.204079 | -0.807900 |
| H | 0.778316 | 2.584372 | -0.452688 |
| H | -0.087703 | 1.986441 | -1.874032 |
| H | -0.914627 | 2.999984 | -0.688519 |



4-(trifluoromethyl)spiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax1 | -650.285932 | -650.063874 | -650.111365 |
| eq1 | -650.283152 | -650.061091 | -650.10883 |

ax1

| | | | |
|---|-----------|-----------|-----------|
| C | -0.890768 | 0.790072 | 0.010694 |
| C | 0.258128 | 0.105991 | 0.735611 |
| H | 0.534379 | 0.708044 | 1.604457 |
| C | -1.798433 | 1.624198 | 0.873665 |
| C | -0.878732 | 2.283212 | -0.120587 |
| C | -0.155122 | -1.296707 | 1.210762 |
| C | -0.828412 | -2.137864 | 0.123139 |
| H | -0.106223 | -2.402382 | -0.651705 |

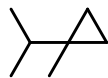
| | | | |
|---|-----------|-----------|-----------|
| H | -1.171715 | -3.073645 | 0.566187 |
| C | -1.562915 | -0.040030 | -1.067354 |
| C | -2.004440 | -1.392932 | -0.507897 |
| H | -2.774131 | -1.229189 | 0.252541 |
| H | -2.454045 | -1.997297 | -1.296773 |
| C | 1.525574 | 0.072226 | -0.086178 |
| H | -1.553806 | 1.721623 | 1.922116 |
| H | -2.854890 | 1.597464 | 0.646874 |
| H | -1.318307 | 2.703350 | -1.014337 |
| H | -0.026888 | 2.820841 | 0.269369 |
| H | -0.865934 | -1.147429 | 2.026410 |
| H | -2.421659 | 0.513657 | -1.450687 |
| H | -0.881837 | -0.194740 | -1.907279 |
| H | 0.703978 | -1.819976 | 1.630364 |
| F | 1.415459 | -0.598776 | -1.246611 |
| F | 1.958233 | 1.304147 | -0.409262 |
| F | 2.537618 | -0.510852 | 0.586021 |

eq1

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.671476 | 0.875504 | -0.183634 |
| C | -0.151578 | -0.396987 | -0.369063 |
| H | -0.111415 | -0.667171 | -1.429743 |
| C | 0.112645 | 2.263326 | -0.277644 |
| C | 0.566741 | 1.719671 | 1.056185 |
| C | 0.478900 | -1.537308 | 0.443242 |
| C | 1.919751 | -1.769489 | -0.013116 |
| H | 2.370769 | -2.558293 | 0.589840 |
| H | 1.905998 | -2.124872 | -1.047747 |
| C | 2.085712 | 0.651396 | -0.690941 |
| C | 2.755663 | -0.493345 | 0.069105 |
| H | 3.756426 | -0.673527 | -0.325875 |
| H | 2.869629 | -0.203121 | 1.117566 |
| C | -1.628344 | -0.287966 | -0.089634 |
| H | -0.948389 | 2.398746 | -0.418260 |
| H | 0.732943 | 3.006842 | -0.758579 |
| H | 1.495698 | 2.093731 | 1.463893 |
| H | -0.193825 | 1.497191 | 1.787934 |
| H | 0.460674 | -1.268125 | 1.502623 |
| H | 2.055219 | 0.416302 | -1.759596 |
| H | 2.657820 | 1.573291 | -0.576456 |
| H | -0.099315 | -2.452494 | 0.322431 |
| F | -1.922218 | 0.110969 | 1.159923 |
| F | -2.256175 | 0.564263 | -0.919779 |
| F | -2.245833 | -1.473822 | -0.255148 |

Acyclic Conformations



1-isopropyl-1-methylcyclopropane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| 1 | -275.098656 | -274.894486 | -274.935986 |
| 2 | -275.096483 | -274.892205 | -274.93343 |

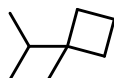
1

| | | | |
|---|-----------|-----------|-----------|
| C | -0.840591 | 0.000639 | -0.480420 |
| H | -0.712907 | 0.002132 | -1.567014 |
| C | 0.559375 | -0.000240 | 0.117877 |
| C | 1.612655 | 0.756830 | -0.636112 |
| C | 1.613042 | -0.754716 | -0.638388 |
| H | 1.317703 | 1.257160 | -1.548351 |
| H | 2.383868 | -1.256109 | -0.070068 |
| H | 1.318088 | -1.252569 | -1.551964 |
| C | 0.659093 | -0.002657 | 1.626883 |
| H | 1.704990 | -0.002595 | 1.934584 |
| H | 0.184531 | 0.879558 | 2.060008 |
| H | 0.185502 | -0.886808 | 2.057144 |
| C | -1.620503 | 1.256511 | -0.096807 |
| H | -2.575914 | 1.291043 | -0.622029 |
| H | -1.831234 | 1.273566 | 0.973996 |
| H | -1.061892 | 2.159913 | -0.347587 |
| H | 2.383120 | 1.257011 | -0.066211 |
| C | -1.620722 | -1.256102 | -0.100311 |
| H | -1.831984 | -1.275799 | 0.970338 |
| H | -2.575870 | -1.289147 | -0.626095 |
| H | -1.062100 | -2.158943 | -0.353088 |

2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.901457 | 0.188705 | -0.417157 |
| H | 1.006100 | 0.613158 | -1.420834 |
| C | -0.598682 | 0.116049 | -0.128402 |
| C | -1.062267 | -0.570976 | 1.123883 |
| C | -1.344209 | -1.185562 | -0.225601 |
| H | -0.321763 | -1.058964 | 1.742542 |
| H | -2.360029 | -1.146305 | -0.593183 |
| H | -0.802202 | -2.083340 | -0.481221 |
| C | -1.369215 | 1.350437 | -0.544121 |
| H | -2.425533 | 1.248199 | -0.294281 |
| H | -0.993899 | 2.245391 | -0.045513 |
| H | -1.290012 | 1.509032 | -1.621846 |
| C | 1.610223 | -1.163242 | -0.412411 |
| H | 2.680997 | -1.018829 | -0.560086 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.477266 | -1.678442 | 0.541651 |
| H | 1.249382 | -1.816240 | -1.205919 |
| H | -1.887989 | -0.128410 | 1.663096 |
| C | 1.589534 | 1.133346 | 0.570120 |
| H | 1.549510 | 0.715721 | 1.578773 |
| H | 2.638757 | 1.270734 | 0.305845 |
| H | 1.118363 | 2.115755 | 0.593102 |



1-isopropyl-1-methylcyclobutane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| 1 | -314.402919 | -314.168723 | -314.212199 |
| 2 | -314.400011 | -314.165515 | -314.208805 |
| 3 | -314.400397 | -314.16589 | -314.208454 |
| 4 | -314.401110 | -314.16668 | -314.210152 |

1

| | | | |
|---|-----------|-----------|-----------|
| C | 1.108323 | 0.000000 | -0.525799 |
| H | 0.904692 | 0.000000 | -1.601611 |
| C | -0.260819 | -0.000000 | 0.158361 |
| C | -1.258052 | -1.078781 | -0.345625 |
| C | -1.258052 | 1.078781 | -0.345624 |
| H | -0.994250 | -1.419449 | -1.347628 |
| H | -1.418244 | 1.944025 | 0.297229 |
| H | -0.994250 | 1.419450 | -1.347626 |
| C | -0.180603 | -0.000000 | 1.680582 |
| H | -1.182999 | -0.000001 | 2.112608 |
| H | 0.338405 | -0.885049 | 2.051943 |
| H | 0.338404 | 0.885049 | 2.051944 |
| C | 1.913098 | -1.257515 | -0.205201 |
| H | 2.813035 | -1.304936 | -0.819942 |
| H | 2.227078 | -1.267778 | 0.839866 |
| H | 1.329776 | -2.161299 | -0.392171 |
| H | -1.418244 | -1.944026 | 0.297226 |
| C | 1.913098 | 1.257515 | -0.205201 |
| H | 2.227079 | 1.267778 | 0.839866 |
| H | 2.813033 | 1.304937 | -0.819944 |
| H | 1.329774 | 2.161299 | -0.392170 |
| C | -2.363786 | 0.000000 | -0.385493 |
| H | -3.027388 | 0.000000 | -1.247027 |
| H | -2.965146 | -0.000000 | 0.521442 |

