

Supporting Information

DFT Mechanistic Study of Functionalizations of ω -Ene-Cyclopropanes and Alkylidenecyclopropanes via Allylic C–H and C–C Bond Cleavage Facilitated by a Zirconocene Complex

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1. Mechanism of eq 1 reaction

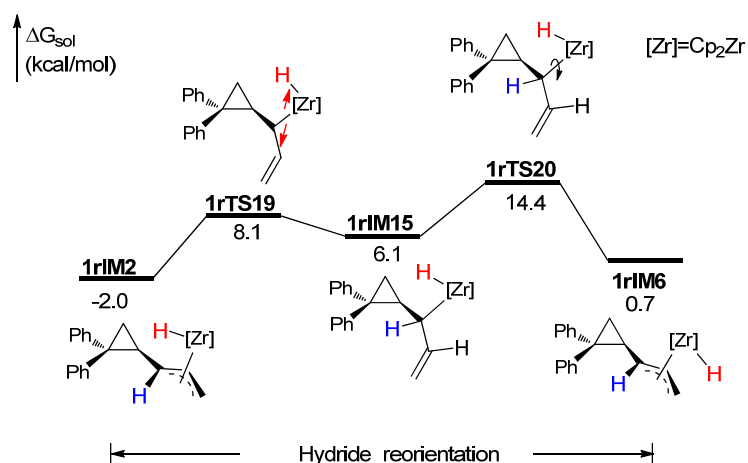


Figure S1. Free energy profile for hydride transfer (stage II) by the pathway of rotation around Zr-C⁴ single bond.

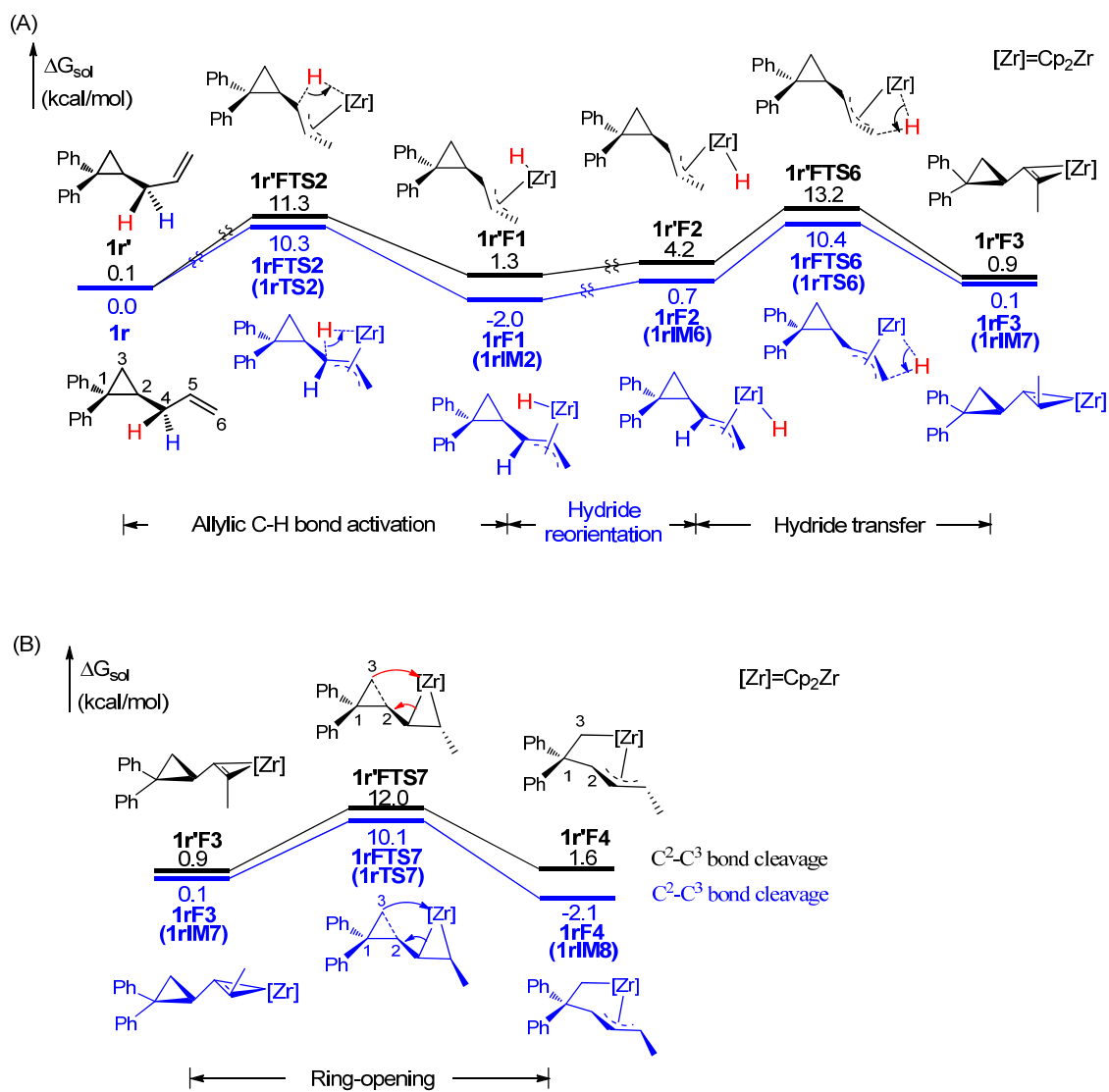


Figure S2. Free energy profile for energetic comparisons of the front side attacking mode of [Zr]C₄H₈ to the C⁵=C⁶ double bond of **1r** and **1r'**.

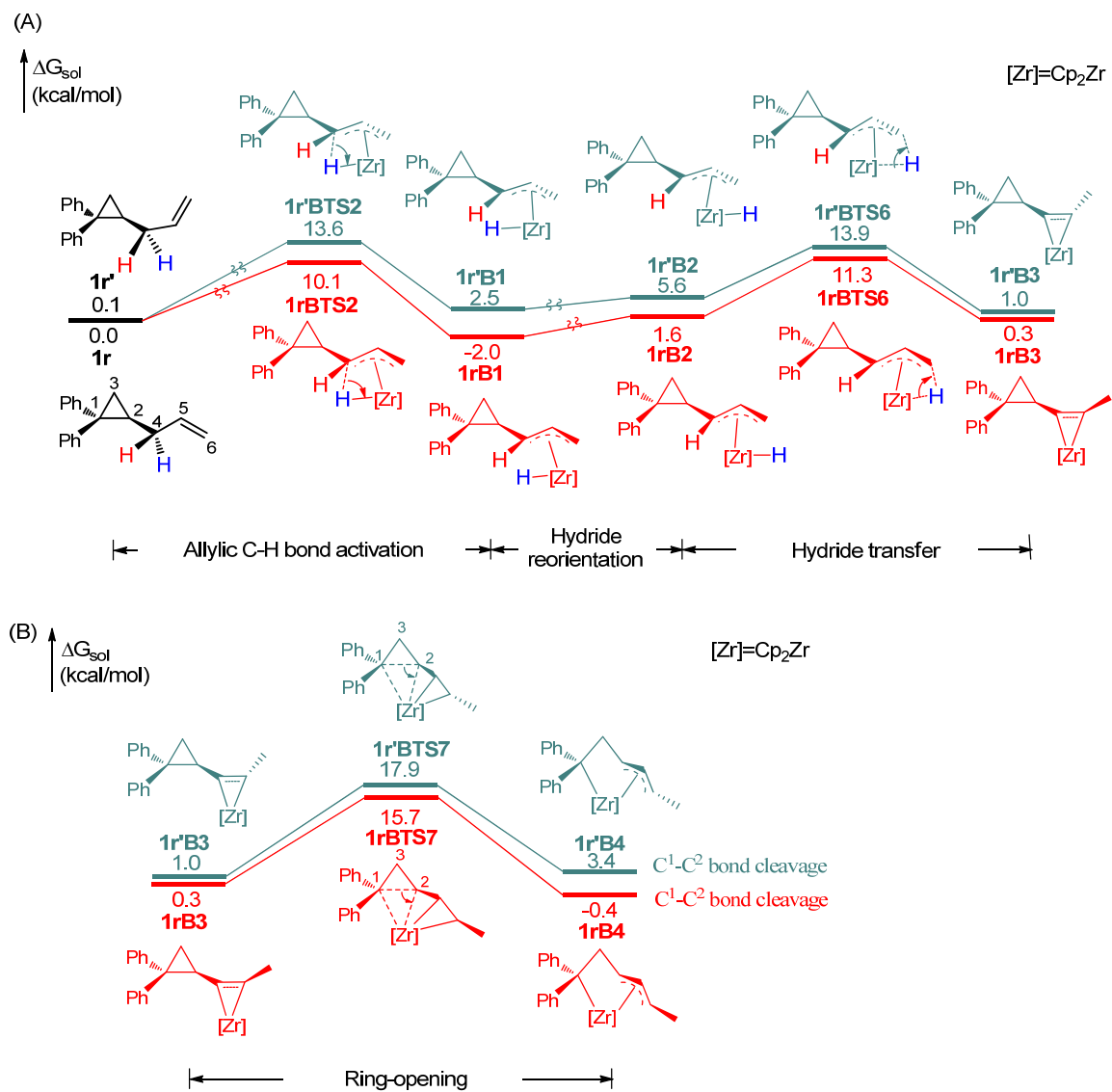


Figure S3. Free energy profile for energetic comparisons of the back side attacking mode of [Zr]C₄H₈ to the C⁵=C⁶ double bond of **1r** and **1r'**.

2. Mechanism for the reaction eq 2

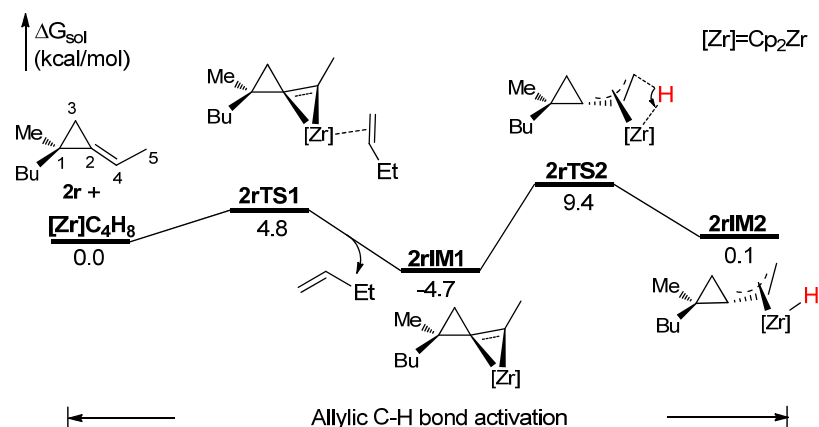


Figure S4. Free energy profile for the allylic C-H bond activation (stage I) of **2r**.

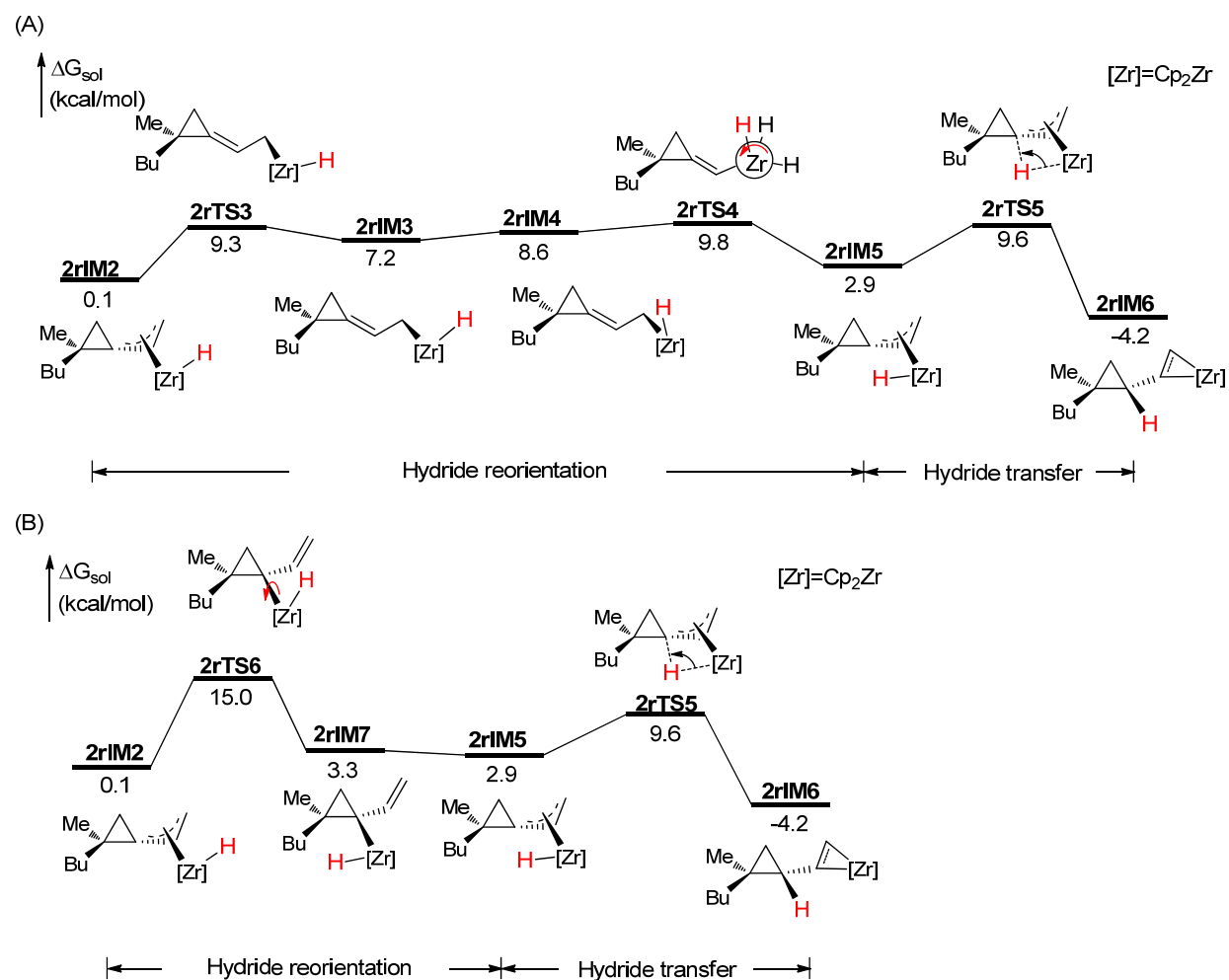


Figure S5. (A) Free energy profile for hydride transfer (stage II) by the pathway of rotation around Zr-C⁵ single bond. (B) Free energy profile for hydride transfer by the pathway of rotation around Zr-C² single bond.

From **2rIM2** to **2rIM5** in Figure S5, the Zr–C⁵ bond is formed for turning the hydride towards C⁵. We examined an alternative via forming Zr–C² single bond. Expectedly, the energetic results indicate that the alternative is less favorable due to the more significant steric hindrance between [Zr] and 3-membered ring which is in accordance with **1r**(see Figure 2 and Figure S1).

3. Energetic results for ring-opening and electrophilic addition of HCl to **4r**

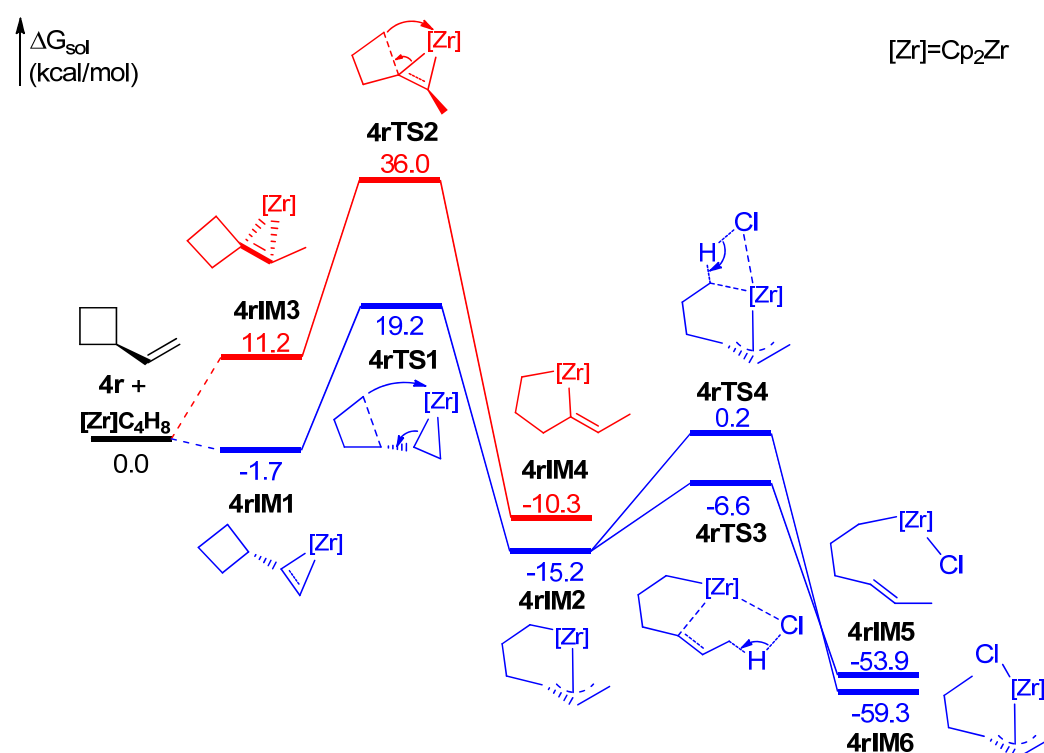


Figure S6. Free energy profile for ring-opening and electrophilic addition of HCl to **4rIM2**.

4. Energies and Cartesian Coordinates of All the Structures

All energies are given in Hartree.

1r

SCF energy in gas phase: -696.718236

Free energy in Et₂O : -696.078521

Enthalpy in Et₂O : -696.016467

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.010667 | -0.278354 | 0.475769 | C | -0.459242 | 1.665574 | -1.158445 |
| C | -0.385143 | 1.141498 | 0.134215 | C | -1.033157 | 1.886503 | 1.168948 |
| C | -0.363800 | 1.564382 | -1.204943 | C | -0.885563 | 2.971659 | -1.391257 |
| C | -0.741254 | 2.073781 | 1.117090 | H | -0.057366 | 1.075091 | -1.977312 |
| C | -0.700520 | 2.871633 | -1.550516 | C | -1.458845 | 3.197571 | 0.939794 |
| H | -0.072650 | 0.859757 | -1.979040 | H | -1.086483 | 1.473609 | 2.171915 |
| C | -1.077430 | 3.386147 | 0.774553 | C | -1.389494 | 3.744001 | -0.341220 |
| H | -0.750571 | 1.774272 | 2.160905 | H | -0.823744 | 3.388580 | -2.392763 |
| C | -1.060856 | 3.789409 | -0.560152 | H | -1.842233 | 3.790643 | 1.765609 |
| H | -0.681010 | 3.175567 | -2.593516 | H | -1.721497 | 4.762473 | -0.521324 |
| H | -1.349227 | 4.092528 | 1.554201 | C | 1.449952 | -0.473333 | 0.140330 |
| H | -1.323106 | 4.808951 | -0.827876 | C | 1.978846 | -1.074702 | -1.008575 |
| C | 1.462701 | -0.588768 | 0.178767 | C | 2.341700 | 0.026104 | 1.101763 |
| C | 1.843057 | -1.336886 | -0.942378 | C | 3.360037 | -1.180975 | -1.191410 |
| C | 2.468652 | -0.090281 | 1.020390 | H | 1.305543 | -1.465764 | -1.766409 |
| C | 3.190541 | -1.586546 | -1.214577 | C | 3.720053 | -0.078855 | 0.923628 |
| H | 1.078629 | -1.730876 | -1.606360 | H | 1.945050 | 0.501192 | 1.995138 |
| C | 3.814002 | -0.338388 | 0.753130 | C | 4.235140 | -0.684332 | -0.225760 |
| H | 2.188117 | 0.496794 | 1.890936 | H | 3.749677 | -1.652606 | -2.089432 |
| C | 4.180288 | -1.089113 | -0.367220 | H | 4.393661 | 0.310722 | 1.682030 |
| H | 3.464303 | -2.171029 | -2.088715 | H | 5.309156 | -0.768001 | -0.365410 |
| H | 4.577881 | 0.052821 | 1.419560 | C | -0.689185 | -1.169932 | 1.420940 |
| H | 5.228318 | -1.284585 | -0.575644 | C | -0.938360 | -1.489379 | -0.033179 |
| C | -0.612063 | -0.954774 | 1.683397 | H | -0.409060 | -2.359501 | -0.415806 |
| C | -1.003071 | -1.403397 | 0.296307 | C | -2.307211 | -1.282720 | -0.647741 |
| H | -0.578794 | -2.354315 | -0.019109 | H | -2.757951 | -0.363973 | -0.248259 |
| C | -2.409496 | -1.158549 | -0.231730 | H | -2.201018 | -1.091902 | -1.726773 |
| H | -2.397907 | -1.110540 | -1.328212 | C | -3.277576 | -2.422883 | -0.457836 |
| C | -3.374988 | -2.223622 | 0.218082 | H | -4.235430 | -2.292554 | -0.963252 |
| H | -3.474211 | -2.345526 | 1.297470 | C | -3.075021 | -3.535057 | 0.249564 |
| C | -4.082888 | -3.010360 | -0.592715 | H | -2.146126 | -3.721369 | 0.780181 |
| H | -4.010240 | -2.926126 | -1.674922 | H | -3.841439 | -4.300673 | 0.325798 |
| H | -4.763907 | -3.764106 | -0.208307 | H | -0.045937 | -1.828806 | 1.996444 |
| H | 0.020044 | -1.604089 | 2.281379 | H | -1.518114 | -0.750112 | 1.983609 |
| H | -1.350704 | -0.399995 | 2.255692 | | | | |
| H | -2.755359 | -0.176377 | 0.116744 | | | | |

Cp₂ZrC₄H₈

SCF energy in gas phase: -590.938822

Free energy in Et₂O : -590.862687

Enthalpy in Et₂O : -590.802287

1r'

SCF energy in gas phase: -696.717298

Free energy in Et₂O : -696.078439

Enthalpy in Et₂O : -696.016662

| | | | | | | | |
|---|-----------|-----------|----------|----|-----------|----------|-----------|
| C | -0.041911 | -0.315670 | 0.346981 | Zr | -0.300118 | 0.099837 | -0.153133 |
| C | -0.532943 | 1.098585 | 0.124478 | C | 0.128985 | 2.539488 | -0.968792 |
| | | | | H | -0.206986 | 2.837620 | -1.954391 |
| | | | | C | 1.401393 | 2.005192 | -0.652765 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 2.203255 | 1.826972 | -1.355105 | C | -3.478098 | 1.582064 | 1.967064 |
| C | 1.439962 | 1.737824 | 0.742121 | H | -3.552123 | 2.645722 | 1.788289 |
| H | 2.286129 | 1.350498 | 1.291483 | C | -1.232971 | 1.850148 | -1.266154 |
| C | 0.175897 | 2.106127 | 1.289165 | H | -0.305007 | 2.258088 | -0.893615 |
| H | -0.105577 | 2.058059 | 2.333328 | C | -1.368201 | 0.731468 | -2.138843 |
| C | -0.631978 | 2.605279 | 0.228339 | H | -0.563169 | 0.120188 | -2.520679 |
| H | -1.642084 | 2.982075 | 0.320827 | C | -2.738237 | 0.563453 | -2.432756 |
| C | -2.806759 | -0.091058 | 0.133242 | H | -3.151268 | -0.202424 | -3.075201 |
| H | -3.404625 | 0.798845 | -0.013429 | C | -3.473785 | 1.558016 | -1.736133 |
| C | -2.510971 | -1.074263 | -0.852084 | H | -4.544623 | 1.706277 | -1.774183 |
| H | -2.814556 | -1.048635 | -1.890974 | C | -2.536351 | 2.363447 | -1.026743 |
| C | -1.741587 | -2.091090 | -0.237803 | H | -2.773015 | 3.238761 | -0.437892 |
| H | -1.338602 | -2.964065 | -0.732852 | C | -7.046614 | -0.641804 | -0.984908 |
| C | -1.559632 | -1.754098 | 1.127073 | H | -7.208252 | -0.573520 | -2.066584 |
| H | -1.021585 | -2.341494 | 1.859511 | H | -6.550672 | 0.279895 | -0.667056 |
| C | -2.217026 | -0.512695 | 1.361500 | H | -8.029066 | -0.681540 | -0.504937 |
| H | -2.295276 | -0.001324 | 2.311985 | C | -6.210513 | -1.879324 | -0.634162 |
| C | 3.259990 | -1.549397 | 1.254477 | H | -6.110135 | -1.986094 | 0.451416 |
| H | 2.988706 | -2.582423 | 1.502277 | H | -6.758758 | -2.772134 | -0.971468 |
| H | 2.726352 | -0.897629 | 1.956421 | C | -4.854443 | -1.907747 | -1.292854 |
| H | 4.334686 | -1.437727 | 1.436965 | H | -4.819503 | -1.466963 | -2.288769 |
| C | 2.894188 | -1.222768 | -0.198231 | C | -3.755429 | -2.532778 | -0.834062 |
| H | 3.211823 | -0.198887 | -0.434219 | H | -3.743944 | -3.045355 | 0.123396 |
| H | 3.494233 | -1.872021 | -0.857480 | H | -2.865748 | -2.633380 | -1.442770 |
| C | 1.415802 | -1.415635 | -0.516954 | C | 3.676154 | -0.286695 | 0.545911 |
| H | 1.092190 | -2.419171 | -0.227888 | C | 3.943415 | 1.139177 | 0.117035 |
| C | 0.864364 | -0.960183 | -1.807359 | C | 3.981479 | 1.457337 | -1.250460 |
| H | 1.516578 | -0.342497 | -2.425626 | C | 4.194761 | 2.162345 | 1.040246 |
| H | 0.304294 | -1.678004 | -2.407071 | C | 4.246247 | 2.756641 | -1.679337 |

1rTS1

SCF energy in gas phase: -1287.658156

Free energy in Et₂O : -1286.924841

Enthalpy in Et₂O : -1286.824041

| | | | | | | | |
|----|-----------|-----------|----------|---|----------|-----------|-----------|
| Zr | -2.467491 | 0.133922 | 0.148765 | H | 3.807432 | 0.672528 | -1.981444 |
| C | -2.387312 | 0.916144 | 2.585975 | C | 4.462644 | 3.466067 | 0.614466 |
| H | -1.476882 | 1.376213 | 2.943303 | H | 4.184716 | 1.936964 | 2.102569 |
| C | -2.725860 | -0.463604 | 2.682785 | C | 4.486646 | 3.769204 | -0.746487 |
| H | -2.101337 | -1.243591 | 3.096348 | H | 4.266164 | 2.980026 | -2.742615 |
| C | -4.011334 | -0.642906 | 2.129457 | H | 4.655690 | 4.242980 | 1.349437 |
| H | -4.537988 | -1.584957 | 2.058175 | H | 4.693735 | 4.782420 | -1.079094 |
| C | -4.482076 | 0.615921 | 1.668440 | C | 4.774729 | -1.249153 | 0.146024 |
| H | -5.450612 | 0.816875 | 1.232432 | C | 4.612916 | -2.159461 | -0.905934 |
| | | | | C | 6.007862 | -1.219428 | 0.815626 |
| | | | | C | 5.649222 | -3.020048 | -1.277184 |
| | | | | H | 3.665648 | -2.197207 | -1.436453 |
| | | | | C | 7.043801 | -2.077084 | 0.449710 |
| | | | | H | 6.150473 | -0.514382 | 1.630394 |
| | | | | C | 6.867927 | -2.982724 | -0.600108 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 5.501504 | -3.719476 | -2.095695 | H | 2.997811 | -2.641599 | -2.075752 |
| H | 7.989236 | -2.040645 | 0.984295 | C | 4.734992 | -1.976570 | -0.851078 |
| H | 7.673957 | -3.652833 | -0.885528 | H | 4.978116 | -2.865227 | -0.282242 |
| C | 2.966133 | -0.548212 | 1.863710 | C | 5.393370 | -0.718534 | -0.763532 |
| C | 2.242382 | -0.808246 | 0.566705 | H | 6.250532 | -0.489098 | -0.144168 |
| H | 2.134002 | -1.857985 | 0.300966 | C | 4.755235 | 0.172758 | -1.675896 |
| C | 1.048094 | 0.045162 | 0.154329 | H | 5.048043 | 1.195766 | -1.873470 |
| H | 0.998436 | 0.069235 | -0.941189 | C | 2.060928 | 1.796872 | 1.306891 |
| C | -0.251008 | -0.489447 | 0.741934 | H | 1.170710 | 2.240618 | 0.883153 |
| H | -0.190770 | -0.508988 | 1.829809 | C | 2.096484 | 0.806854 | 2.326310 |
| C | -0.928499 | -1.629593 | 0.153996 | H | 1.238285 | 0.346765 | 2.794874 |
| H | -0.595072 | -1.956063 | -0.832862 | C | 3.450794 | 0.523754 | 2.626273 |
| H | -1.206573 | -2.469991 | 0.790464 | H | 3.802427 | -0.193950 | 3.357402 |
| H | 3.300462 | -1.393924 | 2.457301 | C | 4.266204 | 1.334157 | 1.792944 |
| H | 2.645077 | 0.309403 | 2.449274 | H | 5.347923 | 1.360781 | 1.792375 |
| H | 1.225541 | 1.078953 | 0.475788 | C | 3.408205 | 2.121729 | 0.973271 |
| butene | | | | H | 3.725334 | 2.867138 | 0.255073 |
| SCF energy in gas phase: -157.229536 | | | | C | -2.972637 | -0.341831 | -0.555337 |
| Free energy in Et ₂ O : -157.04771 | | | | C | -3.118645 | 1.163919 | -0.581415 |
| Enthalpy in Et ₂ O : -157.013997 | | | | C | -3.170099 | 1.879070 | 0.626457 |
| C | -1.730031 | -0.245337 | -0.294362 | C | -3.241861 | 1.880689 | -1.778651 |
| H | -1.930894 | -1.167543 | 0.262419 | C | -3.323597 | 3.264305 | 0.635665 |
| H | -1.530632 | -0.522869 | -1.334307 | H | -3.094458 | 1.337970 | 1.565678 |
| H | -2.640722 | 0.362049 | -0.272250 | C | -3.398471 | 3.269271 | -1.773835 |
| C | -0.539705 | 0.519796 | 0.308565 | H | -3.218516 | 1.347462 | -2.724397 |
| H | -0.365212 | 1.444105 | -0.255226 | C | -3.436680 | 3.967056 | -0.567103 |
| H | -0.798313 | 0.822928 | 1.333540 | H | -3.356714 | 3.796935 | 1.582309 |
| C | 0.723489 | -0.297368 | 0.338633 | H | -3.493282 | 3.803140 | -2.715653 |
| H | 0.672773 | -1.225894 | 0.910541 | H | -3.557084 | 5.046689 | -0.561417 |
| C | 1.861953 | 0.018592 | -0.279142 | C | -4.173532 | -1.050198 | 0.034878 |
| H | 1.958625 | 0.931313 | -0.863208 | C | -4.146943 | -1.597715 | 1.323831 |
| H | 2.740138 | -0.618189 | -0.223676 | C | -5.365459 | -1.137929 | -0.700720 |
| 1rIM1 | | | | C | -5.275950 | -2.219106 | 1.863614 |
| SCF energy in gas phase: -1130.428523 | | | | H | -3.232983 | -1.540131 | 1.908360 |
| Free energy in Et ₂ O : -1129.895804 | | | | C | -6.493550 | -1.758725 | -0.166908 |
| Enthalpy in Et ₂ O : -1129.806616 | | | | H | -5.402563 | -0.712724 | -1.700278 |
| Zr | 3.083985 | -0.237653 | 0.159408 | C | -6.452811 | -2.302582 | 1.119844 |
| C | 3.705245 | -0.540923 | -2.321823 | H | -5.233303 | -2.638148 | 2.865369 |
| H | 3.037563 | -0.150513 | -3.078528 | H | -7.405520 | -1.819643 | -0.754712 |
| C | 3.696324 | -1.861505 | -1.805404 | H | -7.330970 | -2.787527 | 1.536811 |
| | | | | C | -2.236340 | -1.035836 | -1.688862 |
| | | | | C | -1.595089 | -0.956393 | -0.326345 |
| | | | | H | -1.598748 | -1.886112 | 0.239451 |
| | | | | C | -0.347943 | -0.112181 | -0.095293 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -0.341238 | 0.217343 | 0.951598 | H | -0.786281 | -2.657192 | -1.120541 |
| C | 0.936845 | -0.870688 | -0.416545 | C | -2.014301 | -1.332201 | -2.294148 |
| H | 0.921378 | -1.235062 | -1.446292 | H | -1.963372 | -0.492707 | -2.985297 |
| C | 1.491485 | -1.833483 | 0.554935 | H | -2.562416 | -2.181288 | -2.690816 |
| H | 1.039497 | -1.843310 | 1.547507 | H | 2.071114 | -2.149458 | 1.657450 |
| H | 1.725665 | -2.840606 | 0.210271 | H | 0.834436 | -0.816677 | 1.880620 |
| H | -2.622684 | -1.991424 | -2.030924 | H | -0.526704 | -0.067715 | 0.315534 |
| H | -1.813072 | -0.417822 | -2.476688 | Zr | -2.372850 | -0.305308 | -0.175942 |
| H | -0.420571 | 0.801001 | -0.699047 | C | -2.487620 | -1.356801 | 2.132309 |

1rTS2(1rFTS2)

SCF energy in gas phase: -1130.413777

Free energy in Et₂O : -1129.877046

Enthalpy in Et₂O : -1129.791281

| | | | |
|---|-----------|-----------|-----------|
| C | 2.392772 | -0.377101 | 0.333936 |
| C | 2.186449 | 1.120575 | 0.388939 |
| C | 2.371380 | 1.889548 | -0.771632 |
| C | 1.857733 | 1.783889 | 1.578054 |
| C | 2.215708 | 3.275222 | -0.747850 |
| H | 2.652443 | 1.394922 | -1.697529 |
| C | 1.705175 | 3.172508 | 1.607166 |
| H | 1.723311 | 1.210875 | 2.490484 |
| C | 1.879486 | 3.923213 | 0.443590 |
| H | 2.360591 | 3.849985 | -1.658371 |
| H | 1.454242 | 3.666629 | 2.541784 |
| H | 1.760193 | 5.002584 | 0.464798 |
| C | 3.828484 | -0.776750 | 0.063340 |
| C | 4.251049 | -1.207118 | -1.200580 |
| C | 4.780278 | -0.684041 | 1.089923 |
| C | 5.587886 | -1.539813 | -1.433703 |
| H | 3.528820 | -1.286748 | -2.008467 |
| C | 6.114559 | -1.016285 | 0.861344 |
| H | 4.466424 | -0.347733 | 2.074642 |
| C | 6.523676 | -1.446227 | -0.403739 |
| H | 5.895409 | -1.873271 | -2.421026 |
| H | 6.835768 | -0.941445 | 1.670596 |
| H | 7.562770 | -1.707194 | -0.582932 |
| C | 1.578949 | -1.276970 | 1.238118 |
| C | 1.293488 | -1.262441 | -0.246784 |
| H | 1.660494 | -2.127817 | -0.792296 |
| C | 0.018845 | -0.694620 | -0.851166 |
| H | 0.184915 | 0.227605 | -1.415229 |
| C | -0.866727 | -1.636357 | -1.488376 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.829078 | -0.993745 | 2.908949 |
| C | -2.227869 | -2.440737 | 1.247524 |
| H | -1.321962 | -3.030818 | 1.223020 |
| C | -3.373612 | -2.630273 | 0.426803 |
| H | -3.483640 | -3.370387 | -0.353760 |
| C | -4.335562 | -1.660468 | 0.789376 |
| H | -5.313399 | -1.539039 | 0.341496 |
| C | -3.792234 | -0.872888 | 1.843700 |
| H | -4.295077 | -0.061731 | 2.351948 |
| C | -1.893332 | 2.246012 | -0.188879 |
| H | -0.959021 | 2.605884 | 0.219993 |
| C | -2.126710 | 1.865442 | -1.538293 |
| H | -1.402403 | 1.908298 | -2.340934 |
| C | -3.489879 | 1.471027 | -1.664426 |
| H | -3.982319 | 1.149350 | -2.571277 |
| C | -4.089259 | 1.593943 | -0.388107 |
| H | -5.121381 | 1.373517 | -0.147979 |
| C | -3.101878 | 2.069067 | 0.524549 |
| H | -3.251487 | 2.271501 | 1.576908 |

1rIM2 (1rF1)