2

| | | | |
|---|-----------|-----------|-----------|
| C | 1.234850 | -0.011927 | -0.391362 |
| H | 1.516012 | 0.333385 | -1.391910 |
| C | -0.267277 | 0.272238 | -0.216558 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.876267 | 0.015254 | 1.189078 |
| C | -1.304236 | -0.738797 | -0.784793 |
| H | -0.331377 | -0.758472 | 1.729756 |
| H | -1.773655 | -0.472975 | -1.731868 |
| H | -0.906693 | -1.748652 | -0.853383 |
| C | -0.611028 | 1.678734 | -0.701084 |
| H | -1.676635 | 1.882507 | -0.583773 |
| H | -0.067046 | 2.442033 | -0.143976 |
| H | -0.364231 | 1.786792 | -1.759505 |
| C | 1.600919 | -1.492358 | -0.292206 |
| H | 2.685043 | -1.610500 | -0.319920 |
| H | 1.246599 | -1.926041 | 0.645717 |
| H | 1.184719 | -2.075446 | -1.112359 |
| H | -0.999071 | 0.883665 | 1.836274 |
| C | 2.053891 | 0.777202 | 0.633101 |
| H | 1.823534 | 0.434906 | 1.644970 |
| H | 3.121202 | 0.625601 | 0.468397 |
| H | 1.859019 | 1.847946 | 0.587416 |
| C | -2.136076 | -0.561973 | 0.505629 |
| H | -2.567464 | -1.460199 | 0.941334 |
| H | -2.918612 | 0.185217 | 0.392007 |

3

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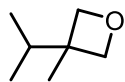
| | | | |
|---|-----------|-----------|-----------|
| C | 0.252982 | 0.499572 | -0.137349 |
| C | 0.931645 | 0.040271 | 1.185551 |
| C | 1.446108 | -0.124025 | -0.916769 |
| H | 1.437664 | 0.868966 | 1.680179 |
| H | 1.198004 | -0.751548 | -1.772072 |
| H | 2.153612 | 0.639999 | -1.236794 |
| C | 0.134678 | 2.008945 | -0.289560 |
| H | 1.117937 | 2.474126 | -0.208222 |
| H | -0.286612 | 2.273676 | -1.263086 |
| H | -0.500424 | 2.442830 | 0.483819 |
| C | -2.212997 | 0.340249 | 0.460560 |
| H | -3.131643 | -0.224363 | 0.296540 |
| H | -1.945278 | 0.238163 | 1.515494 |
| H | -2.429505 | 1.389665 | 0.267291 |
| H | 0.298859 | -0.466559 | 1.913241 |
| C | -1.042125 | -1.719959 | -0.309673 |
| H | -0.841044 | -2.026374 | 0.718941 |
| H | -2.006818 | -2.141993 | -0.593708 |
| H | -0.284234 | -2.165517 | -0.952993 |
| C | 1.907594 | -0.841276 | 0.372743 |
| H | 2.962365 | -0.752887 | 0.623198 |
| H | 1.631098 | -1.893298 | 0.389091 |
| C | -1.090989 | -0.195553 | -0.430448 |
| H | -1.335359 | 0.045773 | -1.471254 |

4

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| | | | |
|---|-----------|-----------|-----------|
| C | -0.291119 | 0.000192 | 0.364374 |
| C | -1.327779 | 1.078568 | -0.064691 |
| C | -1.327684 | -1.078615 | -0.063772 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.897467 | 1.438742 | 0.791955 |
| H | -0.953358 | -1.933681 | -0.624692 |
| H | -1.897311 | -1.438244 | 0.793148 |
| C | 0.076006 | 0.000828 | 1.839184 |
| H | -0.829096 | 0.001005 | 2.447971 |
| H | 0.657367 | -0.882811 | 2.109169 |
| H | 0.657278 | 0.884757 | 2.108425 |
| C | 1.805469 | -1.247737 | -0.386536 |
| H | 2.578156 | -1.283902 | -1.155744 |
| H | 2.308410 | -1.237571 | 0.581889 |
| H | 1.222767 | -2.166630 | -0.454965 |
| H | -0.953573 | 1.933296 | -0.626202 |
| C | 1.805564 | 1.247345 | -0.387523 |
| H | 2.308804 | 1.237738 | 0.580761 |
| H | 2.578035 | 1.283056 | -1.156983 |
| H | 1.222937 | 2.166259 | -0.456318 |
| C | -2.101570 | -0.000394 | -0.852152 |
| H | -3.185108 | -0.000385 | -0.759269 |
| H | -1.839971 | -0.000814 | -1.908515 |
| C | 0.939076 | -0.000213 | -0.562616 |
| H | 0.554357 | -0.000661 | -1.588237 |



3-isopropyl-3-methyloxetane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| 1 | -350.314072 | -350.103248 | -350.146852 |
| 2 | -350.310996 | -350.099815 | -350.143533 |
| 3 | -350.312287 | -350.101218 | -350.143983 |

1

| | | | |
|---|-----------|-----------|-----------|
| C | -1.068825 | -0.000035 | -0.530800 |
| H | -0.829983 | 0.000005 | -1.598796 |
| C | 0.271638 | 0.000070 | 0.202628 |
| C | 1.297393 | 1.029881 | -0.303853 |
| C | 1.297248 | -1.029924 | -0.303723 |
| H | 1.027789 | 1.499358 | -1.252136 |
| H | 1.632566 | -1.784698 | 0.407230 |
| H | 1.027559 | -1.499415 | -1.251978 |
| C | 0.164534 | 0.000212 | 1.720278 |
| H | 1.162457 | 0.000153 | 2.161764 |
| H | -0.360648 | 0.885518 | 2.080268 |
| H | -0.360836 | -0.884906 | 2.080460 |
| C | -1.878718 | 1.258792 | -0.231084 |
| H | -2.759433 | 1.307624 | -0.872309 |
| H | -2.221989 | 1.267229 | 0.804492 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.288031 | 2.161696 | -0.399630 |
| H | 1.632765 | 1.784648 | 0.407077 |
| O | 2.297253 | -0.000092 | -0.504468 |
| C | -1.878508 | -1.258898 | -0.230840 |
| H | -2.221621 | -1.267207 | 0.804780 |
| H | -2.759361 | -1.308051 | -0.871831 |
| H | -1.287835 | -2.161807 | -0.399281 |

2

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.197308 | -0.013445 | -0.413831 |
| H | 1.474583 | 0.339544 | -1.411555 |
| C | -0.287101 | 0.323461 | -0.211488 |
| C | -0.893834 | -0.030509 | 1.159170 |
| C | -1.358682 | -0.643975 | -0.755196 |
| H | -0.303590 | -0.723829 | 1.759897 |
| H | -2.021920 | -0.239007 | -1.519293 |
| H | -1.002894 | -1.627254 | -1.057075 |
| C | -0.610870 | 1.756968 | -0.612888 |
| H | -1.672428 | 1.960392 | -0.463068 |
| H | -0.046759 | 2.477904 | -0.021900 |
| H | -0.379133 | 1.918106 | -1.667305 |
| C | 1.507477 | -1.508561 | -0.341162 |
| H | 2.586058 | -1.663848 | -0.381679 |
| H | 1.147214 | -1.944767 | 0.593102 |
| H | 1.063638 | -2.062809 | -1.166487 |
| H | -1.221311 | 0.807143 | 1.775053 |
| O | -2.011194 | -0.711692 | 0.537494 |
| C | 2.052363 | 0.733959 | 0.612584 |
| H | 1.799466 | 0.409625 | 1.625292 |
| H | 3.109565 | 0.521830 | 0.452425 |
| H | 1.917105 | 1.813107 | 0.559505 |

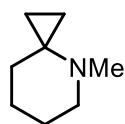
3

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.089552 | -0.154647 | -0.440056 |
| H | 1.310786 | 0.081573 | -1.486178 |
| C | -0.280969 | 0.479457 | -0.141578 |
| C | -1.451037 | -0.235481 | -0.841283 |
| C | -0.949875 | -0.044761 | 1.142631 |
| H | -2.242672 | 0.441328 | -1.166957 |
| H | -0.335054 | -0.603813 | 1.846745 |
| H | -1.523932 | 0.715526 | 1.675505 |
| C | -0.265425 | 1.990470 | -0.292476 |
| H | -1.276678 | 2.390619 | -0.217804 |
| H | 0.336682 | 2.459580 | 0.485480 |
| H | 0.147881 | 2.280395 | -1.260712 |
| C | 1.109588 | -1.676675 | -0.288092 |
| H | 2.078531 | -2.062095 | -0.606302 |
| H | 0.968724 | -1.970435 | 0.753620 |
| H | 0.345090 | -2.170122 | -0.886768 |
| H | -1.213196 | -0.936832 | -1.639923 |
| O | -1.827551 | -0.912400 | 0.382965 |
| C | 2.185307 | 0.454011 | 0.435432 |

| | | | |
|---|----------|-----------|----------|
| H | 1.926507 | 0.353961 | 1.493040 |
| H | 3.130765 | -0.064900 | 0.274910 |
| H | 2.344132 | 1.510175 | 0.224150 |

N-Heterocycles



4-methyl-4-azaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -368.552780 | -368.321815 | -368.363599 |
| eq | -368.551067 | -368.319947 | -368.361743 |

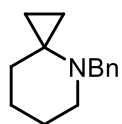
ax

| | | | |
|---|-----------|-----------|-----------|
| C | -0.802696 | -0.158906 | -0.060095 |
| C | -1.710390 | -0.752099 | 0.976735 |
| C | -2.281273 | -0.020304 | -0.216651 |
| C | 1.182573 | 0.664535 | 0.986616 |
| C | 2.062073 | -0.250416 | 0.129888 |
| H | 2.396407 | 0.283199 | -0.763442 |
| H | 2.956526 | -0.519168 | 0.694462 |
| C | -0.032480 | -1.112167 | -0.954141 |
| C | 1.285101 | -1.502559 | -0.279952 |
| H | 1.064689 | -2.095159 | 0.613443 |
| H | 1.883963 | -2.128629 | -0.942747 |
| C | 0.092347 | 1.981578 | -0.744887 |
| H | 0.700661 | 1.601209 | -1.573819 |
| H | -0.883620 | 2.258950 | -1.142930 |
| H | -1.761341 | -0.249614 | 1.931745 |
| H | -1.808916 | -1.828192 | 1.005460 |
| H | -2.763790 | -0.604544 | -0.987430 |
| H | -2.705270 | 0.957361 | -0.037126 |
| H | 0.941722 | 0.148127 | 1.920333 |
| H | -0.641844 | -1.993089 | -1.160678 |
| H | 0.174972 | -0.630616 | -1.914405 |
| H | 1.713258 | 1.582042 | 1.244434 |
| N | -0.087334 | 1.034037 | 0.349700 |
| H | 0.572389 | 2.881891 | -0.360277 |

eq

| | | | |
|---|-----------|-----------|-----------|
| C | 0.553538 | -0.500152 | -0.177710 |
| C | 1.920068 | -1.079197 | -0.331379 |
| C | 1.305104 | -0.958646 | 1.049581 |
| C | -0.875171 | 1.340289 | 0.359529 |
| C | -2.119768 | 0.547426 | -0.015796 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.957985 | 0.879743 | 0.598404 |
| H | -2.369962 | 0.761949 | -1.058129 |
| C | -0.618616 | -1.361902 | -0.599491 |
| C | -1.881277 | -0.950220 | 0.153938 |
| H | -2.741879 | -1.520615 | -0.197829 |
| H | -1.753009 | -1.177871 | 1.216290 |
| C | 1.407761 | 1.809273 | -0.200691 |
| H | 1.773826 | 1.801195 | 0.835418 |
| H | 2.233432 | 1.568993 | -0.866187 |
| H | 2.754344 | -0.431380 | -0.551219 |
| H | 1.982932 | -2.063312 | -0.774407 |
| H | 0.966833 | -1.859319 | 1.542418 |
| H | 1.731425 | -0.211745 | 1.703499 |
| H | -1.035445 | 2.401159 | 0.165190 |
| H | -0.380771 | -2.409852 | -0.413261 |
| H | -0.774889 | -1.241922 | -1.675524 |
| H | -0.673141 | 1.228991 | 1.437783 |
| N | 0.287215 | 0.909819 | -0.423080 |
| H | 1.083955 | 2.824030 | -0.428769 |



4-benzyl-4-azaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax | -599.583802 | -599.266557 | -599.3205 |
| ax2 | -599.578802 | -599.26142 | -599.316007 |
| ax3 | -599.582589 | -599.265272 | -599.318992 |
| ax4 | -599.582590 | -599.265272 | -599.318986 |
| ax5 | -599.582589 | -599.265271 | -599.318983 |
| eq | -599.580380 | -599.262975 | -599.317138 |
| eq1 | -599.580381 | -599.262976 | -599.317144 |
| eq2 | -599.577535 | -599.259711 | -599.312082 |
| eq3 | -599.580320 | -599.263108 | -599.316674 |
| eq4 | -599.577535 | -599.259713 | -599.312085 |
| eq5 | -599.580314 | -599.263149 | -599.316834 |

ax

| | | | |
|---|----------|-----------|-----------|
| C | 2.086892 | -0.673673 | -0.158125 |
| C | 2.813629 | -1.610704 | 0.760992 |
| C | 2.302686 | -2.089831 | -0.578456 |
| C | 0.773059 | 0.842796 | 1.141010 |
| C | 1.507941 | 2.049014 | 0.549993 |
| H | 0.958502 | 2.436571 | -0.311859 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.537371 | 2.847738 | 1.292947 |
| C | 2.882133 | 0.442328 | -0.807800 |
| C | 2.923580 | 1.656416 | 0.123443 |
| H | 3.506739 | 1.400226 | 1.013367 |
| H | 3.426268 | 2.494099 | -0.361732 |
| C | -0.157761 | -0.145443 | -0.895785 |
| H | 0.063755 | 0.758142 | -1.474900 |
| H | 0.000889 | -0.998034 | -1.558800 |
| H | 2.283199 | -1.948797 | 1.639349 |
| H | 3.879676 | -1.475480 | 0.878295 |
| H | 3.024590 | -2.279422 | -1.360213 |
| H | 1.439854 | -2.741061 | -0.570987 |
| H | 1.280175 | 0.533423 | 2.058899 |
| H | 3.889444 | 0.090883 | -1.035447 |
| H | 2.414326 | 0.721670 | -1.756819 |
| H | -0.251383 | 1.105217 | 1.407112 |
| N | 0.739094 | -0.325657 | 0.250315 |
| C | -1.606886 | -0.109461 | -0.472353 |
| C | -2.397657 | 1.009110 | -0.716458 |
| C | -2.176509 | -1.206376 | 0.175119 |
| C | -3.733941 | 1.035713 | -0.326161 |
| H | -1.963077 | 1.867956 | -1.213868 |
| C | -3.507951 | -1.185115 | 0.566222 |
| H | -1.566494 | -2.079667 | 0.371948 |
| C | -4.291737 | -0.061351 | 0.316212 |
| H | -4.334972 | 1.913794 | -0.521866 |
| H | -3.938094 | -2.044261 | 1.063776 |
| H | -5.329287 | -0.043935 | 0.621485 |