SCF energy in gas phase: -1130.435698

Free energy in Et₂O : -1129.896695

Enthalpy in Et₂O : -1129.80866

| | | | |
|---|-----------|-----------|-----------|
| C | -2.556868 | -0.128709 | -0.495989 |
| C | -2.826194 | 1.300637 | -0.083475 |
| C | -3.033166 | 1.612310 | 1.269787 |
| C | -2.914741 | 2.335304 | -1.023739 |
| C | -3.311846 | 2.917887 | 1.670138 |
| H | -2.975353 | 0.820810 | 2.011341 |
| C | -3.195618 | 3.645175 | -0.626281 |
| H | -2.767380 | 2.113976 | -2.076861 |
| C | -3.393771 | 3.941442 | 0.722076 |
| H | -3.464834 | 3.137726 | 2.723185 |

| | | | | | | | |
|----|----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 3.924582 | -0.177039 | -1.446939 | H | 2.602774 | 1.581461 | 0.205734 |
| Zr | 2.683963 | -0.211074 | -0.127915 | C | 3.488377 | -2.148427 | -0.200058 |
| C | 2.527978 | -2.503383 | -1.336792 | H | 1.432532 | -2.576995 | 0.129275 |
| H | 2.048890 | -2.559410 | -2.306469 | C | 4.495855 | -1.190199 | -0.347481 |
| C | 1.916452 | -2.800474 | -0.073708 | H | 4.887378 | 0.933883 | -0.286119 |
| H | 0.876894 | -3.057465 | 0.066341 | H | 3.728470 | -3.206644 | -0.303601 |
| C | 2.893541 | -2.698382 | 0.921983 | H | 5.522884 | -1.476579 | -0.558516 |
| H | 2.748618 | -2.844258 | 1.982460 | C | -0.455887 | -1.139916 | 1.197452 |
| C | 4.128317 | -2.323340 | 0.299788 | C | -1.382122 | -1.790892 | 0.207391 |
| H | 5.086519 | -2.221807 | 0.794093 | H | -0.894857 | -2.258627 | -0.650107 |
| C | 3.911673 | -2.301248 | -1.104802 | C | -2.731649 | -1.769221 | 0.241244 |
| H | 4.666842 | -2.146567 | -1.859664 | H | -3.235177 | -1.293631 | 1.083904 |
| C | 1.946148 | 2.259981 | -0.889772 | C | -3.577985 | -2.354391 | -0.780801 |
| H | 1.036909 | 2.372654 | -1.468223 | H | -3.052472 | -2.793860 | -1.630866 |
| C | 2.051986 | 2.388685 | 0.525989 | C | -4.922008 | -2.408660 | -0.762133 |
| H | 1.239563 | 2.598508 | 1.206897 | H | -5.495961 | -1.982213 | 0.057288 |
| C | 3.410395 | 2.219888 | 0.874124 | H | -5.486886 | -2.871943 | -1.565380 |
| H | 3.823294 | 2.254902 | 1.874340 | H | 0.199144 | -1.901179 | 1.643231 |
| C | 4.148497 | 1.983727 | -0.310120 | H | -1.046909 | -0.742936 | 2.033951 |
| H | 5.216906 | 1.830504 | -0.382666 | | | | |
| C | 3.238572 | 2.040604 | -1.409708 | | | | |
| H | 3.500572 | 1.925644 | -2.451692 | | | | |

1rIM3

SCF energy in gas phase: -696.14498

Free energy in Et₂O : -695.561974

Enthalpy in Et₂O : -695.500405

| | | | |
|---|-----------|-----------|-----------|
| C | 0.398275 | -0.063816 | 0.534498 |
| C | -0.211788 | 1.214363 | 0.263334 |
| C | 0.298695 | 2.152069 | -0.693285 |
| C | -1.428105 | 1.635935 | 0.892573 |
| C | -0.301318 | 3.378918 | -0.939830 |
| H | 1.167840 | 1.878522 | -1.280205 |
| C | -2.020150 | 2.867422 | 0.640102 |
| H | -1.913648 | 0.980517 | 1.607027 |
| C | -1.467392 | 3.773857 | -0.270760 |
| H | 0.141865 | 4.036272 | -1.687889 |
| H | -2.938036 | 3.124256 | 1.168854 |
| H | -1.933689 | 4.736194 | -0.465386 |
| C | 1.752535 | -0.419749 | 0.196598 |
| C | 2.817631 | 0.530270 | 0.051898 |
| C | 2.171784 | -1.784764 | 0.060683 |
| C | 4.127710 | 0.156119 | -0.208290 |

1rIM3(ZrH)

SCF energy in gas phase: -434.068385

Free energy in Et₂O : -434.261959

Enthalpy in Et₂O : -434.214218

| | | | |
|----|-----------|-----------|-----------|
| H | 0.000276 | -1.726028 | 1.073929 |
| Zr | 0.000002 | -0.456686 | -0.207444 |
| C | -2.197814 | -0.512793 | 1.008213 |
| H | -2.366851 | -1.208918 | 1.816958 |
| C | -2.484352 | -0.737651 | -0.368030 |
| H | -2.910893 | -1.642537 | -0.785702 |
| C | -2.184639 | 0.456876 | -1.086880 |
| H | -2.325999 | 0.613538 | -2.150446 |
| C | -1.678898 | 1.408150 | -0.168057 |
| H | -1.388692 | 2.424343 | -0.399221 |
| C | -1.672695 | 0.805089 | 1.127893 |
| H | -1.388374 | 1.291480 | 2.051608 |
| C | 2.197524 | -0.512130 | 1.008797 |
| H | 2.366506 | -1.207660 | 1.818066 |
| C | 2.484442 | -0.737936 | -0.367221 |
| H | 2.911093 | -1.643118 | -0.784132 |
| C | 2.184974 | 0.456089 | -1.086958 |
| H | 2.326504 | 0.612007 | -2.150612 |
| C | 1.678961 | 1.408011 | -0.168944 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|----------|-----------|-----------|
| H | 1.388777 | 2.424027 | -0.400912 | Zr | 3.438121 | -0.367277 | 0.083953 |
| C | 1.672434 | 0.805862 | 1.127434 | C | 5.323998 | -1.076358 | 1.699465 |
| H | 1.387947 | 1.292906 | 2.050753 | H | 5.511085 | -2.129923 | 1.848144 |
| 1rTS4 | | | | C | 4.445155 | -0.267382 | 2.466744 |
| SCF energy in gas phase: -1130.420948 | | | | H | 3.835186 | -0.606457 | 3.293728 |
| Free energy in Et ₂ O : -1129.887275 | | | | C | 4.495674 | 1.054495 | 1.957053 |
| Enthalpy in Et ₂ O : -1129.799512 | | | | H | 3.934360 | 1.901303 | 2.328771 |
| C | -3.329079 | -0.184694 | -0.493043 | C | 5.391668 | 1.063821 | 0.856576 |
| C | -3.581325 | 1.266411 | -0.151884 | H | 5.667017 | 1.928317 | 0.267140 |
| C | -3.451316 | 1.711432 | 1.172695 | C | 5.905638 | -0.255636 | 0.699561 |
| C | -3.989772 | 2.186447 | -1.125860 | H | 6.629714 | -0.572446 | -0.039080 |
| C | -3.719060 | 3.036853 | 1.511640 | C | 3.412259 | -1.342472 | -2.301895 |
| H | -3.132032 | 1.011097 | 1.938801 | H | 3.628197 | -2.392926 | -2.435601 |
| C | -4.261067 | 3.514943 | -0.789583 | C | 2.125917 | -0.775568 | -2.094031 |
| H | -4.097272 | 1.858896 | -2.156233 | H | 1.194193 | -1.318386 | -2.019838 |
| C | -4.126382 | 3.944704 | 0.530644 | C | 2.272608 | 0.627449 | -1.969548 |
| H | -3.607876 | 3.362703 | 2.542268 | H | 1.470178 | 1.331082 | -1.798519 |
| H | -4.578545 | 4.212071 | -1.560363 | C | 3.655734 | 0.934085 | -2.077213 |
| H | -4.335417 | 4.977691 | 0.794216 | H | 4.093322 | 1.923320 | -2.048920 |
| C | -4.434157 | -1.116774 | -0.044918 | C | 4.358368 | -0.287246 | -2.291012 |
| C | -4.346598 | -1.824789 | 1.160854 | H | 5.426171 | -0.388798 | -2.432143 |
| C | -5.594098 | -1.259381 | -0.820147 | 1rIM4 | | | |
| C | -5.388037 | -2.654715 | 1.581240 | SCF energy in gas phase: -1130.421019 | | | |
| H | -3.452286 | -1.728737 | 1.770356 | Free energy in Et ₂ O : -1129.888431 | | | |
| C | -6.635998 | -2.087648 | -0.404145 | Enthalpy in Et ₂ O : -1129.797561 | | | |
| H | -5.675264 | -0.714661 | -1.757074 | C | 3.358923 | -0.240083 | 0.463348 |
| C | -6.536307 | -2.788934 | 0.799939 | C | 3.569587 | 1.251616 | 0.332109 |
| H | -5.299977 | -3.197979 | 2.518191 | C | 3.454223 | 1.873196 | -0.920945 |
| H | -7.525426 | -2.187765 | -1.020345 | C | 3.925613 | 2.038981 | 1.434601 |
| H | -7.346120 | -3.436366 | 1.124237 | C | 3.683265 | 3.240751 | -1.064971 |
| C | -2.606259 | -0.519278 | -1.776462 | H | 3.177667 | 1.276861 | -1.785469 |
| C | -1.893503 | -0.727817 | -0.450029 | C | 4.157940 | 3.409211 | 1.293778 |
| H | -1.822233 | -1.764128 | -0.125239 | H | 4.024215 | 1.574366 | 2.411757 |
| C | -0.739793 | 0.110267 | -0.054505 | C | 4.036758 | 4.015089 | 0.043195 |
| H | -0.756365 | 1.150152 | -0.382039 | H | 3.584019 | 3.703721 | -2.043008 |
| C | 0.292979 | -0.329382 | 0.691973 | H | 4.434912 | 4.001049 | 2.162077 |
| H | 0.254577 | -1.369116 | 1.028280 | H | 4.215348 | 5.080842 | -0.068643 |
| C | 1.495117 | 0.436866 | 1.099926 | C | 4.495261 | -1.065829 | -0.100439 |
| H | 1.374285 | 1.514705 | 0.929445 | C | 4.427305 | -1.619084 | -1.385771 |
| H | 1.689283 | 0.290742 | 2.170701 | C | 5.664531 | -1.260725 | 0.649101 |
| H | -2.924037 | -1.398405 | -2.329489 | C | 5.496614 | -2.349490 | -1.908746 |
| H | -2.262941 | 0.303881 | -2.397202 | H | 3.527143 | -1.480372 | -1.978303 |
| H | 3.329202 | -2.206960 | 0.285457 | | | | |

| | | | | | | | |
|--|-----------|-----------|-----------|--|-----------|-----------|-----------|
| C | 6.733931 | -1.990375 | 0.130889 | Enthalpy in Et ₂ O : -1129.797649 | | | |
| H | 5.731412 | -0.834933 | 1.646871 | | | | |
| C | 6.653452 | -2.538007 | -1.151892 | C | 3.213806 | -0.081151 | 0.574730 |
| H | 5.423541 | -2.772476 | -2.907018 | C | 3.534749 | 1.249534 | -0.067405 |
| H | 7.630191 | -2.133271 | 0.728496 | C | 3.487057 | 1.389995 | -1.462900 |
| H | 7.485049 | -3.108239 | -1.556127 | C | 3.927172 | 2.354260 | 0.699333 |
| C | 2.640594 | -0.769439 | 1.682423 | C | 3.818429 | 2.599512 | -2.071856 |
| C | 1.941532 | -0.814407 | 0.333663 | H | 3.181195 | 0.544212 | -2.071554 |
| H | 1.903835 | -1.799272 | -0.128073 | C | 4.261861 | 3.567097 | 0.092590 |
| C | 0.763662 | 0.033323 | 0.041976 | H | 3.972310 | 2.263416 | 1.781154 |
| H | 0.762759 | 1.034591 | 0.473491 | C | 4.207984 | 3.693950 | -1.295557 |
| C | -0.270354 | -0.352110 | -0.730936 | H | 3.770120 | 2.689268 | -3.153657 |
| H | -0.218790 | -1.352586 | -1.169179 | H | 4.564904 | 4.411302 | 0.706072 |
| C | -1.490661 | 0.426839 | -1.047735 | H | 4.465740 | 4.636793 | -1.769673 |
| H | -1.372663 | 1.489368 | -0.794125 | C | 4.310846 | -1.112471 | 0.421439 |
| H | -1.699995 | 0.372955 | -2.126672 | C | 4.274175 | -2.068597 | -0.602118 |
| H | 2.982055 | -1.706249 | 2.113282 | C | 5.412943 | -1.105767 | 1.288641 |
| H | 2.269318 | -0.049461 | 2.406389 | C | 5.308143 | -2.994667 | -0.754836 |
| H | -3.590032 | -2.102586 | -0.849186 | H | 3.425618 | -2.090458 | -1.280568 |
| Zr | -3.495444 | -0.378027 | -0.173249 | C | 6.447176 | -2.029416 | 1.140025 |
| C | -5.498067 | -0.436191 | -1.803541 | H | 5.454914 | -0.368693 | 2.086270 |
| H | -5.835763 | -1.392927 | -2.174892 | C | 6.398176 | -2.978499 | 0.116135 |
| C | -4.530251 | 0.403126 | -2.416960 | H | 5.259933 | -3.729937 | -1.553504 |
| H | -3.994896 | 0.185327 | -3.331777 | H | 7.291058 | -2.009840 | 1.824361 |
| C | -4.380507 | 1.566418 | -1.622133 | H | 7.202043 | -3.699967 | 0.000416 |
| H | -3.714522 | 2.394157 | -1.825821 | C | 2.408539 | -0.099052 | 1.853132 |
| C | -5.239794 | 1.441561 | -0.498882 | C | 1.766118 | -0.590517 | 0.567159 |
| H | -5.377034 | 2.176599 | 0.283098 | H | 1.678851 | -1.672345 | 0.484412 |
| C | -5.935028 | 0.203381 | -0.615906 | C | 0.661991 | 0.154665 | -0.079012 |
| H | -6.681521 | -0.173433 | 0.070258 | H | 0.698987 | 1.241850 | -0.008400 |
| C | -3.485755 | -1.958315 | 1.861532 | C | -0.349527 | -0.428262 | -0.751458 |
| H | -3.767281 | -2.992015 | 1.720236 | H | -0.332689 | -1.518824 | -0.825604 |
| C | -2.170500 | -1.430429 | 1.763981 | C | -1.510149 | 0.246600 | -1.378467 |
| H | -1.276624 | -1.984915 | 1.514752 | H | -1.323775 | 1.319462 | -1.508857 |
| C | -2.227861 | -0.039423 | 2.023645 | H | -1.728954 | -0.180882 | -2.369355 |
| H | -1.383522 | 0.635448 | 2.009016 | H | 2.665631 | -0.833213 | 2.611299 |
| C | -3.584869 | 0.305171 | 2.263086 | H | 2.059559 | 0.851568 | 2.247212 |
| H | -3.958024 | 1.289066 | 2.515075 | H | -4.670322 | 0.724488 | -1.662268 |
| C | -4.361688 | -0.886141 | 2.167208 | Zr | -3.567310 | 0.048445 | -0.335443 |
| H | -5.430174 | -0.962238 | 2.319399 | C | -4.635145 | 2.202220 | 0.608504 |
| | | | | H | -5.474952 | 2.639263 | 0.087681 |
| | | | | C | -3.265205 | 2.511461 | 0.391296 |
| | | | | H | -2.885040 | 3.215487 | -0.337347 |
| | | | | C | -2.485169 | 1.728244 | 1.276054 |
| 1rIM5 | | | | | | | |
| SCF energy in gas phase: -1130.421323 | | | | | | | |
| Free energy in Et ₂ O : -1129.88946 | | | | | | | |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -1.405456 | 1.713775 | 1.336422 | C | 2.160048 | -0.252879 | 1.754916 |
| C | -3.368596 | 0.911554 | 2.030669 | C | 1.609256 | -0.669202 | 0.400612 |
| H | -3.081785 | 0.214835 | 2.807322 | H | 1.561807 | -1.744779 | 0.239462 |
| C | -4.700463 | 1.211752 | 1.620195 | C | 0.526770 | 0.086929 | -0.266895 |
| H | -5.603881 | 0.770130 | 2.020106 | H | 0.540863 | 1.169985 | -0.148387 |
| C | -4.687832 | -1.980799 | -1.451401 | C | -0.425374 | -0.484440 | -1.037238 |
| H | -5.174567 | -1.839405 | -2.405678 | H | -0.374346 | -1.570541 | -1.148106 |
| C | -3.331559 | -2.346563 | -1.245159 | C | -1.556663 | 0.180926 | -1.723432 |
| H | -2.599791 | -2.536670 | -2.018140 | H | -1.359287 | 1.238987 | -1.919927 |
| C | -3.104735 | -2.429615 | 0.154386 | H | -1.807993 | -0.311893 | -2.669027 |
| H | -2.169271 | -2.686378 | 0.633944 | H | 2.391477 | -1.033629 | 2.473775 |
| C | -4.324222 | -2.124409 | 0.813660 | H | 1.762712 | 0.658919 | 2.192687 |
| H | -4.481974 | -2.113788 | 1.884049 | H | -4.578532 | 0.453745 | -1.657895 |
| C | -5.299276 | -1.839515 | -0.176538 | Zr | -3.397373 | -0.016110 | -0.321078 |
| H | -6.329727 | -1.562524 | 0.004185 | C | -4.489707 | 2.234450 | 0.294257 |

1rTS5

SCF energy in gas phase: -1130.42096

Free energy in Et₂O : -1129.887149

Enthalpy in Et₂O : -1129.798907

| | | | |
|---|----------|-----------|-----------|
| C | 3.038677 | -0.124301 | 0.532775 |
| C | 3.357106 | 1.257364 | 0.007606 |
| C | 3.395587 | 1.496555 | -1.374610 |
| C | 3.664037 | 2.313887 | 0.874652 |
| C | 3.727298 | 2.755419 | -1.873534 |
| H | 3.157367 | 0.688803 | -2.060272 |
| C | 3.998836 | 3.575965 | 0.378396 |
| H | 3.642670 | 2.145431 | 1.947823 |
| C | 4.031056 | 3.801035 | -0.997900 |
| H | 3.746258 | 2.921706 | -2.947118 |
| H | 4.235007 | 4.381414 | 1.068545 |
| H | 4.289139 | 4.782193 | -1.386287 |
| C | 4.172374 | -1.113844 | 0.371408 |
| C | 4.222522 | -1.989363 | -0.721328 |
| C | 5.221849 | -1.145814 | 1.300935 |
| C | 5.290498 | -2.874465 | -0.881779 |
| H | 3.414863 | -1.980046 | -1.448161 |
| C | 6.289708 | -2.029180 | 1.144871 |
| H | 5.196532 | -0.470882 | 2.152420 |
| C | 6.327768 | -2.897592 | 0.051294 |
| H | 5.310038 | -3.547006 | -1.735049 |
| H | 7.092087 | -2.041025 | 1.877562 |
| H | 7.158145 | -3.587307 | -0.070512 |

| | | | |
|---|-----------|-----------|-----------|
| C | -5.306996 | 2.598325 | -0.311065 |
| C | -3.109857 | 2.518200 | 0.094239 |
| H | -2.697126 | 3.125480 | -0.699742 |
| C | -2.373534 | 1.866888 | 1.112862 |
| H | -1.298009 | 1.872565 | 1.224963 |
| C | -3.288861 | 1.158379 | 1.935713 |
| H | -3.036295 | 0.577609 | 2.813026 |
| C | -4.599371 | 1.395194 | 1.431878 |
| H | -5.519364 | 1.005220 | 1.847832 |
| C | -4.624015 | -2.133859 | -1.115893 |
| H | -5.217472 | -2.078163 | -2.016758 |
| C | -3.246407 | -2.470092 | -1.038026 |
| H | -2.606187 | -2.723536 | -1.871670 |
| C | -2.862917 | -2.436233 | 0.331323 |
| H | -1.875416 | -2.643468 | 0.722037 |
| C | -4.001914 | -2.079323 | 1.096872 |
| H | -4.036655 | -1.977580 | 2.173462 |
| C | -5.087424 | -1.885235 | 0.203163 |
| H | -6.094466 | -1.598346 | 0.476705 |

1rIM6 (1rF2)

SCF energy in gas phase: -1130.433394

Free energy in Et₂O : -1129.892428

Enthalpy in Et₂O : -1129.80602

| | | | |
|---|----------|-----------|-----------|
| C | 2.325236 | -0.177702 | 0.401127 |
| C | 2.525997 | 1.294943 | 0.124984 |
| C | 2.818490 | 1.731263 | -1.177234 |
| C | 2.461235 | 2.252372 | 1.146035 |

| | | | |
|---|----------|-----------|-----------|
| H | 3.639379 | -2.074535 | -2.255941 |
| C | 4.000971 | -2.276896 | -0.055627 |
| H | 5.070168 | -2.133468 | 0.028906 |

1rTS7(1rFTS7)

SCF energy in gas phase: -1130.418955

Free energy in Et₂O : -1129.877452

Enthalpy in Et₂O : -1129.79305

| | | | |
|----|-----------|-----------|-----------|
| Zr | 1.958511 | -0.174566 | -0.081849 |
| C | 3.879225 | 1.536129 | -0.388739 |
| H | 4.805095 | 1.375455 | 0.148196 |
| C | 2.778494 | 2.295730 | 0.071494 |
| H | 2.724616 | 2.821066 | 1.013477 |
| C | 1.759408 | 2.241916 | -0.916731 |
| H | 0.801000 | 2.740859 | -0.867423 |
| C | 2.236588 | 1.444657 | -1.998528 |
| H | 1.720285 | 1.247763 | -2.929352 |
| C | 3.551509 | 1.015253 | -1.668186 |
| H | 4.192326 | 0.404616 | -2.289067 |
| C | 3.284189 | -2.124448 | 0.966568 |
| H | 3.732503 | -1.977265 | 1.938977 |
| C | 1.994738 | -2.673994 | 0.706636 |
| H | 1.289719 | -3.015448 | 1.452705 |
| C | 1.817652 | -2.743135 | -0.697568 |
| H | 0.944133 | -3.124874 | -1.209706 |
| C | 2.980476 | -2.229056 | -1.317244 |
| H | 3.156193 | -2.157162 | -2.382617 |
| C | 3.890867 | -1.856198 | -0.284460 |
| H | 4.882411 | -1.448870 | -0.431346 |
| C | -1.812362 | -0.121978 | -0.146055 |
| C | -2.346288 | 1.296566 | -0.113301 |
| C | -2.835966 | 1.825882 | 1.090472 |
| C | -2.420675 | 2.085355 | -1.268337 |
| C | -3.377138 | 3.110077 | 1.138475 |
| H | -2.788267 | 1.224906 | 1.993818 |
| C | -2.965078 | 3.371206 | -1.224040 |
| H | -2.057733 | 1.689360 | -2.212760 |
| C | -3.442842 | 3.888552 | -0.019595 |
| H | -3.746989 | 3.503933 | 2.081046 |
| H | -3.017009 | 3.965750 | -2.131938 |
| H | -3.863658 | 4.889241 | 0.017219 |
| C | -2.916831 | -1.163309 | -0.127543 |
| C | -3.289231 | -1.813417 | 1.055686 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.617716 | -1.461876 | -1.304794 |
| C | -4.331407 | -2.743499 | 1.062639 |
| H | -2.759684 | -1.591574 | 1.978399 |
| C | -4.658038 | -2.389888 | -1.301447 |
| H | -3.341885 | -0.961829 | -2.229541 |
| C | -5.018450 | -3.035332 | -0.115821 |
| H | -4.604347 | -3.239531 | 1.989940 |
| H | -5.187232 | -2.610854 | -2.224295 |
| H | -5.827484 | -3.760091 | -0.112245 |
| C | -0.622349 | -0.418983 | -1.045103 |
| C | -0.577360 | -0.441612 | 0.642157 |
| H | -0.533970 | -1.476152 | 0.974374 |
| C | 0.244837 | 0.512675 | 1.375093 |
| H | -0.035706 | 1.558581 | 1.294179 |
| H | 1.285208 | 1.102672 | 4.152975 |
| C | 1.384598 | 0.168752 | 2.189128 |
| H | 1.394741 | -0.855916 | 2.567064 |
| C | 1.876657 | 1.158912 | 3.226302 |
| H | 1.801484 | 2.191685 | 2.870017 |
| H | 2.923092 | 0.979036 | 3.496318 |
| H | -0.661027 | -1.345491 | -1.606888 |
| H | -0.253288 | 0.443178 | -1.590541 |

1rIM8(1rF4)

SCF energy in gas phase: -1130.442952

Free energy in Et₂O : -1129.896859

Enthalpy in Et₂O : -1129.813229

| | | | |
|----|----------|-----------|-----------|
| Zr | 1.735823 | -0.199534 | -0.113398 |
| C | 3.423862 | 1.247801 | -1.383769 |
| H | 4.313316 | 0.757767 | -1.754677 |
| C | 3.283329 | 1.864520 | -0.114284 |
| H | 4.045087 | 1.940514 | 0.649779 |
| C | 1.975517 | 2.419158 | -0.052087 |
| H | 1.568758 | 2.987069 | 0.772236 |
| C | 1.304158 | 2.117581 | -1.257085 |
| H | 0.289773 | 2.396461 | -1.499545 |
| C | 2.192209 | 1.373603 | -2.079375 |
| H | 1.977120 | 0.998099 | -3.071198 |
| C | 3.108169 | -2.207906 | 0.842962 |
| H | 3.422424 | -2.182839 | 1.876860 |
| C | 1.903981 | -2.772461 | 0.342435 |
| H | 1.144357 | -3.274187 | 0.926860 |
| C | 1.906727 | -2.630880 | -1.071290 |

| | | | | | | | |
|---------------------------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 1.140804 | -2.981516 | -1.747383 | Free energy in Et ₂ O : -1129.886515 | | | |
| C | 3.091529 | -1.955083 | -1.440225 | Enthalpy in Et ₂ O : -1129.802487 | | | |
| H | 3.386264 | -1.696779 | -2.448854 | | | | |
| C | 3.834816 | -1.688872 | -0.253102 | Zr | 1.717918 | -0.221650 | -0.274921 |
| H | 4.797712 | -1.199197 | -0.197553 | C | 3.558861 | 1.590081 | -0.443648 |
| C | -1.463952 | -0.190753 | -0.077607 | H | 4.554489 | 1.334408 | -0.105424 |
| C | -2.083468 | 1.220483 | -0.102363 | C | 2.532131 | 2.165049 | 0.346059 |
| C | -2.543440 | 1.814940 | 1.084510 | H | 2.601944 | 2.407855 | 1.398431 |
| C | -2.314553 | 1.908493 | -1.302234 | C | 1.390010 | 2.348314 | -0.476520 |
| C | -3.174984 | 3.058660 | 1.077439 | H | 0.445814 | 2.779121 | -0.179568 |
| H | -2.413160 | 1.292199 | 2.026797 | C | 1.716832 | 1.892940 | -1.782813 |
| C | -2.950195 | 3.152708 | -1.315468 | H | 1.066781 | 1.920257 | -2.644506 |
| H | -2.007227 | 1.467337 | -2.244573 | C | 3.053507 | 1.424022 | -1.763587 |
| C | -3.377125 | 3.739068 | -0.124524 | H | 3.597394 | 1.016968 | -2.606357 |
| H | -3.514295 | 3.493227 | 2.013914 | C | 2.472348 | -2.373285 | 0.977477 |
| H | -3.112980 | 3.660673 | -2.262297 | H | 2.198666 | -2.475840 | 2.019697 |
| H | -3.867779 | 4.708092 | -0.132974 | C | 1.723181 | -2.837461 | -0.128705 |
| C | -2.649587 | -1.178042 | -0.042859 | H | 0.769421 | -3.345033 | -0.081916 |
| C | -3.135077 | -1.697256 | 1.164095 | C | 2.422202 | -2.488476 | -1.313943 |
| C | -3.297819 | -1.549497 | -1.229635 | H | 2.104291 | -2.703304 | -2.325480 |
| C | -4.229006 | -2.565788 | 1.187236 | C | 3.611949 | -1.812251 | -0.936516 |
| H | -2.652854 | -1.420812 | 2.098131 | H | 4.369450 | -1.432556 | -1.609133 |
| C | -4.391790 | -2.413579 | -1.211464 | C | 3.639844 | -1.729065 | 0.483075 |
| H | -2.936864 | -1.158664 | -2.176574 | H | 4.425037 | -1.286335 | 1.081926 |
| C | -4.862613 | -2.928457 | -0.001055 | C | -1.206174 | -0.212689 | -0.269837 |
| H | -4.584126 | -2.958344 | 2.136468 | C | -1.890690 | 1.170075 | -0.373789 |
| H | -4.876770 | -2.687622 | -2.144670 | C | -2.624887 | 1.658357 | 0.723694 |
| H | -5.712338 | -3.605098 | 0.014064 | C | -1.899611 | 1.944915 | -1.541511 |
| C | -0.434389 | -0.496599 | -1.199467 | C | -3.306500 | 2.871815 | 0.666674 |
| C | -0.508342 | -0.430561 | 1.095292 | H | -2.673801 | 1.068652 | 1.633042 |
| H | -0.346722 | -1.488559 | 1.296173 | C | -2.584193 | 3.163218 | -1.606518 |
| C | 0.266916 | 0.476923 | 1.793960 | H | -1.375284 | 1.601269 | -2.425038 |
| H | 0.019638 | 1.533144 | 1.705279 | C | -3.286701 | 3.637949 | -0.501651 |
| H | 1.933795 | 1.083796 | 4.255834 | H | -3.861396 | 3.216072 | 1.535365 |
| C | 1.553174 | 0.140412 | 2.327842 | H | -2.566713 | 3.736401 | -2.529788 |
| H | 1.645240 | -0.898617 | 2.646467 | H | -3.818602 | 4.583825 | -0.550121 |
| C | 2.303600 | 1.106320 | 3.220166 | C | -2.373512 | -1.230463 | -0.173673 |
| H | 2.211288 | 2.140335 | 2.871109 | C | -2.799421 | -1.776005 | 1.044894 |
| H | 3.372468 | 0.869039 | 3.258291 | C | -3.067883 | -1.604621 | -1.335934 |
| H | -0.545643 | -1.534770 | -1.512265 | C | -3.871260 | -2.672017 | 1.100526 |
| H | -0.520059 | 0.130991 | -2.088056 | H | -2.292673 | -1.499060 | 1.964197 |
| | | | | C | -4.136218 | -2.497678 | -1.285324 |
| 1rTS8 | | | | H | -2.763676 | -1.187626 | -2.291535 |
| SCF energy in gas phase: -1130.423703 | | | | C | -4.543349 | -3.040512 | -0.063646 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -4.177615 | -3.081747 | 2.059622 | C | -1.839114 | 1.107197 | -0.590495 |
| H | -4.653210 | -2.770530 | -2.201720 | C | -2.852794 | 1.452472 | 0.324481 |
| H | -5.373561 | -3.739983 | -0.022169 | C | -1.639752 | 1.976089 | -1.671971 |
| C | -0.250392 | -0.574136 | -1.459987 | C | -3.613985 | 2.608704 | 0.173647 |
| C | -0.221977 | -0.339100 | 0.945065 | H | -3.051705 | 0.798364 | 1.165708 |
| H | -0.237059 | -1.363774 | 1.320304 | C | -2.402657 | 3.138666 | -1.830873 |
| C | -0.014637 | 0.615625 | 2.037009 | H | -0.880174 | 1.760341 | -2.412580 |
| H | -0.255384 | 1.659970 | 1.838838 | C | -3.393171 | 3.464272 | -0.908537 |
| H | 0.269664 | 1.147108 | 5.231245 | H | -4.387197 | 2.838329 | 0.901878 |
| C | 0.542006 | 0.336633 | 3.242061 | H | -2.216698 | 3.784905 | -2.684718 |
| H | 0.770707 | -0.701567 | 3.490282 | H | -3.988128 | 4.364817 | -1.031128 |
| C | 0.829000 | 1.355584 | 4.308473 | C | -2.125376 | -1.332410 | -0.290486 |
| H | 0.557505 | 2.364487 | 3.979463 | C | -2.561836 | -1.886259 | 0.921545 |
| H | 1.890649 | 1.371961 | 4.592493 | C | -2.741911 | -1.784728 | -1.470512 |
| H | -0.351028 | -1.637483 | -1.686370 | C | -3.557973 | -2.867899 | 0.952422 |
| H | -0.425309 | -0.038419 | -2.393350 | H | -2.137431 | -1.541231 | 1.858103 |

1rIM9

SCF energy in gas phase: -1130.426572

Free energy in Et₂O : -1129.886111

Enthalpy in Et₂O : -1129.799985

| | | | |
|----|-----------|-----------|-----------|
| Zr | 1.773826 | -0.174556 | -0.278776 |
| C | 3.575887 | 1.634908 | 0.026184 |
| H | 4.489254 | 1.359232 | 0.536275 |
| C | 2.410211 | 2.168116 | 0.631778 |
| H | 2.263284 | 2.348145 | 1.688789 |
| C | 1.454964 | 2.405227 | -0.389610 |
| H | 0.462676 | 2.808203 | -0.253082 |
| C | 2.025275 | 2.013766 | -1.627819 |
| H | 1.554034 | 2.083620 | -2.598034 |
| C | 3.336140 | 1.529471 | -1.371908 |
| H | 4.039522 | 1.171328 | -2.112749 |
| C | 2.417811 | -2.211828 | 1.205863 |
| H | 2.063645 | -2.223938 | 2.228159 |
| C | 1.749784 | -2.762040 | 0.083147 |
| H | 0.784813 | -3.251372 | 0.095600 |
| C | 2.549207 | -2.529989 | -1.064939 |
| H | 2.311073 | -2.831170 | -2.076478 |
| C | 3.713532 | -1.830425 | -0.653793 |
| H | 4.528119 | -1.517332 | -1.293712 |
| C | 3.631542 | -1.632016 | 0.752218 |
| H | 4.374653 | -1.147295 | 1.371472 |
| C | -1.050289 | -0.211930 | -0.375948 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.839114 | 1.107197 | -0.590495 |
| C | -2.852794 | 1.452472 | 0.324481 |
| C | -1.639752 | 1.976089 | -1.671971 |
| C | -3.613985 | 2.608704 | 0.173647 |
| H | -3.051705 | 0.798364 | 1.165708 |
| C | -2.402657 | 3.138666 | -1.830873 |
| H | -0.880174 | 1.760341 | -2.412580 |
| C | -3.393171 | 3.464272 | -0.908537 |
| H | -4.387197 | 2.838329 | 0.901878 |
| H | -2.216698 | 3.784905 | -2.684718 |
| H | -3.988128 | 4.364817 | -1.031128 |
| C | -2.125376 | -1.332410 | -0.290486 |
| C | -2.561836 | -1.886259 | 0.921545 |
| C | -2.741911 | -1.784728 | -1.470512 |
| C | -3.557973 | -2.867899 | 0.952422 |
| H | -2.137431 | -1.541231 | 1.858103 |
| C | -3.735465 | -2.760747 | -1.443674 |
| H | -2.438766 | -1.359829 | -2.422479 |
| C | -4.146691 | -3.314677 | -0.228475 |
| H | -3.872592 | -3.278914 | 1.908190 |
| H | -4.191061 | -3.088981 | -2.374303 |
| H | -4.918380 | -4.078956 | -0.204991 |
| C | -0.052290 | -0.547697 | -1.562790 |
| C | -0.160758 | -0.167836 | 0.957694 |
| H | -0.168522 | -1.170032 | 1.390532 |
| C | -0.411702 | 0.815871 | 2.031018 |
| H | -0.578809 | 1.849577 | 1.727690 |
| H | -1.440186 | 1.363618 | 5.077072 |
| C | -0.406495 | 0.560551 | 3.352945 |
| H | -0.260176 | -0.467627 | 3.691645 |
| C | -0.582706 | 1.593892 | 4.430135 |
| H | -0.745209 | 2.589793 | 4.004448 |
| H | 0.293500 | 1.653165 | 5.090986 |
| H | -0.124131 | -1.608372 | -1.808081 |
| H | -0.254765 | 0.001541 | -2.480647 |

1rTS9

SCF energy in gas phase: -1591.231643

Free energy in Et₂O : -1590.691852

Enthalpy in Et₂O : -1590.604378

| | | | |
|----|----------|-----------|-----------|
| Zr | 1.661512 | -0.176230 | 0.205317 |
| C | 3.477924 | 1.578381 | -0.127116 |
| H | 4.489888 | 1.343398 | 0.172259 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -0.245836 | -0.843347 | 3.159322 | C | -1.903186 | -1.544373 | 0.301530 |
| C | 0.628278 | -0.116007 | 1.299547 | H | -2.383920 | -0.716647 | -0.217637 |
| H | 0.840778 | -1.174352 | 1.021004 | H | -2.027319 | -3.591383 | -1.633241 |
| C | 0.520079 | -0.126001 | 2.841403 | C | -2.665366 | -2.842294 | 0.316471 |
| H | 0.232202 | 0.860010 | 3.214772 | H | -2.112167 | -3.593113 | 0.893680 |
| H | 1.460239 | -0.402259 | 3.325341 | C | -2.956675 | -3.378669 | -1.095084 |
| H | -2.407251 | -1.570713 | -2.367990 | H | -3.521681 | -2.649292 | -1.685756 |
| H | -3.602935 | -0.323154 | -2.739465 | H | -3.544296 | -4.301507 | -1.052954 |
| Cl | 2.006061 | -2.693253 | -0.893643 | H | 0.898086 | -0.630216 | 2.906167 |
| H | -1.886765 | 0.098985 | -2.635194 | H | 0.848940 | 1.119183 | 2.659248 |
| Cl | 1.614623 | 2.723355 | 1.599150 | H | -0.646116 | 0.221870 | 2.992972 |
| H | 1.347379 | 1.265042 | 1.272156 | H | -3.621665 | -2.691948 | 0.838230 |