ax2

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.744672 | -0.581763 | -0.112848 |
| C | 3.193571 | -0.992322 | -0.038134 |
| C | 2.095427 | -2.025364 | 0.044213 |
| C | 1.372514 | 1.548056 | 0.947930 |
| C | 0.883579 | 2.150731 | -0.373291 |
| H | -0.201245 | 2.060873 | -0.450712 |
| H | 1.125383 | 3.215386 | -0.384928 |
| C | 1.268854 | -0.066596 | -1.461134 |
| C | 1.533799 | 1.436234 | -1.557030 |
| H | 2.614005 | 1.612622 | -1.538582 |
| H | 1.156667 | 1.832486 | -2.500672 |
| C | -0.014343 | -0.406513 | 1.630039 |
| H | 0.148521 | -1.451460 | 1.896912 |
| H | -0.173653 | 0.143263 | 2.559188 |
| H | 3.721370 | -0.764492 | 0.876237 |
| H | 3.779223 | -0.944487 | -0.945498 |
| H | 1.939525 | -2.671883 | -0.807975 |
| H | 1.921877 | -2.481120 | 1.008221 |
| H | 2.438481 | 1.782220 | 1.047889 |
| H | 1.786586 | -0.605004 | -2.256687 |
| H | 0.199166 | -0.253098 | -1.579687 |
| H | 0.859564 | 2.004121 | 1.795538 |
| N | 1.234389 | 0.095082 | 1.057658 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.280982 | -0.328303 | 0.797948 |
| C | -1.646144 | -1.386574 | -0.032866 |
| C | -2.108248 | 0.792219 | 0.852271 |
| C | -2.793530 | -1.317118 | -0.814232 |
| H | -1.019465 | -2.270459 | -0.070411 |
| C | -3.257121 | 0.869001 | 0.073626 |
| H | -1.846709 | 1.613766 | 1.509231 |
| C | -3.599876 | -0.185031 | -0.766471 |
| H | -3.060951 | -2.146153 | -1.456078 |
| H | -3.887348 | 1.746989 | 0.125884 |
| H | -4.494758 | -0.129076 | -1.371604 |

ax3

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| | | | |
|---|-----------|-----------|-----------|
| C | 1.196654 | -0.813604 | 0.228660 |
| C | 1.471995 | -1.774155 | 1.349813 |
| C | 0.195625 | -1.878058 | 0.551584 |
| C | 2.156784 | 1.280677 | 0.836043 |
| C | 3.072741 | 1.269662 | -0.390175 |
| H | 2.600467 | 1.816404 | -1.210541 |
| H | 4.000077 | 1.792701 | -0.150408 |
| C | 2.057414 | -0.945539 | -1.014645 |
| C | 3.362652 | -0.167914 | -0.824893 |
| H | 3.956774 | -0.660638 | -0.049115 |
| H | 3.953786 | -0.182222 | -1.741539 |
| C | 0.002500 | 1.256105 | -0.289439 |
| H | 0.001415 | 2.304292 | 0.015795 |
| H | 0.354571 | 1.224534 | -1.326225 |
| H | 1.390142 | -1.389522 | 2.356264 |
| H | 2.236741 | -2.521928 | 1.193916 |
| H | 0.097047 | -2.695425 | -0.149270 |
| H | -0.716788 | -1.574938 | 1.042272 |
| H | 2.677843 | 0.807639 | 1.672629 |
| H | 2.259092 | -2.000276 | -1.206497 |
| H | 1.519728 | -0.559114 | -1.885260 |
| H | 1.915549 | 2.302301 | 1.131402 |
| N | 0.896256 | 0.548579 | 0.638401 |
| C | -1.410753 | 0.729858 | -0.239230 |
| C | -2.179762 | 0.899528 | 0.912141 |
| C | -1.963791 | 0.053676 | -1.321286 |
| C | -3.469467 | 0.392408 | 0.984057 |
| H | -1.755101 | 1.425357 | 1.758916 |
| C | -3.256671 | -0.458737 | -1.254815 |
| H | -1.374317 | -0.083177 | -2.220091 |
| C | -4.010821 | -0.293478 | -0.100615 |
| H | -4.055103 | 0.530926 | 1.883266 |
| H | -3.671092 | -0.988335 | -2.102407 |
| H | -5.015234 | -0.691217 | -0.045118 |

ax4

```
=====
```

| | | | |
|---|----------|----------|-----------|
| C | 1.196782 | 0.813959 | -0.227659 |
| C | 1.472703 | 1.775933 | -1.347481 |
| C | 0.195954 | 1.878848 | -0.549794 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.157090 | -1.279462 | -0.837579 |
| C | 3.072538 | -1.270172 | 0.389066 |
| H | 2.599880 | -1.818026 | 1.208470 |
| H | 3.999949 | -1.792917 | 0.148968 |
| C | 2.056912 | 0.944083 | 1.016215 |
| C | 3.362284 | 0.166789 | 0.825956 |
| H | 3.956742 | 0.660611 | 0.051139 |
| H | 3.952998 | 0.179767 | 1.742888 |
| C | 0.002382 | -1.256672 | 0.286912 |
| H | 0.001187 | -2.304214 | -0.020487 |
| H | 0.354289 | -1.227240 | 1.323816 |
| H | 1.391525 | 1.392621 | -2.354485 |
| H | 2.237339 | 2.523505 | -1.190070 |
| H | 0.096875 | 2.695410 | 0.151926 |
| H | -0.716187 | 1.576254 | -1.041305 |
| H | 2.678562 | -0.805330 | -1.673295 |
| H | 2.258428 | 1.998535 | 1.209790 |
| H | 1.518823 | 0.556276 | 1.885988 |
| H | 1.916051 | -2.300702 | -1.134415 |
| N | 0.896500 | -0.547640 | -0.639485 |
| C | -1.410802 | -0.730160 | 0.237630 |
| C | -1.963945 | -0.056661 | 1.321433 |
| C | -2.179737 | -0.896988 | -0.914106 |
| C | -3.256794 | 0.455773 | 1.256232 |
| H | -1.374376 | 0.077878 | 2.220518 |
| C | -3.469526 | -0.389714 | -0.984794 |
| H | -1.755141 | -1.420695 | -1.762230 |
| C | -4.010943 | 0.293345 | 0.101536 |
| H | -3.671434 | 0.983140 | 2.105109 |
| H | -4.055032 | -0.525969 | -1.884432 |
| H | -5.015374 | 0.691182 | 0.047110 |

ax5

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=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.196879 | 0.813994 | 0.227548 |
| C | -1.472573 | 1.776014 | 1.347377 |
| C | -0.196014 | 1.878944 | 0.549381 |
| C | -2.156927 | -1.279512 | 0.837626 |
| C | -3.072581 | -1.270281 | -0.388857 |
| H | -2.599958 | -1.818000 | -1.208377 |
| H | -3.999880 | -1.793176 | -0.148653 |
| C | -2.057301 | 0.944046 | -1.016136 |
| C | -3.362581 | 0.166671 | -0.825612 |
| H | -3.956912 | 0.660398 | -0.050638 |
| H | -3.953497 | 0.179636 | -1.742415 |
| C | -0.002347 | -1.256515 | -0.287188 |
| H | -0.001264 | -2.304129 | 0.019963 |
| H | -0.354187 | -1.226795 | -1.324108 |
| H | -1.391106 | 1.392744 | 2.354373 |
| H | -2.237292 | 2.523535 | 1.190123 |
| H | -0.097131 | 2.695455 | -0.152424 |
| H | 0.716247 | 1.576430 | 1.040721 |
| H | -2.678286 | -0.805430 | 1.673443 |
| H | -2.258891 | 1.998478 | -1.209735 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.519385 | 0.556189 | -1.885992 |
| H | -1.915746 | -2.300732 | 1.134410 |
| N | -0.896439 | -0.547589 | 0.639315 |
| C | 1.410890 | -0.730132 | -0.237728 |
| C | 2.179630 | -0.896913 | 0.914136 |
| C | 1.964224 | -0.056730 | -1.321497 |
| C | 3.469430 | -0.389678 | 0.984983 |
| H | 1.754881 | -1.420526 | 1.762240 |
| C | 3.257081 | 0.455659 | -1.256137 |
| H | 1.374796 | 0.077770 | -2.220680 |
| C | 4.011040 | 0.293283 | -0.101306 |
| H | 4.054805 | -0.525899 | 1.884712 |
| H | 3.671861 | 0.982969 | -2.104981 |
| H | 5.015470 | 0.691101 | -0.046717 |

eq

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```

| | | | |
|---|-----------|-----------|-----------|
| C | 2.084826 | -0.609470 | 0.251476 |
| C | 2.356616 | -2.023684 | 0.645855 |
| C | 2.673108 | -1.559571 | -0.763245 |
| C | 0.746901 | 1.073139 | -0.803191 |
| C | 1.639819 | 2.189019 | -0.281645 |
| H | 1.627208 | 3.019414 | -0.989022 |
| H | 1.230290 | 2.555087 | 0.663624 |
| C | 3.025791 | 0.434833 | 0.819525 |
| C | 3.060106 | 1.679635 | -0.062114 |
| H | 3.684835 | 2.451449 | 0.389195 |
| H | 3.505851 | 1.423614 | -1.027843 |
| C | -0.279226 | -1.040807 | -0.324133 |
| H | -0.163760 | -1.309461 | -1.383318 |
| H | -0.168440 | -1.951651 | 0.260169 |
| H | 1.549695 | -2.729077 | 0.764761 |
| H | 3.184621 | -2.175896 | 1.323986 |
| H | 3.709138 | -1.433659 | -1.045134 |
| H | 2.025956 | -1.931070 | -1.545115 |
| H | -0.276147 | 1.434189 | -0.905833 |
| H | 4.021624 | 0.001300 | 0.916543 |
| H | 2.682308 | 0.704559 | 1.822647 |
| H | 1.087731 | 0.759351 | -1.803555 |
| N | 0.734100 | -0.080405 | 0.105324 |
| C | -1.681058 | -0.516695 | -0.105386 |
| C | -2.590860 | -0.445090 | -1.155349 |
| C | -2.089026 | -0.112067 | 1.165945 |
| C | -3.886956 | 0.017566 | -0.944338 |
| H | -2.281435 | -0.749722 | -2.147806 |
| C | -3.379328 | 0.352169 | 1.380805 |
| H | -1.385797 | -0.161683 | 1.987859 |
| C | -4.283861 | 0.418533 | 0.324169 |
| H | -4.581605 | 0.068930 | -1.772242 |
| H | -3.682703 | 0.660932 | 2.372481 |
| H | -5.289185 | 0.781169 | 0.491089 |

eq1

```
=====
```


| | | | |
|---|-----------|-----------|-----------|
| C | -2.084640 | -0.609707 | -0.251360 |
| C | -2.355823 | -2.023929 | -0.646037 |
| C | -2.672587 | -1.560257 | 0.763091 |
| C | -0.747387 | 1.073685 | 0.803088 |
| C | -1.640505 | 2.189183 | 0.281109 |
| H | -1.628051 | 3.019807 | 0.988218 |
| H | -1.231067 | 2.555006 | -0.664293 |
| C | -3.025888 | 0.434283 | -0.819537 |
| C | -3.060620 | 1.679300 | 0.061767 |
| H | -3.685612 | 2.450734 | -0.389823 |
| H | -3.506296 | 1.423439 | 1.027569 |
| C | 0.279281 | -1.040143 | 0.325447 |
| H | 0.163966 | -1.307501 | 1.384982 |
| H | 0.168456 | -1.951715 | -0.257693 |
| H | -1.548662 | -2.729012 | -0.765250 |
| H | -3.183742 | -2.176310 | -1.324248 |
| H | -3.708661 | -1.434943 | 1.045112 |
| H | -2.025342 | -1.931587 | 1.544978 |
| H | 0.275577 | 1.434972 | 0.905818 |
| H | -4.021591 | 0.000409 | -0.916450 |
| H | -2.682519 | 0.703873 | -1.822735 |
| H | -1.088299 | 0.760161 | 1.803526 |
| N | -0.734106 | -0.080239 | -0.104949 |
| C | 1.681097 | -0.516270 | 0.105946 |
| C | 2.088741 | -0.112325 | -1.165703 |
| C | 2.591246 | -0.444296 | 1.155590 |
| C | 3.379058 | 0.351589 | -1.381185 |
| H | 1.385244 | -0.162194 | -1.987368 |
| C | 3.887350 | 0.018030 | 0.943952 |
| H | 2.282059 | -0.748332 | 2.148307 |
| C | 4.283942 | 0.418302 | -0.324876 |
| H | 3.682161 | 0.659831 | -2.373106 |
| H | 4.582244 | 0.069696 | 1.771633 |
| H | 5.289282 | 0.780669 | -0.492280 |

eq2

| | | | |
|---|-----------|-----------|-----------|
| C | -1.485745 | 0.893575 | 0.031196 |
| C | -0.832610 | 2.231822 | 0.096423 |
| C | -0.668969 | 1.379115 | -1.146173 |
| C | -1.357451 | -1.489821 | 0.210339 |
| C | -2.858403 | -1.635720 | -0.017564 |
| H | -3.056615 | -2.581637 | -0.524159 |
| H | -3.358869 | -1.668924 | 0.953670 |
| C | -2.986467 | 0.858406 | -0.185604 |
| C | -3.397993 | -0.463060 | -0.832202 |
| H | -4.483245 | -0.524079 | -0.923743 |
| H | -2.984605 | -0.507242 | -1.844263 |
| C | 0.228121 | -0.155631 | 1.546637 |
| H | 0.246305 | 0.744771 | 2.159759 |
| H | 0.242521 | -1.005920 | 2.231714 |
| H | 0.038859 | 2.365518 | 0.717230 |
| H | -1.481109 | 3.095051 | 0.039662 |
| H | -1.202894 | 1.674402 | -2.038876 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.304472 | 0.941410 | -1.312740 |
| H | -0.995274 | -2.293962 | 0.852184 |
| H | -3.281594 | 1.701941 | -0.810986 |
| H | -3.485043 | 0.968603 | 0.781644 |
| H | -0.837385 | -1.575296 | -0.755652 |
| N | -1.061935 | -0.215546 | 0.863400 |
| C | 1.499609 | -0.198555 | 0.710622 |
| C | 2.347251 | 0.906753 | 0.651578 |
| C | 1.864022 | -1.348468 | 0.006394 |
| C | 3.505258 | 0.884222 | -0.117884 |
| H | 2.101478 | 1.796827 | 1.217694 |
| C | 3.015877 | -1.374233 | -0.770348 |
| H | 1.250103 | -2.236586 | 0.073510 |
| C | 3.836950 | -0.253985 | -0.842138 |
| H | 4.147565 | 1.754372 | -0.149390 |
| H | 3.278092 | -2.273086 | -1.312606 |
| H | 4.734081 | -0.273855 | -1.446112 |