(E)1p

SCF energy in gas phase: -697.973461

Free energy in Et₂O : -697.286735

Enthalpy in Et₂O : -697.223296

1rTS11

SCF energy in gas phase: -1591.232285

Free energy in Et₂O : -1590.690135

Enthalpy in Et₂O : -1590.599754

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 0.111781 | -0.074793 | 0.950649 | Zr | 1.516843 | -0.378289 | -0.612031 |
| C | -0.611079 | 1.094688 | 0.253250 | C | 3.362357 | 1.276790 | -1.207435 |
| C | -0.602874 | 1.178938 | -1.149101 | H | 4.351079 | 1.078066 | -0.816874 |
| C | -1.314291 | 2.077350 | 0.961553 | C | 2.367763 | 2.066677 | -0.579461 |
| C | -1.269916 | 2.204124 | -1.816304 | H | 2.464993 | 2.541442 | 0.386759 |
| H | -0.060026 | 0.433470 | -1.721545 | C | 1.222049 | 2.079270 | -1.414122 |
| C | -1.980128 | 3.110596 | 0.296192 | H | 0.294327 | 2.596484 | -1.218409 |
| H | -1.349857 | 2.050067 | 2.044647 | C | 1.511192 | 1.307296 | -2.571535 |
| C | -1.961835 | 3.179448 | -1.095028 | H | 0.851099 | 1.141319 | -3.410593 |
| H | -1.244013 | 2.244295 | -2.901712 | C | 2.833008 | 0.809651 | -2.444556 |
| H | -2.512244 | 3.862087 | 0.872884 | H | 3.354358 | 0.202119 | -3.172499 |
| H | -2.477337 | 3.983221 | -1.612613 | C | 2.325447 | -2.252939 | 0.965786 |
| C | 1.511043 | -0.261169 | 0.314432 | H | 2.187251 | -2.100837 | 2.027548 |
| C | 1.877972 | -1.423289 | -0.374268 | C | 1.423362 | -2.886271 | 0.077466 |
| C | 2.461150 | 0.768411 | 0.417156 | H | 0.459622 | -3.302671 | 0.339130 |
| C | 3.155057 | -1.562451 | -0.926237 | C | 1.988071 | -2.852040 | -1.225502 |
| H | 1.158922 | -2.226565 | -0.493706 | H | 1.538501 | -3.252035 | -2.124505 |
| C | 3.734343 | 0.633480 | -0.130639 | C | 3.245522 | -2.201011 | -1.138158 |
| H | 2.196330 | 1.695237 | 0.917516 | H | 3.932143 | -2.033128 | -1.957012 |
| C | 4.090516 | -0.538114 | -0.803227 | C | 3.449987 | -1.815856 | 0.215129 |
| H | 3.412325 | -2.475697 | -1.455715 | H | 4.307965 | -1.295115 | 0.616937 |
| H | 4.448860 | 1.446491 | -0.036331 | C | -1.349270 | -0.270064 | -0.299938 |
| H | 5.083104 | -0.645221 | -1.230930 | C | -2.121579 | 1.030404 | -0.653970 |
| C | 0.313630 | 0.184974 | 2.470508 | C | -2.947725 | 1.619893 | 0.322588 |
| C | -0.706279 | -1.361625 | 0.863659 | C | -2.102026 | 1.636282 | -1.916664 |
| H | -0.249107 | -2.205725 | 1.383732 | C | -3.696989 | 2.762999 | 0.057275 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -3.015030 | 1.165629 | 1.305672 | C | -1.187960 | -2.126198 | -0.661198 |
| C | -2.854413 | 2.784284 | -2.191522 | H | -0.143581 | -2.199031 | -0.917829 |
| H | -1.499124 | 1.220650 | -2.714036 | C | -2.245723 | -1.785263 | -1.545946 |
| C | -3.653882 | 3.357074 | -1.206746 | H | -2.148105 | -1.578219 | -2.603641 |
| H | -4.322835 | 3.185900 | 0.838346 | C | -3.463321 | -1.821257 | -0.808634 |
| H | -2.811384 | 3.223424 | -3.184612 | H | -4.452310 | -1.628239 | -1.201669 |
| H | -4.239768 | 4.246672 | -1.418867 | C | -3.541921 | 2.306377 | 0.340052 |
| C | -2.441988 | -1.288287 | 0.138009 | H | -3.800988 | 2.607098 | 1.345061 |
| C | -2.720995 | -1.593880 | 1.477123 | C | -2.393443 | 2.712141 | -0.378118 |
| C | -3.235929 | -1.900171 | -0.847874 | H | -1.630065 | 3.390918 | -0.023308 |
| C | -3.739058 | -2.490548 | 1.818564 | C | -2.409297 | 2.060900 | -1.642514 |
| H | -2.151087 | -1.125296 | 2.272223 | H | -1.674617 | 2.176417 | -2.427575 |
| C | -4.251968 | -2.791559 | -0.512016 | C | -3.566672 | 1.248949 | -1.701005 |
| H | -3.055422 | -1.667540 | -1.892868 | H | -3.875690 | 0.643095 | -2.541634 |
| C | -4.506825 | -3.097571 | 0.827572 | C | -4.261344 | 1.383429 | -0.464176 |
| H | -3.928046 | -2.709544 | 2.866148 | H | -5.192068 | 0.899820 | -0.198064 |
| H | -4.847495 | -3.247895 | -1.298241 | C | 1.488481 | 0.187259 | 0.009133 |
| H | -5.295571 | -3.795988 | 1.092085 | C | 2.045343 | -0.484118 | -1.261444 |
| C | -0.527643 | -0.875679 | -1.496770 | C | 3.370866 | -0.956637 | -1.269904 |
| C | -0.304908 | -0.042337 | 0.875645 | C | 1.306040 | -0.612715 | -2.444078 |
| H | -0.238669 | -0.944155 | 1.486959 | C | 3.920806 | -1.556483 | -2.400573 |
| C | -0.272889 | 1.143602 | 1.688622 | H | 3.980571 | -0.835924 | -0.379850 |
| H | -0.479629 | 2.089901 | 1.186859 | C | 1.855527 | -1.208712 | -3.584503 |
| H | -0.865956 | 2.517539 | 4.462276 | H | 0.289565 | -0.238853 | -2.481075 |
| C | 0.105405 | 1.224933 | 3.012758 | C | 3.162990 | -1.688599 | -3.567307 |
| H | 0.125736 | 0.296072 | 3.587151 | H | 4.947123 | -1.912453 | -2.374119 |
| C | 0.024274 | 2.502632 | 3.820247 | H | 1.256793 | -1.290483 | -4.487964 |
| H | -0.023971 | 3.380655 | 3.167443 | H | 3.591694 | -2.150720 | -4.451958 |
| H | 0.894660 | 2.624476 | 4.475169 | C | 2.466896 | 1.341955 | 0.386728 |
| H | -0.672557 | -1.955359 | -1.527608 | C | 3.046939 | 1.464583 | 1.655624 |
| H | -0.812033 | -0.493913 | -2.475375 | C | 2.768684 | 2.329494 | -0.567945 |
| Cl | 3.081887 | 0.881372 | 2.665256 | C | 3.884367 | 2.541209 | 1.966628 |
| H | 1.648936 | 1.099940 | 2.729606 | H | 2.857177 | 0.711455 | 2.412125 |
| | | | | C | 3.602938 | 3.401529 | -0.262403 |
| | | | | H | 2.356482 | 2.246744 | -1.569492 |
| | | | | C | 4.164320 | 3.516423 | 1.012726 |
| | | | | H | 4.319206 | 2.609003 | 2.960311 |
| | | | | H | 3.820848 | 4.146706 | -1.022971 |
| | | | | H | 4.815378 | 4.352016 | 1.253466 |
| Zr | -2.105695 | 0.153813 | 0.100190 | C | 0.091097 | 0.861191 | -0.210491 |
| C | -3.152236 | -2.152927 | 0.531302 | C | 1.364861 | -0.785907 | 1.179879 |
| H | -3.854884 | -2.226483 | 1.350526 | H | 0.849586 | -0.354895 | 2.039564 |
| C | -1.745838 | -2.335961 | 0.622908 | C | 1.778180 | -2.053260 | 1.279604 |
| H | -1.196002 | -2.570042 | 1.522309 | H | 2.292815 | -2.525885 | 0.444005 |

1rIM11

SCF energy in gas phase: -1591.320056

Free energy in Et₂O : -1590.768377

Enthalpy in Et₂O : -1590.676161

| | | | | | | | |
|----|-----------|-----------|-----------|---|----------|-----------|-----------|
| H | 3.540803 | -2.505642 | 3.428963 | H | 1.853854 | -2.676200 | -0.338406 |
| C | 1.602774 | -2.909862 | 2.507411 | C | 2.059887 | -2.074328 | -3.675946 |
| H | 1.024665 | -2.363159 | 3.262379 | H | 2.053434 | -0.110709 | -4.569269 |
| C | 2.943687 | -3.365629 | 3.108900 | H | 2.042359 | -3.867257 | -2.478470 |
| H | 3.535163 | -3.926358 | 2.376587 | H | 2.136535 | -2.601524 | -4.622605 |
| H | 2.786410 | -4.013253 | 3.977714 | C | 2.397397 | 1.468072 | 0.008660 |
| H | -0.033261 | 1.564613 | 0.634242 | C | 3.793822 | 1.497139 | -0.152600 |
| H | 0.170289 | 1.513809 | -1.084061 | C | 1.723200 | 2.694930 | 0.051583 |
| Cl | -2.153184 | 0.355203 | 2.559831 | C | 4.487276 | 2.697911 | -0.267676 |
| H | 1.016681 | -3.804489 | 2.249285 | H | 4.343646 | 0.562684 | -0.184284 |

1rTS12

SCF energy in gas phase: -2052.103538

Free energy in Et₂O : -2051.550174

Enthalpy in Et₂O : -2051.453908

| | | | |
|----|-----------|-----------|-----------|
| Zr | -2.213152 | 0.244394 | 0.122435 |
| C | -3.827695 | 1.231110 | 1.878793 |
| H | -4.390188 | 2.107926 | 1.590855 |
| C | -2.540190 | 1.231638 | 2.481663 |
| H | -1.969793 | 2.112946 | 2.742797 |
| C | -2.142090 | -0.115460 | 2.668039 |
| H | -1.214329 | -0.461671 | 3.099676 |
| C | -3.165150 | -0.952757 | 2.152151 |
| H | -3.147345 | -2.032865 | 2.149018 |
| C | -4.214917 | -0.115016 | 1.676369 |
| H | -5.153578 | -0.448588 | 1.256622 |
| C | -1.895552 | -0.312437 | -2.372896 |
| H | -1.149680 | 0.233227 | -2.934235 |
| C | -1.675466 | -1.521325 | -1.658652 |
| H | -0.738275 | -2.052846 | -1.585685 |
| C | -2.893856 | -1.890671 | -1.036890 |
| H | -3.047888 | -2.768194 | -0.424896 |
| C | -3.877338 | -0.916795 | -1.389440 |
| H | -4.921505 | -0.933999 | -1.109704 |
| C | -3.258985 | 0.047317 | -2.223679 |
| H | -3.729641 | 0.930094 | -2.632162 |
| C | 1.687443 | 0.074638 | 0.119513 |
| C | 1.877525 | -0.701827 | -1.205699 |
| C | 1.925240 | -0.005247 | -2.425357 |
| C | 1.915283 | -2.104600 | -1.255161 |
| C | 2.012702 | -0.679962 | -3.644530 |
| H | 1.906233 | 1.079642 | -2.423776 |
| C | 2.009842 | -2.781091 | -2.474473 |

| | | | |
|----|-----------|-----------|-----------|
| H | 0.645558 | 2.737416 | 0.158004 |
| C | 3.801178 | 3.915107 | -0.216832 |
| H | 5.566500 | 2.684180 | -0.393750 |
| H | 1.865228 | 4.839488 | -0.020444 |
| H | 4.340074 | 4.854486 | -0.301263 |
| C | 0.148850 | 0.278893 | 0.364544 |
| C | 2.298088 | -0.582436 | 1.357998 |
| H | 1.837824 | -0.248733 | 2.288569 |
| C | 3.344281 | -1.407523 | 1.445381 |
| H | 3.841886 | -1.755163 | 0.540616 |
| H | 5.487442 | -0.412969 | 2.976041 |
| C | 3.918470 | -1.913986 | 2.741529 |
| H | 3.312011 | -1.551466 | 3.580013 |
| C | 5.387085 | -1.502643 | 2.942590 |
| H | 6.016447 | -1.869475 | 2.123862 |
| H | 5.786208 | -1.910477 | 3.877202 |
| H | 0.063388 | 0.923043 | 1.250830 |
| H | -0.148858 | 0.892334 | -0.512349 |
| Cl | -2.328418 | 2.636135 | -0.587526 |
| H | 3.851831 | -3.011188 | 2.762496 |
| Cl | -0.311843 | -2.664172 | 1.376376 |
| H | -0.220798 | -1.328003 | 0.838317 |

Me₂CO_1rTS11-like^a

SCF energy in gas phase: -1323.589799

Free energy in Et₂O : -1322.897191

Enthalpy in Et₂O : -1322.795787

| | | | |
|----|----------|-----------|-----------|
| Zr | 1.283236 | -0.877026 | -0.589732 |
| C | 1.377991 | -3.450215 | -0.091159 |
| H | 0.749810 | -4.105029 | -0.679662 |
| C | 1.019031 | -2.832796 | 1.139978 |
| H | 0.063317 | -2.920044 | 1.639151 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 2.112952 | -2.053976 | 1.572746 | H | -3.081403 | 1.745676 | 0.762200 |
| H | 2.146541 | -1.440659 | 2.461602 | C | -3.255179 | 1.560387 | -3.085821 |
| C | 3.152741 | -2.173263 | 0.607700 | H | -1.946629 | -0.118773 | -2.936700 |
| H | 4.121701 | -1.695966 | 0.655892 | C | -3.966231 | 2.550930 | -2.414979 |
| C | 2.702263 | -3.061881 | -0.403778 | H | -4.442921 | 3.366653 | -0.474329 |
| H | 3.268003 | -3.374863 | -1.271055 | H | -3.303168 | 1.491537 | -4.169590 |
| C | 0.952473 | 0.805150 | -2.572399 | H | -4.573829 | 3.264299 | -2.964703 |
| H | 0.050849 | 1.399429 | -2.601232 | C | -2.557608 | -0.919616 | 0.897565 |
| C | 2.162392 | 1.157168 | -1.932051 | C | -3.491401 | -1.879780 | 0.467841 |
| H | 2.332547 | 2.060628 | -1.364845 | C | -2.622313 | -0.512896 | 2.237562 |
| C | 3.086423 | 0.094585 | -2.109063 | C | -4.431521 | -2.423713 | 1.339927 |
| H | 4.099641 | 0.060493 | -1.732194 | H | -3.480393 | -2.199474 | -0.569978 |
| C | 2.443773 | -0.911640 | -2.883516 | C | -3.563857 | -1.056832 | 3.117959 |
| H | 2.886681 | -1.841952 | -3.212495 | H | -1.941968 | 0.248522 | 2.603273 |
| C | 1.124648 | -0.476564 | -3.160729 | C | -4.469911 | -2.018711 | 2.677026 |
| H | 0.384971 | -1.020989 | -3.730475 | H | -5.138003 | -3.164746 | 0.974687 |
| C | -1.554281 | -0.327272 | -0.130320 | H | -3.585347 | -0.720934 | 4.151669 |
| C | -0.908662 | -1.484185 | -0.965155 | H | -5.199161 | -2.444338 | 3.360707 |
| H | -1.124326 | -2.446236 | -0.501732 | | | | |
| H | -1.262480 | -1.554355 | -1.992701 | | | | |
| C | -0.313229 | 0.374283 | 0.584705 | | | | |
| C | -0.251520 | 1.845792 | 0.656585 | | | | |
| H | -0.416493 | 2.382554 | -0.279681 | | | | |
| C | -0.003464 | 2.601065 | 1.745467 | | | | |
| H | 0.122209 | 2.108903 | 2.711973 | Zr | -1.713593 | -0.089313 | 0.085838 |
| H | -0.207407 | -0.044012 | 1.591362 | C | -3.282459 | -0.075593 | -1.985229 |
| C | 3.877275 | 3.032636 | 1.151412 | H | -4.229874 | -0.588578 | -1.894259 |
| H | 4.209311 | 2.830798 | 0.132032 | C | -2.052532 | -0.654039 | -2.408041 |
| H | 4.712765 | 3.405775 | 1.752303 | H | -1.892944 | -1.683153 | -2.700319 |
| H | 3.117057 | 3.822649 | 1.126940 | C | -1.071095 | 0.368931 | -2.408367 |
| C | 3.263399 | 1.792125 | 1.766665 | H | -0.041369 | 0.271835 | -2.711117 |
| O | 2.919845 | 0.840722 | 1.081210 | C | -1.679894 | 1.558379 | -1.943276 |
| C | 3.124487 | 1.779995 | 3.273889 | H | -1.187749 | 2.514306 | -1.845969 |
| H | 4.120392 | 1.687283 | 3.725718 | C | -3.050705 | 1.284037 | -1.687002 |
| H | 2.696328 | 2.721020 | 3.633170 | H | -3.778205 | 1.982518 | -1.297944 |
| H | 2.504802 | 0.942813 | 3.595511 | C | -1.998878 | -2.525918 | 0.963332 |
| C | 0.057284 | 4.104692 | 1.749506 | H | -1.271172 | -3.252235 | 0.634690 |
| H | -0.714285 | 4.541262 | 2.399018 | C | -1.927752 | -1.724417 | 2.139026 |
| H | 1.017040 | 4.494523 | 2.122766 | H | -1.131065 | -1.742286 | 2.871129 |
| H | -0.092734 | 4.509955 | 0.743020 | C | -3.091770 | -0.924786 | 2.188028 |
| C | -2.381950 | 0.678901 | -0.976695 | H | -3.331191 | -0.187595 | 2.940359 |
| C | -3.115311 | 1.686881 | -0.319748 | C | -3.861596 | -1.185078 | 1.028978 |
| C | -2.477223 | 0.639211 | -2.374112 | H | -4.804117 | -0.718286 | 0.775897 |
| C | -3.890410 | 2.606686 | -1.020676 | C | -3.193534 | -2.201215 | 0.286257 |

Me₂CO_1rTS13-like^b

SCF energy in gas phase: -1323.577179

Free energy in Et₂O : -1322.883017

Enthalpy in Et₂O : -1322.788809

| | | | |
|---|-----------|-----------|-----------|
| C | 4.111328 | -1.086381 | 0.620337 |
| C | 4.393961 | -2.502612 | -1.753851 |
| H | 2.468702 | -1.716915 | -2.280995 |
| C | 5.265937 | -1.826212 | 0.384078 |
| H | 4.014842 | -0.528783 | 1.547420 |
| C | 5.412726 | -2.547096 | -0.805971 |
| H | 4.494911 | -3.046449 | -2.689693 |
| H | 6.056711 | -1.840692 | 1.129655 |
| H | 6.312050 | -3.128031 | -0.989913 |
| C | 1.118195 | -0.785278 | 1.288625 |
| C | 0.725389 | -0.444576 | -1.049795 |
| H | 0.494346 | -1.499980 | -1.196557 |
| C | 0.113841 | 0.458490 | -1.885379 |
| H | 0.432802 | 1.496510 | -1.829703 |
| H | -1.046313 | 0.979011 | -4.614680 |
| C | -1.076460 | 0.130152 | -2.613039 |
| H | -1.091945 | -0.907744 | -2.938815 |
| C | -1.619005 | 1.059934 | -3.679823 |
| H | -1.585683 | 2.111856 | -3.380434 |
| H | -2.661151 | 0.823829 | -3.926101 |
| H | 1.037037 | -1.867869 | 1.137782 |
| H | 1.787102 | -0.640702 | 2.144819 |
| C | -0.121596 | -2.103521 | 3.477208 |
| H | 0.946727 | -2.088216 | 3.698897 |
| H | -0.337212 | -2.919859 | 2.786461 |
| H | -0.659409 | -2.308140 | 4.413906 |
| C | -0.650939 | -0.776589 | 2.945160 |
| O | -1.778930 | -0.765095 | 2.387212 |
| C | -0.204773 | 0.439102 | 3.749299 |
| H | 0.858406 | 0.420624 | 3.996525 |
| H | -0.448150 | 1.370868 | 3.239434 |
| H | -0.767364 | 0.423325 | 4.694953 |

CH₃COCH₃

SCF energy in gas phase: -193.164213

Free energy in Et₂O : -193.031777

Enthalpy in Et₂O : -192.997544

| | | | |
|---|-----------|-----------|-----------|
| C | 0.000000 | -1.292621 | -0.614475 |
| H | -0.880433 | -1.340353 | -1.265863 |
| H | 0.000706 | -2.146350 | 0.064204 |
| H | 0.879574 | -1.339750 | -1.267056 |
| C | 0.000000 | 0.000000 | 0.184621 |
| O | 0.000000 | 0.000000 | 1.400425 |

| | | | |
|---|-----------|----------|-----------|
| C | 0.000000 | 1.292621 | -0.614475 |
| H | -0.879574 | 1.339750 | -1.267056 |
| H | -0.000706 | 2.146350 | 0.064204 |
| H | 0.880433 | 1.340353 | -1.265863 |

CH₃CHO_1rTS11-like

SCF energy in gas phase: -1284.264251

Free energy in Et₂O : -1283.619137

Enthalpy in Et₂O : -1283.52187

| | | | |
|----|-----------|-----------|-----------|
| Zr | -1.401531 | 0.667781 | -0.656856 |
| C | -1.666714 | 3.254359 | -0.394530 |
| H | -1.109858 | 3.895803 | -1.064101 |
| C | -1.222142 | 2.778651 | 0.868909 |
| H | -0.258865 | 2.979618 | 1.318927 |
| C | -2.242281 | 1.966097 | 1.415543 |
| H | -2.206734 | 1.435006 | 2.356098 |
| C | -3.318580 | 1.925145 | 0.488048 |
| H | -4.242288 | 1.379829 | 0.619937 |
| C | -2.966624 | 2.739193 | -0.621917 |
| H | -3.581300 | 2.927474 | -1.492398 |
| C | -1.125285 | -1.354137 | -2.290517 |
| H | -0.207714 | -1.923476 | -2.264098 |
| C | -2.287422 | -1.607878 | -1.523254 |
| H | -2.400841 | -2.396651 | -0.792992 |
| C | -3.255908 | -0.623347 | -1.845161 |
| H | -4.248071 | -0.545312 | -1.421858 |
| C | -2.690754 | 0.235618 | -2.829290 |
| H | -3.183463 | 1.077487 | -3.297396 |
| C | -1.374424 | -0.214731 | -3.101248 |
| H | -0.687282 | 0.229246 | -3.807584 |
| C | 1.417162 | 0.347865 | -0.211245 |
| C | 0.708431 | 1.321545 | -1.228053 |
| H | 0.892505 | 2.357656 | -0.947326 |
| H | 1.047709 | 1.212959 | -2.256633 |
| C | 0.244262 | -0.308479 | 0.664240 |
| C | 0.283327 | -1.748607 | 0.968889 |
| H | 0.492151 | -2.417070 | 0.132060 |
| C | 0.080406 | -2.332604 | 2.168351 |
| H | -0.086658 | -1.699034 | 3.042200 |
| H | 0.146143 | 0.255623 | 1.595193 |
| C | -3.053343 | -2.049470 | 2.088922 |
| O | -3.154313 | -0.954726 | 1.565992 |
| C | -3.384355 | -2.325898 | 3.529838 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -0.882597 | -3.104145 | 3.704131 | C | 0.268435 | -1.282639 | 1.596362 |
| H | -1.024511 | -2.223666 | 4.339941 | H | 0.467317 | -2.208839 | 1.055966 |
| H | -0.017863 | -3.659371 | 4.093891 | C | 0.062276 | -1.385783 | 2.924424 |
| H | -0.362002 | -0.383136 | -2.196368 | H | -0.109257 | -0.476934 | 3.504909 |
| H | -0.735943 | 1.310437 | -2.007502 | H | 0.172087 | 0.813877 | 1.469778 |
| C | 1.603621 | 1.620552 | -2.547093 | C | -3.553442 | -1.331636 | 3.257481 |
| O | 2.573960 | 1.368471 | -1.802785 | O | -3.782191 | -0.511410 | 2.398207 |
| C | 1.130327 | 3.027803 | -2.769898 | C | 0.083091 | -2.676530 | 3.696364 |
| H | 1.269981 | 3.637566 | -1.875441 | H | 0.859557 | -2.671505 | 4.473671 |
| H | 1.750627 | 3.452886 | -3.571923 | H | -0.865177 | -2.872915 | 4.218277 |
| H | 0.091449 | 3.060679 | -3.104900 | H | 0.279896 | -3.529856 | 3.038711 |
| H | 1.254090 | 0.868195 | -3.270272 | C | 2.164460 | -1.019646 | -0.648056 |

CH₂O_1rTS11-like

SCF energy in gas phase: -1244.932442

Free energy in Et₂O : -1244.345001

Enthalpy in Et₂O : -1244.247396

| | | | |
|----|-----------|-----------|-----------|
| Zr | -1.455331 | 0.407582 | -0.717122 |
| C | -1.838186 | 2.950492 | -1.115141 |
| H | -1.333574 | 3.416821 | -1.950649 |
| C | -1.334080 | 2.839949 | 0.206890 |
| H | -0.369031 | 3.191100 | 0.548015 |
| C | -2.300599 | 2.160510 | 0.990457 |
| H | -2.217598 | 1.909870 | 2.039192 |
| C | -3.401740 | 1.843330 | 0.154859 |
| H | -4.296877 | 1.326422 | 0.469761 |
| C | -3.116327 | 2.334834 | -1.148651 |
| H | -3.765288 | 2.263843 | -2.011931 |
| C | -1.233463 | -2.088550 | -1.439965 |
| H | -0.288805 | -2.590032 | -1.289427 |
| C | -2.302491 | -2.025699 | -0.511140 |
| H | -2.303258 | -2.456823 | 0.480605 |
| C | -3.349402 | -1.269477 | -1.094775 |
| H | -4.299429 | -1.042306 | -0.631365 |
| C | -2.922621 | -0.857243 | -2.388204 |
| H | -3.502298 | -0.277665 | -3.095030 |
| C | -1.614962 | -1.368733 | -2.601226 |
| H | -1.019764 | -1.236624 | -3.494382 |
| C | 1.342886 | 0.256032 | -0.316092 |
| C | 0.591120 | 0.856265 | -1.576427 |
| H | 0.759195 | 1.931947 | -1.628485 |
| H | 0.918152 | 0.438261 | -2.526708 |
| C | 0.222212 | -0.043609 | 0.796767 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.268435 | -1.282639 | 1.596362 |
| H | 0.467317 | -2.208839 | 1.055966 |
| C | 0.062276 | -1.385783 | 2.924424 |
| H | -0.109257 | -0.476934 | 3.504909 |
| H | 0.172087 | 0.813877 | 1.469778 |
| C | -3.553442 | -1.331636 | 3.257481 |
| O | -3.782191 | -0.511410 | 2.398207 |
| C | 0.083091 | -2.676530 | 3.696364 |
| H | 0.859557 | -2.671505 | 4.473671 |
| H | -0.865177 | -2.872915 | 4.218277 |
| H | 0.279896 | -3.529856 | 3.038711 |
| C | 2.164460 | -1.019646 | -0.648056 |
| C | 3.038038 | -1.542311 | 0.325383 |
| C | 2.116879 | -1.688453 | -1.878838 |
| C | 3.815860 | -2.671552 | 0.083136 |
| H | 3.115190 | -1.049076 | 1.287681 |
| C | 2.896563 | -2.823670 | -2.129358 |
| H | 1.467893 | -1.334196 | -2.669909 |
| C | 3.751286 | -3.323234 | -1.150944 |
| H | 4.479953 | -3.039649 | 0.860644 |
| H | 2.831834 | -3.310024 | -3.099206 |
| H | 4.360710 | -4.201302 | -1.344950 |
| C | 2.373686 | 1.300868 | 0.199380 |
| C | 3.206029 | 1.956027 | -0.725940 |
| C | 2.567460 | 1.590007 | 1.557832 |
| C | 4.169407 | 2.874923 | -0.316366 |
| H | 3.097125 | 1.735649 | -1.783344 |
| C | 3.532007 | 2.514239 | 1.973669 |
| H | 1.976009 | 1.079519 | 2.309818 |
| C | 4.334160 | 3.166485 | 1.040338 |
| H | 4.794581 | 3.364205 | -1.058736 |
| H | 3.653444 | 2.717559 | 3.034515 |
| H | 5.081037 | 3.886681 | 1.362306 |
| H | -3.163860 | -2.341378 | 3.023139 |
| H | -3.720260 | -1.119777 | 4.333037 |

CH₂O_1rTS13-like

SCF energy in gas phase: -1244.925129

Free energy in Et₂O : -1244.332137

Enthalpy in Et₂O : -1244.24015

| | | | |
|----|----------|-----------|-----------|
| Zr | 1.724124 | -0.124160 | -0.211815 |
| C | 3.344353 | 1.542538 | 0.960901 |
| H | 4.271820 | 1.157677 | 1.362269 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 2.109021 | 1.639477 | 1.653624 | C | -0.617716 | -0.105780 | 2.231357 |
| H | 1.919752 | 1.337251 | 2.674779 | H | -0.786316 | 0.961113 | 2.380472 |
| C | 1.159741 | 2.219865 | 0.772284 | H | -1.627943 | -0.831389 | 5.248495 |
| H | 0.131383 | 2.448388 | 1.001756 | C | -0.604174 | -0.870848 | 3.341025 |
| C | 1.791396 | 2.433419 | -0.475145 | H | -0.466032 | -1.949551 | 3.238966 |
| H | 1.333583 | 2.871411 | -1.350449 | C | -0.774746 | -0.357921 | 4.743988 |
| C | 3.149168 | 2.013818 | -0.357280 | H | -0.940191 | 0.724702 | 4.755314 |
| H | 3.894188 | 2.048934 | -1.139217 | H | 0.105344 | -0.566262 | 5.368529 |
| C | 2.159927 | -2.319651 | 1.123837 | H | -0.296093 | -1.411302 | -1.793791 |
| H | 1.576405 | -2.476737 | 2.019908 | H | -0.561639 | 0.187979 | -2.437417 |
| C | 1.824753 | -2.756410 | -0.187056 | C | 1.726832 | 0.004030 | -3.359750 |
| H | 0.934093 | -3.303293 | -0.465468 | O | 2.667194 | 0.269750 | -2.623097 |
| C | 2.847426 | -2.330072 | -1.062738 | H | 1.273079 | 0.773554 | -4.009389 |
| H | 2.884552 | -2.500002 | -2.130655 | H | 1.339609 | -1.020527 | -3.474708 |
| C | 3.816326 | -1.617318 | -0.304780 | | | | |
| H | 4.720435 | -1.167107 | -0.692113 | HCl | | | |
| C | 3.397906 | -1.636913 | 1.052655 | SCF energy in gas phase: -460.800777 | | | |
| H | 3.925568 | -1.202627 | 1.890557 | Free energy in Et ₂ O : -460.808828 | | | |
| C | -1.289108 | -0.145701 | -0.361775 | Enthalpy in Et ₂ O : -460.787636 | | | |
| C | -1.868833 | 1.281554 | -0.273914 | | | | |
| C | -2.787568 | 1.593988 | 0.746529 | Cl | 0.000000 | 0.000000 | 0.071441 |
| C | -1.588484 | 2.289454 | -1.207650 | H | 0.000000 | 0.000000 | -1.214502 |
| C | -3.364555 | 2.858178 | 0.849680 | | | | |
| H | -3.065638 | 0.826863 | 1.461366 | [Zr]Cl₂ | | | |
| C | -2.170425 | 3.558037 | -1.114669 | SCF energy in gas phase: -1354.251515 | | | |
| H | -0.901892 | 2.094252 | -2.022576 | Free energy in Et ₂ O : -1354.373683 | | | |
| C | -3.056361 | 3.853421 | -0.081166 | Enthalpy in Et ₂ O : -1354.318208 | | | |
| H | -4.066814 | 3.062388 | 1.653551 | | | | |
| H | -1.927728 | 4.313549 | -1.857615 | Zr | 0.000062 | -0.096796 | -0.000090 |
| H | -3.508704 | 4.838185 | -0.006173 | C | -2.567470 | -0.185421 | 0.236390 |
| C | -2.517708 | -1.078257 | -0.541876 | H | -3.005697 | -1.143400 | 0.479462 |
| C | -2.984483 | -1.925562 | 0.472260 | C | -2.320844 | 0.313312 | -1.064184 |
| C | -3.208267 | -1.084025 | -1.766248 | H | -2.533814 | -0.200229 | -1.990389 |
| C | -4.090316 | -2.757369 | 0.266545 | C | -1.671979 | 1.569589 | -0.940300 |
| H | -2.491863 | -1.930182 | 1.438279 | H | -1.363466 | 2.208333 | -1.757201 |
| C | -4.307771 | -1.912920 | -1.976117 | C | -1.560937 | 1.867739 | 0.450820 |
| H | -2.877685 | -0.425236 | -2.564369 | H | -1.142542 | 2.769543 | 0.876219 |
| C | -4.754897 | -2.760221 | -0.958136 | C | -2.108311 | 0.782262 | 1.174239 |
| H | -4.430154 | -3.403630 | 1.071986 | H | -2.147139 | 0.686503 | 2.250501 |
| H | -4.819770 | -1.896448 | -2.934994 | C | 2.319935 | 0.316322 | 1.064849 |
| H | -5.611688 | -3.408640 | -1.118974 | H | 2.531896 | -0.194115 | 1.993000 |
| C | -0.275944 | -0.347878 | -1.525932 | C | 2.567563 | -0.186926 | -0.233834 |
| C | -0.375196 | -0.562651 | 0.847425 | H | 3.005753 | -1.145840 | -0.473275 |
| H | -0.373980 | -1.654616 | 0.841796 | C | 2.109707 | 0.777801 | -1.175350 |

| | | | |
|----|-----------|-----------|-----------|
| H | 2.149543 | 0.678372 | -2.251241 |
| C | 1.561900 | 1.865838 | -0.456123 |
| H | 1.144254 | 2.766354 | -0.884984 |
| C | 1.671673 | 1.572392 | 0.936114 |
| H | 1.362643 | 2.213955 | 1.750599 |
| Cl | -0.052231 | -1.672284 | 1.879122 |
| Cl | 0.051565 | -1.676251 | -1.875876 |

1rTS14

SCF energy in gas phase: -1130.414339

Free energy in Et₂O : -1129.875342

Enthalpy in Et₂O : -1129.791673

| | | | |
|----|-----------|-----------|-----------|
| Zr | -1.763514 | 0.224029 | -0.179686 |
| C | -3.693304 | -1.501233 | -0.324495 |
| H | -4.657961 | -1.220273 | 0.076382 |
| C | -2.652315 | -2.148069 | 0.386706 |
| H | -2.687081 | -2.442584 | 1.427403 |
| C | -1.563135 | -2.343840 | -0.504262 |
| H | -0.617623 | -2.809178 | -0.267294 |
| C | -1.934239 | -1.812612 | -1.766924 |
| H | -1.338153 | -1.826777 | -2.667013 |
| C | -3.245850 | -1.281984 | -1.653912 |
| H | -3.813174 | -0.813460 | -2.448064 |
| C | -2.431501 | 2.147459 | 1.453408 |
| H | -2.072506 | 2.093754 | 2.472736 |
| C | -1.781363 | 2.789810 | 0.370989 |
| H | -0.825516 | 3.294932 | 0.413003 |
| C | -2.582035 | 2.624647 | -0.788257 |
| H | -2.354267 | 3.001644 | -1.776535 |
| C | -3.733173 | 1.881062 | -0.421796 |
| H | -4.544178 | 1.597749 | -1.079633 |
| C | -3.637098 | 1.578008 | 0.963743 |
| H | -4.366675 | 1.034218 | 1.549580 |
| C | 1.072252 | 0.297905 | -0.274227 |
| C | 1.837374 | -1.011237 | -0.577437 |
| C | 2.890343 | -1.397442 | 0.273685 |
| C | 1.581971 | -1.836708 | -1.679960 |
| C | 3.633011 | -2.552929 | 0.045424 |
| H | 3.147313 | -0.767707 | 1.117720 |
| C | 2.322418 | -3.000696 | -1.915986 |
| H | 0.801154 | -1.578850 | -2.382898 |
| C | 3.350171 | -3.369032 | -1.052673 |
| H | 4.440799 | -2.812483 | 0.724465 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.092515 | -3.611595 | -2.785089 |
| H | 3.929478 | -4.269715 | -1.235162 |
| C | 2.146777 | 1.415277 | -0.156688 |
| C | 2.432808 | 2.115192 | 1.021913 |
| C | 2.893577 | 1.746958 | -1.303286 |
| C | 3.413052 | 3.114880 | 1.054923 |
| H | 1.898212 | 1.885503 | 1.936683 |
| C | 3.869653 | 2.738229 | -1.275600 |
| H | 2.703108 | 1.211417 | -2.228762 |
| C | 4.134369 | 3.434317 | -0.091634 |
| H | 3.609237 | 3.638543 | 1.986983 |
| H | 4.427495 | 2.968763 | -2.179475 |
| H | 4.894405 | 4.210073 | -0.067055 |
| C | 0.061924 | 0.725970 | -1.424425 |
| C | 0.169410 | 0.161562 | 1.054174 |
| H | 0.112864 | 1.187261 | 1.433657 |
| C | 0.657182 | -0.665281 | 2.204024 |
| H | 1.448788 | -0.213095 | 2.814159 |
| H | 0.023012 | -2.888599 | 4.502379 |
| C | 0.245502 | -1.874866 | 2.604160 |
| H | -0.536934 | -2.380110 | 2.043868 |
| C | 0.806080 | -2.624805 | 3.779204 |
| H | 1.565756 | -2.037136 | 4.304617 |
| H | 1.270299 | -3.568978 | 3.464641 |
| H | 0.136853 | 1.802648 | -1.587145 |
| H | 0.270169 | 0.249613 | -2.381456 |