eq3

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | -1.375334 | 0.733471 | 0.288357 |
| C | -0.515094 | 1.922486 | 0.560042 |
| C | -1.665343 | 2.038271 | -0.416562 |
| C | -1.988208 | -1.052870 | -1.172441 |
| C | -3.058958 | -1.534475 | -0.199769 |
| H | -3.883369 | -1.977058 | -0.760895 |
| H | -2.628099 | -2.319757 | 0.427021 |
| C | -2.377029 | 0.316265 | 1.343861 |
| C | -3.558299 | -0.394359 | 0.684827 |
| H | -4.251747 | -0.769677 | 1.438500 |
| H | -4.106285 | 0.326050 | 0.070485 |
| C | 0.287027 | -0.199136 | -1.279291 |
| H | 0.315305 | -1.004346 | -2.015840 |
| H | 0.231027 | 0.732717 | -1.858388 |
| H | 0.480589 | 1.959645 | 0.144680 |
| H | -0.618771 | 2.389691 | 1.529530 |
| H | -2.545810 | 2.588380 | -0.115627 |
| H | -1.406297 | 2.124369 | -1.462541 |
| H | -1.589082 | -1.899735 | -1.730147 |
| H | -2.712910 | 1.195261 | 1.895366 |
| H | -1.885577 | -0.356169 | 2.053178 |
| H | -2.431864 | -0.353506 | -1.899085 |
| N | -0.882744 | -0.421487 | -0.447450 |
| C | 1.601292 | -0.224638 | -0.523150 |
| C | 1.722670 | -0.816330 | 0.730547 |
| C | 2.734717 | 0.335415 | -1.112376 |
| C | 2.952749 | -0.851455 | 1.380155 |
| H | 0.846056 | -1.242261 | 1.199269 |
| C | 3.964876 | 0.298051 | -0.468817 |
| H | 2.648789 | 0.809854 | -2.083032 |
| C | 4.078360 | -0.296823 | 0.783593 |
| H | 3.029976 | -1.311870 | 2.356432 |
| H | 4.833157 | 0.738407 | -0.940998 |
| H | 5.033559 | -0.322832 | 1.290394 |

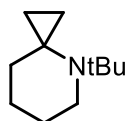
eq4

```
=====
C -1.486006      0.893663      0.030987
C -0.832528      2.231726      0.095852
C -0.669170      1.378698     -1.146551
C -1.357385     -1.489662      0.210327
C -2.858374     -1.635830     -0.017291
H -3.056591     -2.581750     -0.523883
H -3.358615     -1.669127      0.954048
C -2.986690      0.858385     -0.185397
C -3.398334     -0.463175     -0.831768
H -4.483615     -0.524161     -0.922958
H -2.985261     -0.507378     -1.843954
C  0.228023     -0.155142      1.546595
H  0.246340      0.745461      2.159448
H  0.242498     -1.005114      2.232077
H  0.038696      2.365726      0.716936
H -1.481048      3.094903      0.038597
H -1.202623      1.674209     -2.039462
H  0.304046      0.940327     -1.312599
H -0.994877     -2.293794      0.851958
H -3.282077      1.701765     -0.810885
H -3.485031      0.968721      0.781957
H -0.837468     -1.574936     -0.755826
N -1.061913     -0.215356      0.863303
C  1.499763     -0.198361      0.710710
C  2.347687      0.906764      0.651665
C  1.863903     -1.348302      0.006386
C  3.505701      0.884017     -0.117755
H  2.102075      1.796870      1.217771
C  3.015773     -1.374281     -0.770329
H  1.249726     -2.236246      0.073227
C  3.837130     -0.254247     -0.842041
H  4.148203      1.754022     -0.149217
H  3.277755     -2.273124     -1.312727
H  4.734288     -0.274400     -1.445964
```

eq5

```
=====
C  1.384483      0.757929     -0.215231
C  0.534642      1.974529     -0.375527
C  1.684809      1.989398      0.607709
C  1.976300     -1.163516      1.074153
C  3.041430     -1.566117      0.060753
H  3.860070     -2.069226      0.577547
H  2.601017     -2.283990     -0.636296
C  2.383575      0.429014     -1.304175
C  3.555216     -0.354590     -0.713753
H  4.244880     -0.666080     -1.499310
H  4.111201      0.298647     -0.034883
C -0.291747     -0.300836      1.254359
H -0.324102     -1.164052      1.921578
H -0.235832      0.579062      1.909849
```

| | | | |
|---|-----------|-----------|-----------|
| H | -0.461201 | 1.980573 | 0.041412 |
| H | 0.642504 | 2.528734 | -1.297586 |
| H | 2.570079 | 2.557832 | 0.359526 |
| H | 1.424699 | 1.979645 | 1.656987 |
| H | 1.566007 | -2.053355 | 1.550891 |
| H | 2.731392 | 1.351284 | -1.771133 |
| H | 1.885248 | -0.168268 | -2.073451 |
| H | 2.428005 | -0.540009 | 1.862213 |
| N | 0.879633 | -0.454647 | 0.410342 |
| C | -1.604386 | -0.260405 | 0.495719 |
| C | -2.754870 | 0.169862 | 1.157026 |
| C | -1.708065 | -0.665137 | -0.831431 |
| C | -3.983882 | 0.186694 | 0.510933 |
| H | -2.683826 | 0.496888 | 2.187960 |
| C | -2.937456 | -0.644546 | -1.483582 |
| H | -0.818705 | -0.990334 | -1.353839 |
| C | -4.079675 | -0.221297 | -0.815830 |
| H | -4.865882 | 0.522192 | 1.040371 |
| H | -3.000743 | -0.958610 | -2.517231 |
| H | -5.034480 | -0.204293 | -1.323736 |



4-(*tert*-butyl)-4-azaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax2 | -486.464721 | -486.144757 | -486.194045 |
| ax | -486.466407 | -486.146681 | -486.19568 |
| eq | -486.462170 | -486.142531 | -486.191924 |

ax2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.832747 | 0.809403 | 0.006744 |
| C | 1.654516 | 1.660536 | -0.928758 |
| C | 0.745395 | 2.303963 | 0.085121 |
| C | 0.343862 | -1.168980 | -1.184075 |
| C | 1.080574 | -2.041570 | -0.165610 |
| H | 1.491121 | -2.918206 | -0.671326 |
| H | 0.379255 | -2.403033 | 0.590449 |
| C | 1.656990 | 0.078401 | 1.061687 |
| C | 2.200220 | -1.234203 | 0.491372 |
| H | 2.694664 | -1.812815 | 1.273036 |
| H | 2.955546 | -1.006111 | -0.267071 |
| C | -1.550488 | -0.035298 | 0.085345 |
| H | 1.335673 | 1.701253 | -1.960151 |
| H | 2.722189 | 1.701078 | -0.765336 |
| H | 1.192501 | 2.780389 | 0.946687 |
| H | -0.133375 | 2.789244 | -0.305184 |
| H | -0.415042 | -1.738806 | -1.709757 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.480559 | 0.722234 | 1.375847 |
| H | 1.058300 | -0.129417 | 1.947251 |
| H | 1.069872 | -0.849762 | -1.938820 |
| C | -1.460660 | -0.251549 | 1.603967 |
| H | -0.954317 | -1.181865 | 1.858147 |
| H | -0.943379 | 0.575268 | 2.090674 |
| H | -2.471352 | -0.294951 | 2.014408 |
| C | -2.385230 | -1.174499 | -0.505965 |
| H | -3.379512 | -1.143701 | -0.061183 |
| H | -2.495215 | -1.067075 | -1.586219 |
| H | -1.956494 | -2.153777 | -0.292508 |
| C | -2.338928 | 1.264132 | -0.143637 |
| H | -2.364881 | 1.515395 | -1.204589 |
| H | -3.364260 | 1.136891 | 0.207460 |
| H | -1.910810 | 2.100056 | 0.404656 |
| N | -0.237861 | 0.059386 | -0.626231 |