1rIM12

SCF energy in gas phase: -1130.419019

Free energy in Et₂O : -1129.878697

Enthalpy in Et₂O : -1129.793191

| | | | |
|----|-----------|-----------|-----------|
| Zr | -1.802186 | 0.154403 | -0.184507 |
| C | -3.595324 | -1.677421 | 0.000200 |
| H | -4.507531 | -1.445372 | 0.533686 |
| C | -2.417164 | -2.231950 | 0.560064 |
| H | -2.248686 | -2.480562 | 1.599422 |
| C | -1.467778 | -2.387096 | -0.481890 |
| H | -0.467622 | -2.774705 | -0.364137 |
| C | -2.054373 | -1.925742 | -1.687786 |
| H | -1.592246 | -1.923101 | -2.665217 |
| C | -3.368249 | -1.473645 | -1.389237 |
| H | -4.081809 | -1.074160 | -2.098541 |
| C | -2.449518 | 2.095134 | 1.433359 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -2.087356 | 2.055963 | 2.452270 | H | 0.223480 | 0.092035 | -2.376619 |
| C | -1.798653 | 2.718891 | 0.339042 | | | | |
| H | -0.838870 | 3.217342 | 0.371513 | 1rTS15 | | | |
| C | -2.609975 | 2.549940 | -0.811886 | SCF energy in gas phase: -1591.217369 | | | |
| H | -2.386439 | 2.914818 | -1.805621 | Free energy in Et ₂ O : -1590.671437 | | | |
| C | -3.762483 | 1.814904 | -0.431695 | Enthalpy in Et ₂ O : -1590.582483 | | | |
| H | -4.581356 | 1.532869 | -1.080489 | | | | |
| C | -3.662085 | 1.530389 | 0.958149 | Zr | 1.696885 | 0.126249 | -0.135957 |
| H | -4.393570 | 1.001056 | 1.554369 | C | 3.327278 | -1.791130 | -0.669674 |
| C | 1.021675 | 0.310582 | -0.278805 | H | 4.199367 | -1.580492 | -1.273184 |
| C | 1.955042 | -0.880204 | -0.616690 | C | 2.057941 | -2.204457 | -1.150249 |
| C | 3.145798 | -1.054248 | 0.112554 | H | 1.771268 | -2.347255 | -2.183073 |
| C | 1.688934 | -1.813688 | -1.628704 | C | 1.208592 | -2.398067 | -0.029808 |
| C | 4.020148 | -2.105930 | -0.152566 | H | 0.177042 | -2.710674 | -0.070619 |
| H | 3.394055 | -0.352552 | 0.900093 | C | 1.940985 | -2.076314 | 1.138184 |
| C | 2.558678 | -2.876307 | -1.895134 | H | 1.584549 | -2.123446 | 2.156996 |
| H | 0.792013 | -1.727590 | -2.228532 | C | 3.252581 | -1.685208 | 0.742581 |
| C | 3.731061 | -3.029738 | -1.159050 | H | 4.049789 | -1.383190 | 1.408019 |
| H | 4.931308 | -2.202760 | 0.431634 | C | 2.162438 | 1.828734 | -2.059518 |
| H | 2.314946 | -3.578353 | -2.688244 | H | 1.629254 | 1.721152 | -2.994601 |
| H | 4.411400 | -3.850285 | -1.368509 | C | 1.758787 | 2.618223 | -0.950272 |
| C | 1.946927 | 1.548516 | -0.088389 | H | 0.848907 | 3.199791 | -0.883399 |
| C | 2.298276 | 2.071560 | 1.164051 | C | 2.738254 | 2.490507 | 0.062825 |
| C | 2.525650 | 2.147965 | -1.222199 | H | 2.712183 | 2.952474 | 1.040362 |
| C | 3.166391 | 3.163045 | 1.280251 | C | 3.751429 | 1.613750 | -0.411840 |
| H | 1.910142 | 1.616288 | 2.068602 | H | 4.642915 | 1.323494 | 0.128051 |
| C | 3.392184 | 3.232674 | -1.112003 | C | 3.398810 | 1.216577 | -1.731310 |
| H | 2.296716 | 1.749397 | -2.205631 | H | 3.978625 | 0.576654 | -2.382085 |
| C | 3.713562 | 3.754024 | 0.144183 | C | -1.202233 | 0.325586 | 0.199643 |
| H | 3.414779 | 3.543957 | 2.267418 | C | -1.958496 | -0.916167 | 0.728847 |
| H | 3.819993 | 3.670993 | -2.009833 | C | -3.194198 | -1.277696 | 0.160473 |
| H | 4.385154 | 4.603216 | 0.233008 | C | -1.502869 | -1.688478 | 1.807148 |
| C | -0.001189 | 0.632389 | -1.458788 | C | -3.922678 | -2.368456 | 0.630572 |
| C | 0.147583 | 0.055556 | 1.044925 | H | -3.593372 | -0.692597 | -0.659908 |
| H | 0.076887 | 1.018988 | 1.549410 | C | -2.228399 | -2.785674 | 2.282441 |
| C | 0.405527 | -0.956411 | 2.098515 | H | -0.570448 | -1.436070 | 2.296091 |
| H | 0.070455 | -0.604997 | 3.080492 | C | -3.442263 | -3.134353 | 1.695263 |
| H | 0.483444 | -4.010778 | 3.222035 | H | -4.873637 | -2.615518 | 0.166465 |
| C | 0.901435 | -2.208664 | 2.089070 | H | -1.841216 | -3.358629 | 3.120691 |
| H | 1.266090 | -2.657797 | 1.170587 | H | -4.011694 | -3.981546 | 2.066597 |
| C | 1.025344 | -3.060097 | 3.323515 | C | -2.271198 | 1.447079 | 0.032733 |
| H | 0.634033 | -2.545880 | 4.208458 | C | -2.754522 | 1.857785 | -1.217547 |
| H | 2.071486 | -3.325810 | 3.529353 | C | -2.816998 | 2.061910 | 1.173491 |
| H | 0.032011 | 1.695072 | -1.699044 | C | -3.729312 | 2.855121 | -1.326826 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -2.384484 | 1.385622 | -2.121197 | H | -4.133097 | 1.344753 | -2.256465 |
| C | -3.785995 | 3.057245 | 1.068817 | C | -4.010524 | 1.672420 | -0.056029 |
| H | -2.481866 | 1.754539 | 2.159095 | H | -4.927594 | 1.225539 | 0.302082 |
| C | -4.245864 | 3.465098 | -0.186033 | C | -3.013364 | 2.308446 | 0.743500 |
| H | -4.083112 | 3.150004 | -2.311262 | H | -3.041954 | 2.436660 | 1.817371 |
| H | -4.184021 | 3.514880 | 1.970549 | C | 1.622264 | 0.081891 | -0.726780 |
| H | -4.999035 | 4.243338 | -0.269895 | C | 1.778013 | -1.410535 | -0.344999 |
| C | -0.122294 | 0.840470 | 1.247099 | C | 2.605580 | -1.821781 | 0.714852 |
| C | -0.400608 | 0.122459 | -1.149747 | C | 1.108274 | -2.419636 | -1.056372 |
| H | -0.348696 | 1.121751 | -1.582522 | C | 2.735027 | -3.166030 | 1.068287 |
| C | -0.746668 | -0.789595 | -2.268198 | H | 3.185094 | -1.081717 | 1.254994 |
| H | -0.417534 | -0.385247 | -3.231950 | C | 1.240268 | -3.768049 | -0.712574 |
| H | -1.040639 | -3.738084 | -3.609406 | H | 0.466819 | -2.163126 | -1.890812 |
| C | -1.318219 | -2.006992 | -2.335166 | C | 2.049030 | -4.151035 | 0.356690 |
| H | -1.679737 | -2.500555 | -1.438894 | H | 3.385794 | -3.441253 | 1.893981 |
| C | -1.530665 | -2.754879 | -3.623276 | H | 0.711746 | -4.519638 | -1.293426 |
| H | -1.140250 | -2.198082 | -4.482327 | H | 2.153780 | -5.198873 | 0.623045 |
| H | -2.596280 | -2.947163 | -3.808341 | C | 2.977267 | 0.830957 | -0.539102 |
| H | -0.074844 | 1.931278 | 1.173635 | C | 3.068839 | 2.154563 | -0.087386 |
| H | -0.483758 | 0.636238 | 2.257681 | C | 4.166918 | 0.223597 | -0.982328 |
| Cl | 2.325279 | 0.778860 | 3.142275 | C | 4.289969 | 2.833855 | -0.058283 |
| H | 1.263899 | 0.658293 | 2.214111 | H | 2.182245 | 2.672294 | 0.254800 |

1rIM13

SCF energy in gas phase: -1591.308324

Free energy in Et₂O : -1590.760574

Enthalpy in Et₂O : -1590.670459

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| Zr | -1.936988 | 0.178849 | -0.172040 | H | 4.139237 | -0.795667 | -1.354712 |
| C | -3.323762 | -0.853559 | 1.722854 | C | 5.458727 | 2.208918 | -0.487682 |
| H | -4.199345 | -0.325955 | 2.075056 | H | 4.320741 | 3.857819 | 0.304960 |
| C | -2.001878 | -0.693981 | 2.214698 | H | 6.284961 | 0.390108 | -1.303364 |
| H | -1.688019 | -0.022046 | 3.000457 | H | 6.408481 | 2.735705 | -0.462324 |
| C | -1.157327 | -1.591430 | 1.503608 | C | 1.358798 | 0.211294 | -2.257687 |
| H | -0.095075 | -1.711256 | 1.647727 | C | 0.423126 | 0.811432 | -0.000643 |
| C | -1.956238 | -2.287436 | 0.566381 | H | 0.303740 | 1.730662 | -0.584064 |
| H | -1.601015 | -3.014844 | -0.147587 | C | 0.538971 | 1.249227 | 1.423219 |
| C | -3.293488 | -1.823940 | 0.689029 | H | 0.021497 | 2.191689 | 1.626989 |
| H | -4.134413 | -2.146295 | 0.089326 | H | 0.724069 | 0.669865 | 4.626008 |
| C | -2.009929 | 2.796238 | -0.130066 | C | 1.144471 | 0.711580 | 2.499136 |
| H | -1.127505 | 3.346102 | 0.163438 | H | 1.690821 | -0.221881 | 2.414118 |
| C | -2.360637 | 2.434876 | -1.454747 | C | 1.141358 | 1.342901 | 3.863858 |
| H | -1.782226 | 2.636815 | -2.346471 | H | 0.558153 | 2.270636 | 3.878794 |
| C | -3.608257 | 1.762123 | -1.409101 | H | 2.159092 | 1.587453 | 4.196936 |
| | | | | H | 1.397532 | 1.267379 | -2.542267 |
| | | | | H | 2.127614 | -0.313321 | -2.831309 |
| | | | | Cl | -2.150156 | -0.919868 | -2.374751 |
| | | | | H | 0.383203 | -0.178053 | -2.549973 |

1rTS16

SCF energy in gas phase: -2052.100271

Free energy in Et₂O : -2051.554497Enthalpy in Et₂O : -2051.460303

| | | | |
|----|-----------|-----------|-----------|
| Zr | 1.925850 | 0.160094 | -0.571963 |
| C | 3.453560 | 1.408215 | 1.024485 |
| H | 4.486260 | 1.098762 | 1.109059 |
| C | 2.362920 | 0.909910 | 1.794978 |
| H | 2.402229 | 0.138210 | 2.553558 |
| C | 1.195448 | 1.611602 | 1.393782 |
| H | 0.203430 | 1.476677 | 1.798678 |
| C | 1.560054 | 2.517563 | 0.364035 |
| H | 0.894925 | 3.182422 | -0.164025 |
| C | 2.956560 | 2.397438 | 0.142276 |
| H | 3.529920 | 2.945117 | -0.592966 |
| C | 2.154154 | -2.321807 | -1.377104 |
| H | 1.302048 | -2.845076 | -1.790167 |
| C | 3.094371 | -1.572258 | -2.119008 |
| H | 3.060912 | -1.380146 | -3.181479 |
| C | 4.059962 | -1.057882 | -1.211412 |
| H | 4.911487 | -0.443849 | -1.474656 |
| C | 3.732038 | -1.533223 | 0.089438 |
| H | 4.285463 | -1.356629 | 1.000336 |
| C | 2.547058 | -2.296178 | -0.005270 |
| H | 2.063040 | -2.779383 | 0.832059 |
| C | -1.776429 | 0.370144 | -0.792292 |
| C | -2.016900 | 1.478780 | 0.261053 |
| C | -2.619511 | 1.191518 | 1.498862 |
| C | -1.710862 | 2.824242 | 0.005499 |
| C | -2.839059 | 2.179719 | 2.458188 |
| H | -2.964990 | 0.185041 | 1.700136 |
| C | -1.935674 | 3.823013 | 0.958292 |
| H | -1.299246 | 3.115236 | -0.953459 |
| C | -2.487304 | 3.505435 | 2.197319 |
| H | -3.302280 | 1.913014 | 3.403993 |
| H | -1.682277 | 4.852743 | 0.721261 |
| H | -2.659972 | 4.278724 | 2.939944 |
| C | -3.073216 | -0.491477 | -0.931993 |
| C | -3.060236 | -1.856813 | -1.250310 |
| C | -4.328716 | 0.141220 | -0.885223 |
| C | -4.242575 | -2.566720 | -1.477717 |
| H | -2.121226 | -2.390155 | -1.332917 |
| C | -5.511353 | -0.560854 | -1.114297 |

| | | | |
|----|-----------|-----------|-----------|
| H | -4.385097 | 1.201186 | -0.661081 |
| C | -5.476931 | -1.924951 | -1.406533 |
| H | -4.190381 | -3.626007 | -1.714184 |
| H | -6.461803 | -0.036760 | -1.062593 |
| H | -6.396670 | -2.476019 | -1.579759 |
| C | -1.603102 | 1.000095 | -2.202706 |
| C | -0.503374 | -0.548583 | -0.548608 |
| H | -0.260807 | -0.974964 | -1.532389 |
| C | -0.540874 | -1.649054 | 0.388023 |
| H | -0.121334 | -2.576643 | -0.007379 |
| H | -1.358098 | -3.229900 | 3.280731 |
| C | -0.969731 | -1.784405 | 1.705928 |
| H | -1.449616 | -0.931482 | 2.177060 |
| C | -1.453838 | -3.145648 | 2.195260 |
| H | -0.871393 | -3.958097 | 1.746771 |
| H | -2.505558 | -3.301057 | 1.926805 |
| H | -1.545551 | 0.206813 | -2.953333 |
| H | -2.463138 | 1.627041 | -2.451689 |
| Cl | 1.918251 | 1.311520 | -2.748221 |
| H | -0.693861 | 1.595620 | -2.288875 |
| Cl | 1.404846 | -2.041121 | 3.457961 |
| H | 0.268286 | -1.805210 | 2.433832 |