ax

```
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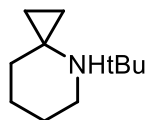
| | | | |
|---|-----------|-----------|-----------|
| C | -0.857675 | 0.795647 | -0.029563 |
| C | -1.758003 | 1.546428 | 0.921502 |
| C | -0.867607 | 2.291955 | -0.034209 |
| C | -0.263310 | -1.157789 | 1.173561 |
| C | -1.081821 | -2.039684 | 0.214642 |
| H | -1.533939 | -2.847342 | 0.794692 |
| H | -0.429800 | -2.506511 | -0.521723 |
| C | -1.589028 | 0.035203 | -1.121085 |
| C | -2.168246 | -1.244283 | -0.512038 |
| H | -2.640770 | -1.862273 | -1.277073 |
| H | -2.948942 | -0.961956 | 0.200170 |
| C | 1.565334 | 0.003839 | -0.087343 |
| H | -1.473951 | 1.555143 | 1.963855 |
| H | -2.821036 | 1.524648 | 0.726179 |
| H | -1.320097 | 2.782692 | -0.885016 |
| H | -0.021109 | 2.802888 | 0.395718 |
| H | 0.569418 | -1.727990 | 1.582711 |
| H | -2.385720 | 0.654327 | -1.537472 |
| H | -0.901003 | -0.205098 | -1.935920 |
| H | -0.907099 | -0.889129 | 2.016659 |
| C | 1.759142 | -1.247343 | -0.962555 |
| H | 1.686625 | -2.164211 | -0.378284 |
| H | 1.035239 | -1.292092 | -1.775554 |
| H | 2.757148 | -1.218072 | -1.402775 |
| C | 2.640137 | -0.016198 | 1.007370 |
| H | 3.634720 | -0.082039 | 0.562978 |
| H | 2.584655 | 0.894791 | 1.604207 |
| H | 2.516755 | -0.870670 | 1.673672 |
| C | 1.820037 | 1.225085 | -0.971605 |
| H | 1.826530 | 2.148013 | -0.395306 |
| H | 2.800908 | 1.114151 | -1.434791 |
| H | 1.079546 | 1.314325 | -1.766721 |
| N | 0.242595 | 0.097034 | 0.599676 |

eq

```

=====
C  -0.720006    0.813089   -0.151559
C  -0.902750    1.666498    1.088210
C  -0.290284    2.246153   -0.163937
C  -0.458170   -1.382639    0.668805
C  -1.787779   -1.826722    0.058932
H  -2.246229   -2.581502    0.700744
H  -1.576859   -2.298680   -0.904566
C  -2.022585    0.493115   -0.866185
C  -2.737078   -0.649377   -0.145281
H  -3.624645   -0.961786   -0.697711
H  -3.075817   -0.288810    0.830297
C   1.632579   -0.208880   -0.101657
H  -0.232740    1.497740    1.918494
H  -1.908060    1.958570    1.359020
H  -0.890776    2.917430   -0.762933
H   0.751552    2.510379   -0.116626
H   0.192759   -2.247151    0.733951
H  -2.656365    1.380942   -0.891596
H  -1.800133    0.209764   -1.898514
H  -0.626280   -1.016282    1.693061
C   2.149312    0.490552    1.168293
H   1.916416    1.552727    1.198918
H   1.727094    0.018578    2.057643
H   3.234998    0.391322    1.223562
C   2.121542    0.502233   -1.370767
H   3.199222    0.661741   -1.309915
H   1.918712   -0.127025   -2.239229
H   1.648021    1.463694   -1.538716
C   2.277985   -1.603393   -0.136224
H   1.820327   -2.225737   -0.906705
H   3.336014   -1.489645   -0.372751
H   2.212964   -2.120229    0.820342
N   0.157603   -0.349973   -0.169794
=====

```



4-(*tert*-butyl)-4λ⁴-azaspiro[2.5]octane

| Conformation | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| ax2 | -486.933348 | -486.59698 | -486.645817 |
| ax | -486.934942 | -486.599028 | -486.647865 |
| eq | -486.930527 | -486.594672 | -486.643616 |

ax2

```

=====
C  0.891502      0.816948      0.030892
C  1.700060      1.664490     -0.904793
C  0.801622      2.304781      0.121554
C  0.347230     -1.208583     -1.206626
C  1.026595     -2.065300     -0.157322
H  1.399949     -2.956314     -0.662035
H  0.303758     -2.398614      0.588656
C  1.662598      0.026662      1.068315
C  2.170432     -1.294496      0.494410
H  2.634163     -1.887686      1.281353
H  2.934919     -1.091955     -0.259753
C -1.593456     -0.025859      0.124511
H  1.378011      1.729582     -1.934980
H  2.768514      1.670164     -0.749635
H  1.244910      2.755688      0.997268
H -0.075503      2.799993     -0.261723
H -0.444461     -1.727006     -1.731489
H  2.498623      0.653254      1.378888
H  1.061214     -0.159341      1.954231
H  1.078403     -0.871620     -1.940660
C -1.427188     -0.201220      1.626250
H -0.928739     -1.130165      1.892038
H -0.902336      0.640815      2.073454
H -2.431297     -0.227769      2.049673
C -2.396539     -1.183964     -0.456833
H -3.382231     -1.159981      0.004863
H -2.527505     -1.082579     -1.534662
H -1.946114     -2.150175     -0.234698
C -2.341497      1.281147     -0.143032
H -2.370754      1.517137     -1.208211
H -3.367258      1.157146      0.200801
H -1.910117      2.116918      0.400904
N -0.227907      0.070571     -0.632525
H -0.468958      0.620876     -1.460573

```

ax

```

=====
C -0.901963      0.807692     -0.054840
C -1.806965      1.546430      0.885244
C -0.897513      2.298615     -0.048530
C -0.286898     -1.195280      1.202340
C -1.072570     -2.053178      0.216210
H -1.530178     -2.847548      0.806702
H -0.405675     -2.535436     -0.492677
C -1.552492     -0.000567     -1.147518
C -2.144985     -1.270127     -0.538262
H -2.582765     -1.899324     -1.312136
H -2.946716     -0.987241      0.147369
C  1.605074      0.005036     -0.123695
H -1.549525      1.557289      1.935486

```

| | | | |
|---|-----------|-----------|-----------|
| H | -2.863782 | 1.500966 | 0.667408 |
| H | -1.319393 | 2.784329 | -0.916272 |
| H | -0.059146 | 2.805221 | 0.404788 |
| H | 0.561930 | -1.731105 | 1.616394 |
| H | -2.331098 | 0.614425 | -1.597954 |
| H | -0.832654 | -0.239707 | -1.932104 |
| H | -0.932972 | -0.886809 | 2.022367 |
| C | 1.753419 | -1.282036 | -0.925786 |
| H | 1.708172 | -2.168608 | -0.296783 |
| H | 1.024512 | -1.363127 | -1.728651 |
| H | 2.744305 | -1.252708 | -1.377896 |
| C | 2.657495 | 0.039298 | 0.982138 |
| H | 3.643387 | -0.022385 | 0.524336 |
| H | 2.602140 | 0.972561 | 1.544949 |
| H | 2.553647 | -0.799132 | 1.670475 |
| C | 1.789393 | 1.204991 | -1.043740 |
| H | 1.792191 | 2.143818 | -0.494907 |
| H | 2.762352 | 1.094659 | -1.521206 |
| H | 1.031546 | 1.244206 | -1.824553 |
| N | 0.232305 | 0.103634 | 0.615048 |
| H | 0.451626 | 0.684966 | 1.428165 |

eq

```
=====
```

| | | | |
|---|-----------|-----------|-----------|
| C | 0.754936 | 0.849009 | 0.168061 |
| C | 0.886633 | 1.640912 | -1.091727 |
| C | 0.312350 | 2.274920 | 0.150816 |
| C | 0.468141 | -1.405240 | -0.663458 |
| C | 1.811081 | -1.816638 | -0.075810 |
| H | 2.246216 | -2.568227 | -0.733628 |
| H | 1.626474 | -2.299080 | 0.888265 |
| C | 2.053693 | 0.493109 | 0.862890 |
| C | 2.756351 | -0.634511 | 0.109272 |
| H | 3.651011 | -0.949960 | 0.644828 |
| H | 3.072576 | -0.264019 | -0.868238 |
| C | -1.697903 | -0.196161 | 0.085148 |
| H | 0.199514 | 1.454295 | -1.901951 |
| H | 1.895168 | 1.887262 | -1.391160 |
| H | 0.928517 | 2.954409 | 0.721943 |
| H | -0.731137 | 2.532045 | 0.119147 |
| H | -0.193810 | -2.259639 | -0.705112 |
| H | 2.676475 | 1.385679 | 0.895629 |
| H | 1.848868 | 0.197791 | 1.896227 |
| H | 0.562733 | -0.968784 | -1.655042 |
| C | -2.096855 | 0.482390 | -1.217022 |
| H | -1.882154 | 1.547189 | -1.235513 |
| H | -1.624829 | 0.000553 | -2.073277 |
| H | -3.174860 | 0.363470 | -1.324313 |
| C | -2.186620 | 0.547169 | 1.326978 |
| H | -3.263236 | 0.683853 | 1.236079 |
| H | -1.997742 | -0.051268 | 2.220082 |
| H | -1.732142 | 1.521719 | 1.463202 |
| C | -2.305246 | -1.600837 | 0.124701 |
| H | -1.857304 | -2.208101 | 0.912744 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.365860 | -1.491686 | 0.345492 |
| H | -2.216845 | -2.119730 | -0.827242 |
| N | -0.162486 | -0.349391 | 0.216871 |
| H | -0.069607 | -0.706771 | 1.174639 |

Butane Model Conformations

| Dihed. Angle | Electronic Energy | Enthalpy | Gibbs Free Energy |
|--------------|-------------------|-------------|-------------------|
| 34 | -158.413077 | -158.273797 | -158.307667 |
| 38 | -158.413778 | -158.274573 | -158.308345 |
| 47 | -158.415067 | -158.275868 | -158.309478 |
| 56 | -158.415735 | -158.276558 | -158.310369 |
| 64 | -158.415821 | -158.276732 | -158.310776 |
| 77 | -158.415239 | -158.27623 | -158.310808 |

34

| | | | |
|---|-----------|-----------|-----------|
| C | -0.411909 | -0.649415 | 0.700226 |
| C | 0.411909 | 0.649415 | 0.700226 |
| H | 0.054500 | 1.300347 | 1.499617 |
| C | 0.411909 | 1.405967 | -0.625203 |
| H | 0.880168 | 0.822269 | -1.417264 |
| H | -0.603193 | 1.650174 | -0.946659 |
| H | 0.963725 | 2.341898 | -0.531818 |
| C | -0.411909 | -1.405967 | -0.625203 |
| H | 0.603193 | -1.650174 | -0.946659 |
| H | -0.963725 | -2.341898 | -0.531818 |
| H | -0.880168 | -0.822269 | -1.417264 |
| H | -1.449558 | -0.406666 | 0.945987 |
| H | -0.054500 | -1.300347 | 1.499617 |
| H | 1.449558 | 0.406666 | 0.945987 |

38

| | | | |
|---|-----------|-----------|-----------|
| C | -0.446282 | -0.624885 | 0.693830 |
| C | 0.446282 | 0.624885 | 0.693830 |
| H | 0.144865 | 1.279131 | 1.513565 |
| C | 0.446282 | 1.402783 | -0.619169 |
| H | 0.871478 | 0.813739 | -1.431327 |
| H | -0.566060 | 1.691417 | -0.911299 |
| H | 1.037302 | 2.314365 | -0.525959 |
| C | -0.446282 | -1.402783 | -0.619169 |
| H | 0.566060 | -1.691417 | -0.911299 |
| H | -1.037302 | -2.314365 | -0.525959 |
| H | -0.871478 | -0.813739 | -1.431327 |
| H | -1.475157 | -0.321563 | 0.907053 |
| H | -0.144865 | -1.279131 | 1.513565 |
| H | 1.475157 | 0.321563 | 0.907053 |

47

```
=====  
C -0.510934 -0.570467 0.675844  
C 0.510934 0.570467 0.675844  
H 0.324110 1.215309 1.536690  
C 0.510934 1.403639 -0.602565  
H 0.838945 0.817906 -1.461112  
H -0.488152 1.787207 -0.822892  
H 1.182319 2.257732 -0.509216  
C -0.510934 -1.403639 -0.602565  
H 0.488152 -1.787207 -0.822892  
H -1.182319 -2.257732 -0.509216  
H -0.838945 -0.817906 -1.461112  
H -1.510541 -0.149263 0.816857  
H -0.324110 -1.215309 1.536690  
H 1.510541 0.149263 0.816857
```

56

```
=====  
C -0.559751 -0.520833 0.652540  
C 0.559751 0.520833 0.652540  
H 0.471316 1.137005 1.549825  
C 0.559751 1.417231 -0.581689  
H 0.790050 0.853414 -1.485941  
H -0.415989 1.887919 -0.721987  
H 1.302668 2.210145 -0.489755  
C -0.559751 -1.417231 -0.581689  
H 0.415989 -1.887919 -0.721987  
H -1.302668 -2.210145 -0.489755  
H -0.790050 -0.853414 -1.485941  
H -1.522989 -0.007540 0.722752  
H -0.471316 -1.137005 1.549825  
H 1.522989 0.007540 0.722752
```

64

```
=====  
C -0.591740 -0.483739 0.627569  
C 0.591740 0.483739 0.627569  
H 0.576793 1.062673 1.553634  
C 0.591740 1.442094 -0.559848  
H 0.710651 0.911604 -1.505058  
H -0.346089 1.999931 -0.606202  
H 1.405880 2.163505 -0.483211  
C -0.591740 -1.442094 -0.559848  
H 0.346089 -1.999931 -0.606202  
H -1.405880 -2.163505 -0.483211  
H -0.710651 -0.911604 -1.505058  
H -1.522493 0.090540 0.634509  
H -0.576793 -1.062673 1.553634  
H 1.522493 -0.090540 0.634509
```

```
=====
C  -0.632720    -0.430231     0.581394
C   0.632720     0.430231     0.581394
H   0.729649     0.930587     1.547325
C   0.632720     1.488239    -0.518518
H   0.545898     1.037460    -1.508405
H  -0.207382     2.173098    -0.389742
H   1.550262     2.077445    -0.503839
C  -0.632720    -1.488239    -0.518518
H   0.207382    -2.173098    -0.389742
H  -1.550262    -2.077445    -0.503839
H  -0.545898    -1.037460    -1.508405
H  -1.507512     0.217336     0.477403
H  -0.729649    -0.930587     1.547325
H   1.507512    -0.217336     0.477403
```