1rTS17

SCF energy in gas phase: -1591.217849

Free energy in Et₂O : -1590.670826Enthalpy in Et₂O : -1590.582217

| | | | |
|----|----------|-----------|-----------|
| Zr | 1.667829 | -0.349586 | -0.320543 |
| C | 3.473639 | 1.273254 | -1.187518 |
| H | 4.480425 | 1.151127 | -0.810891 |
| C | 2.479772 | 2.124673 | -0.643969 |
| H | 2.594657 | 2.741313 | 0.234983 |
| C | 1.307203 | 1.997784 | -1.424471 |
| H | 0.374898 | 2.520500 | -1.271667 |
| C | 1.587024 | 1.089355 | -2.484463 |
| H | 0.911142 | 0.803660 | -3.276235 |
| C | 2.922436 | 0.648339 | -2.342165 |
| H | 3.436484 | -0.033019 | -3.006482 |
| C | 2.468215 | -2.266669 | 1.231286 |
| H | 2.258365 | -2.158881 | 2.286633 |
| C | 1.645370 | -2.900642 | 0.275460 |
| H | 0.687421 | -3.363476 | 0.468995 |
| C | 2.268892 | -2.783178 | -0.995790 |

| | | | | | | | |
|----|-----------|-----------|-----------|---------------|-----------|-----------|---|
| H | 1.881827 | -3.164174 | -1.931362 | 1rIM14 | | | |
| C | 3.498462 | -2.099148 | -0.813659 | | | | SCF energy in gas phase: -1591.307475 |
| H | 4.220955 | -1.874569 | -1.585886 | | | | Free energy in Et ₂ O : -1590.759231 |
| C | 3.614732 | -1.756161 | 0.557556 | | | | Enthalpy in Et ₂ O : -1590.666922 |
| H | 4.436744 | -1.226188 | 1.018961 | | | | |
| C | -1.326466 | -0.366295 | -0.235091 | Zr | -2.086938 | -0.109902 | 0.037418 |
| C | -2.018672 | 0.950787 | -0.651648 | C | -4.060793 | -0.147329 | 1.648057 |
| C | -2.877321 | 1.596889 | 0.258281 | H | -5.002587 | 0.243292 | 1.285832 |
| C | -1.930468 | 1.501481 | -1.937437 | C | -3.067622 | 0.588152 | 2.348317 |
| C | -3.576700 | 2.751514 | -0.085357 | H | -3.100773 | 1.646184 | 2.564956 |
| H | -3.018157 | 1.174178 | 1.246438 | C | -2.002971 | -0.290083 | 2.649651 |
| C | -2.631521 | 2.659500 | -2.291450 | H | -1.088548 | -0.027728 | 3.163031 |
| H | -1.314400 | 1.026026 | -2.690027 | C | -2.341974 | -1.582510 | 2.159157 |
| C | -3.452693 | 3.297328 | -1.365360 | H | -1.731068 | -2.472026 | 2.235731 |
| H | -4.230524 | 3.219397 | 0.645869 | C | -3.619861 | -1.498659 | 1.559048 |
| H | -2.534200 | 3.054650 | -3.299209 | H | -4.166015 | -2.317346 | 1.111527 |
| H | -3.998849 | 4.195916 | -1.637755 | C | -2.018176 | -0.052251 | -2.553047 |
| C | -2.497942 | -1.350562 | 0.046712 | H | -1.323070 | 0.642960 | -2.999563 |
| C | -2.901047 | -1.725018 | 1.334270 | C | -1.736149 | -1.391313 | -2.187896 |
| C | -3.216819 | -1.880137 | -1.039518 | H | -0.805452 | -1.913645 | -2.347440 |
| C | -3.975266 | -2.598946 | 1.533684 | C | -2.891356 | -1.931256 | -1.566564 |
| H | -2.377133 | -1.333781 | 2.200204 | H | -2.998623 | -2.940873 | -1.192294 |
| C | -4.285836 | -2.751440 | -0.846994 | C | -3.902747 | -0.927019 | -1.579040 |
| H | -2.933187 | -1.598792 | -2.049479 | H | -4.909025 | -1.031342 | -1.196225 |
| C | -4.671814 | -3.119054 | 0.445418 | C | -3.360719 | 0.229902 | -2.186791 |
| H | -4.262744 | -2.871199 | 2.545979 | H | -3.864967 | 1.177758 | -2.315800 |
| H | -4.821342 | -3.143935 | -1.707551 | C | 1.489954 | -0.369720 | -0.199683 |
| H | -5.504118 | -3.800175 | 0.598362 | C | 2.062695 | 0.749870 | 0.696178 |
| C | -0.358747 | -0.981942 | -1.290697 | C | 3.416905 | 1.108428 | 0.568465 |
| C | -0.358437 | -0.242978 | 1.011133 | C | 1.298982 | 1.434410 | 1.647120 |
| H | -0.319907 | -1.251748 | 1.427701 | C | 3.975983 | 2.118130 | 1.347812 |
| C | -0.504271 | 0.683565 | 2.128251 | H | 4.039604 | 0.585937 | -0.150716 |
| H | -0.600470 | 0.221613 | 3.117974 | C | 1.854837 | 2.449068 | 2.433066 |
| H | 0.175938 | 3.637793 | 3.533251 | H | 0.249174 | 1.201033 | 1.761895 |
| C | -0.356904 | 2.044498 | 2.164306 | C | 3.195689 | 2.797127 | 2.287837 |
| H | -0.229840 | 2.577737 | 1.222323 | H | 5.025223 | 2.372629 | 1.224315 |
| C | -0.611950 | 2.890052 | 3.385056 | H | 1.230740 | 2.967819 | 3.155815 |
| H | -0.674860 | 2.277182 | 4.290409 | H | 3.630157 | 3.583559 | 2.898454 |
| H | -1.557080 | 3.439681 | 3.288678 | C | 2.505841 | -1.554480 | -0.126925 |
| H | -0.445259 | -2.068709 | -1.249456 | C | 3.250109 | -1.997169 | -1.228889 |
| H | -0.562816 | -0.700563 | -2.323853 | C | 2.716613 | -2.208834 | 1.100411 |
| Cl | 2.572684 | 0.998247 | 2.396448 | C | 4.145239 | -3.067408 | -1.119315 |
| H | 1.199998 | 1.440603 | 2.380234 | H | 3.151340 | -1.496136 | -2.185472 |
| | | | | C | 3.606241 | -3.273584 | 1.214279 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 2.187723 | -1.867955 | 1.985001 | H | 4.319507 | 0.547604 | -2.297478 |
| C | 4.323607 | -3.716518 | 0.099165 | C | 3.845877 | -1.441432 | -1.396923 |
| H | 4.706026 | -3.384894 | -1.994536 | H | 4.793793 | -1.754121 | -0.979128 |
| H | 3.745345 | -3.755807 | 2.178309 | C | -1.617846 | 0.279751 | -0.294451 |
| H | 5.017538 | -4.547812 | 0.185458 | C | -2.650358 | -0.181551 | 0.754428 |
| C | 0.108628 | -0.930256 | 0.326534 | C | -4.012461 | 0.057420 | 0.497401 |
| C | 1.333779 | 0.055361 | -1.656790 | C | -2.305051 | -0.755351 | 1.982153 |
| H | 1.123922 | -0.802503 | -2.294822 | C | -4.993687 | -0.288771 | 1.421728 |
| C | 1.377807 | 1.231299 | -2.302004 | H | -4.302282 | 0.522420 | -0.440069 |
| H | 1.217594 | 1.161775 | -3.381894 | C | -3.289337 | -1.100732 | 2.914814 |
| H | 2.908472 | 4.347764 | -2.223067 | H | -1.270554 | -0.972039 | 2.216768 |
| C | 1.590977 | 2.649577 | -1.841611 | C | -4.635137 | -0.872501 | 2.640479 |
| H | 1.666652 | 2.721002 | -0.758286 | H | -6.038672 | -0.097484 | 1.193615 |
| C | 2.823165 | 3.292235 | -2.501125 | H | -2.992462 | -1.555670 | 3.855533 |
| H | 2.766749 | 3.237918 | -3.594763 | H | -5.397753 | -1.142281 | 3.365494 |
| H | 3.742196 | 2.785710 | -2.189626 | C | -1.875342 | 1.812543 | -0.487838 |
| H | 0.012637 | -1.946988 | -0.080026 | C | -2.221526 | 2.386409 | -1.718095 |
| H | 0.229189 | -1.082533 | 1.401695 | C | -1.768730 | 2.672265 | 0.621706 |
| Cl | -1.842867 | 2.323100 | -0.107772 | C | -2.418620 | 3.766708 | -1.844745 |
| H | 0.698017 | 3.224610 | -2.124606 | H | -2.362636 | 1.758108 | -2.589877 |

1rTS18

SCF energy in gas phase: -2052.08049

Free energy in Et₂O : -2051.535907

Enthalpy in Et₂O : -2051.440415

| | | | | | | | |
|----|----------|-----------|-----------|----|-----------|-----------|-----------|
| Zr | 2.289027 | -0.118513 | 0.101555 | H | -1.560911 | 2.253763 | 1.602187 |
| C | 4.171572 | 1.583954 | 0.444652 | C | -2.279381 | 4.605404 | -0.742657 |
| H | 5.137594 | 1.349737 | 0.018325 | H | -2.689039 | 4.178706 | -2.813293 |
| C | 3.749920 | 1.277927 | 1.757897 | H | -1.874231 | 4.680859 | 1.376877 |
| H | 4.314500 | 0.722581 | 2.491986 | H | -2.431727 | 5.676257 | -0.841007 |
| C | 2.426299 | 1.765988 | 1.922947 | C | -0.116424 | 0.157053 | 0.207087 |
| H | 1.824568 | 1.668263 | 2.816747 | C | -1.714051 | -0.418989 | -1.646008 |
| C | 2.051142 | 2.426178 | 0.724895 | H | -1.110174 | 0.093479 | -2.395552 |
| H | 1.104519 | 2.915886 | 0.538820 | C | -2.331724 | -1.525572 | -2.085159 |
| C | 3.111306 | 2.291664 | -0.203161 | H | -2.169551 | -1.743876 | -3.144215 |
| H | 3.134866 | 2.702743 | -1.203440 | H | -5.167556 | -3.465723 | -1.600202 |
| C | 2.634576 | -2.187616 | -1.366274 | C | -3.197272 | -2.550434 | -1.405369 |
| H | 2.479793 | -3.139121 | -0.879296 | H | -3.285448 | -2.364118 | -0.336904 |
| C | 1.634193 | -1.426276 | -2.010315 | C | -4.589666 | -2.652645 | -2.051018 |
| H | 0.598644 | -1.713925 | -2.116540 | H | -4.519629 | -2.849422 | -3.127364 |
| C | 2.220520 | -0.200166 | -2.441995 | H | -5.155423 | -1.724631 | -1.919213 |
| H | 1.717530 | 0.592973 | -2.980449 | H | 0.373098 | 0.890270 | -0.482885 |
| C | 3.593666 | -0.224805 | -2.085377 | H | -0.082357 | 0.641306 | 1.189160 |
| | | | | Cl | 2.858388 | -1.716582 | 1.857724 |
| | | | | H | -2.686201 | -3.517683 | -1.501724 |
| | | | | Cl | -0.211834 | -2.916815 | 0.434014 |
| | | | | H | -0.027475 | -1.463175 | 0.303386 |

(Z)1p

SCF energy in gas phase: -697.966277

Free energy in Et₂O : -697.280987Enthalpy in Et₂O : -697.218676**1rTS19**

SCF energy in gas phase: -1130.409426

Free energy in Et₂O : -1129.880598Enthalpy in Et₂O : -1129.792651

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 0.234186 | 0.129283 | 1.055097 | C | -2.251608 | -0.147405 | -0.470680 |
| C | 1.611819 | 0.072853 | 0.346136 | C | -2.573248 | 1.324016 | -0.339233 |
| C | 2.517496 | -0.970488 | 0.599156 | C | -2.731577 | 1.907736 | 0.927690 |
| C | 1.988708 | 1.041736 | -0.594762 | C | -2.767599 | 2.130320 | -1.469021 |
| C | 3.747288 | -1.040248 | -0.056382 | C | -3.068629 | 3.254526 | 1.059078 |
| H | 2.266233 | -1.747809 | 1.311648 | H | -2.574940 | 1.302739 | 1.815393 |
| C | 3.217085 | 0.975333 | -1.254116 | C | -3.108063 | 3.478942 | -1.341481 |
| H | 1.319179 | 1.867477 | -0.803403 | H | -2.651697 | 1.696132 | -2.458114 |
| C | 4.105435 | -0.065438 | -0.987338 | C | -3.259728 | 4.046310 | -0.076035 |
| H | 4.425658 | -1.859588 | 0.164773 | H | -3.180339 | 3.687308 | 2.049614 |
| H | 3.479402 | 1.745009 | -1.974720 | H | -3.255868 | 4.084159 | -2.231943 |
| H | 5.063775 | -0.116134 | -1.495918 | H | -3.523097 | 5.095407 | 0.026014 |
| C | -0.823924 | -0.730711 | 0.321605 | C | -3.428755 | -1.054421 | -0.185129 |
| C | -0.516553 | -1.541893 | -0.777721 | C | -3.631100 | -1.600491 | 1.089825 |
| C | -2.141847 | -0.761497 | 0.809966 | C | -4.366419 | -1.341364 | -1.187817 |
| C | -1.490660 | -2.349716 | -1.372470 | C | -4.737561 | -2.408972 | 1.357427 |
| H | 0.489443 | -1.544217 | -1.180559 | H | -2.911525 | -1.391148 | 1.876942 |
| C | -3.113302 | -1.568031 | 0.221623 | C | -5.472601 | -2.149530 | -0.925456 |
| H | -2.413198 | -0.133982 | 1.653244 | H | -4.222838 | -0.925661 | -2.181679 |
| C | -2.791995 | -2.369202 | -0.876687 | C | -5.662466 | -2.686603 | 0.349902 |
| H | -1.223501 | -2.964977 | -2.227211 | H | -4.875285 | -2.823239 | 2.352632 |
| H | -4.123771 | -1.569872 | 0.621128 | H | -6.186434 | -2.361615 | -1.716954 |
| H | -3.548064 | -2.997647 | -1.338201 | H | -6.522742 | -3.317486 | 0.555194 |
| C | 0.363608 | -0.449611 | 2.496707 | C | -1.268905 | -0.579769 | -1.541518 |
| C | -0.201455 | 1.588495 | 1.235037 | C | -0.851403 | -0.660345 | -0.093669 |
| H | 0.184085 | 2.023306 | 2.157471 | H | -0.875387 | -1.666554 | 0.324521 |
| C | -0.930951 | 2.406487 | 0.464342 | C | 0.227438 | 0.220141 | 0.503586 |
| H | -1.086424 | 3.412972 | 0.858720 | H | 0.063971 | 1.262859 | 0.211776 |
| H | -3.489568 | 2.366796 | -1.891839 | C | 0.328182 | 0.101971 | 1.977560 |
| C | -1.561444 | 2.182445 | -0.885120 | H | 0.167795 | -0.905583 | 2.369703 |
| H | -1.363579 | 1.174355 | -1.253135 | C | 0.617993 | 1.058178 | 2.882680 |
| C | -3.074543 | 2.455428 | -0.882871 | H | 0.758385 | 2.097647 | 2.596949 |
| H | -3.295006 | 3.464791 | -0.517184 | H | 0.699962 | 0.828924 | 3.940853 |
| H | -3.597906 | 1.742884 | -0.238753 | H | -1.470969 | -1.502024 | -2.080195 |
| H | -0.562795 | -0.284672 | 3.052546 | H | -0.802397 | 0.193331 | -2.145220 |
| H | 0.549161 | -1.525692 | 2.487745 | H | 1.984874 | -0.114400 | -2.025805 |
| H | -1.085513 | 2.873803 | -1.596977 | Zr | 2.425689 | -0.207718 | -0.240996 |
| H | 1.178676 | 0.041854 | 3.037416 | C | 2.999810 | -2.475527 | -1.330079 |
| | | | | H | 3.088108 | -2.521366 | -2.405989 |

| | | | | | | | |
|---|----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 1.815310 | -2.714874 | -0.580742 | H | 4.943175 | -2.820607 | -2.172341 |
| H | 0.844887 | -2.951911 | -0.993892 | H | 5.762761 | -2.533351 | 2.039659 |
| C | 2.123349 | -2.565106 | 0.791326 | H | 6.344944 | -3.426072 | -0.208276 |
| H | 1.436004 | -2.693636 | 1.615778 | C | 0.997249 | -0.543414 | 1.386495 |
| C | 3.494804 | -2.204214 | 0.900683 | C | 0.714495 | -0.635704 | -0.110424 |
| H | 4.039984 | -2.044211 | 1.821673 | H | 0.762061 | -1.651074 | -0.501297 |
| C | 4.037647 | -2.168427 | -0.415440 | C | -0.298979 | 0.247802 | -0.810670 |
| H | 5.064853 | -1.944991 | -0.671648 | H | -0.130567 | 1.291480 | -0.520353 |
| C | 3.256604 | 2.040359 | -1.191421 | C | -0.282874 | 0.131915 | -2.286829 |
| H | 2.876556 | 2.368162 | -2.148143 | H | -0.237784 | -0.887806 | -2.677544 |
| C | 2.686963 | 2.320103 | 0.078926 | C | -0.328914 | 1.126943 | -3.189363 |
| H | 1.802346 | 2.913629 | 0.262298 | H | -0.334806 | 2.172650 | -2.890197 |
| C | 3.502785 | 1.708808 | 1.070400 | H | -0.354145 | 0.925947 | -4.256196 |
| H | 3.331045 | 1.735672 | 2.137530 | H | 1.116339 | -1.465129 | 1.948579 |
| C | 4.574638 | 1.053633 | 0.411846 | H | 0.517428 | 0.252646 | 1.948122 |
| H | 5.370160 | 0.499557 | 0.892611 | H | -1.981372 | -0.333657 | 2.145299 |
| C | 4.419352 | 1.252641 | -0.984789 | Zr | -2.309854 | -0.227055 | 0.330867 |
| H | 5.065767 | 0.863208 | -1.760585 | C | -3.123799 | -2.554383 | 1.107805 |

1rIM15

SCF energy in gas phase: -1130.41101

Free energy in Et₂O : -1129.883778

Enthalpy in Et₂O : -1129.79481

| | | | |
|---|----------|-----------|-----------|
| C | 2.076808 | -0.148431 | 0.403773 |
| C | 2.444782 | 1.314584 | 0.296936 |
| C | 2.684590 | 1.902938 | -0.954503 |
| C | 2.606497 | 2.103297 | 1.444240 |
| C | 3.070555 | 3.239580 | -1.053661 |
| H | 2.547934 | 1.313078 | -1.855316 |
| C | 2.995865 | 3.441116 | 1.348507 |
| H | 2.428726 | 1.663501 | 2.421831 |
| C | 3.229623 | 4.014175 | 0.098027 |
| H | 3.244886 | 3.677759 | -2.032611 |
| H | 3.117752 | 4.033266 | 2.251528 |
| H | 3.531012 | 5.055055 | 0.020556 |
| C | 3.251957 | -1.087545 | 0.234036 |
| C | 3.591082 | -1.598116 | -1.026583 |
| C | 4.051095 | -1.436686 | 1.331859 |
| C | 4.697652 | -2.433739 | -1.187026 |
| H | 2.978910 | -1.340081 | -1.886706 |
| C | 5.157092 | -2.272596 | 1.175919 |
| H | 3.800508 | -1.048651 | 2.315648 |
| C | 5.484830 | -2.773944 | -0.085606 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.319567 | -2.703524 | 2.160047 |
| C | -1.885533 | -2.784042 | 0.450502 |
| H | -0.977134 | -3.133274 | 0.922475 |
| C | -2.045667 | -2.470711 | -0.921611 |
| H | -1.291740 | -2.566346 | -1.688882 |
| C | -3.376976 | -2.014170 | -1.114352 |
| H | -3.817912 | -1.719223 | -2.057285 |
| C | -4.045613 | -2.083163 | 0.141614 |
| H | -5.080615 | -1.827039 | 0.323279 |
| C | -3.380371 | 1.801181 | 1.517278 |
| H | -3.307194 | 1.878600 | 2.592129 |
| C | -2.465047 | 2.337208 | 0.573656 |
| H | -1.562700 | 2.886854 | 0.809132 |
| C | -2.931913 | 2.025562 | -0.729225 |
| H | -2.443383 | 2.273936 | -1.661268 |
| C | -4.128581 | 1.277564 | -0.594995 |
| H | -4.738417 | 0.903848 | -1.406773 |
| C | -4.404522 | 1.135889 | 0.796275 |
| H | -5.257231 | 0.630762 | 1.229620 |

1rTS20

SCF energy in gas phase: -1130.401653

Free energy in Et₂O : -1129.870627

Enthalpy in Et₂O : -1129.785965

| | | | |
|---|-----------|-----------|-----------|
| C | -2.255030 | -0.337996 | -0.375661 |
|---|-----------|-----------|-----------|

| | | | | | | | |
|---|----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 2.037700 | -1.839606 | -1.820637 | H | 1.307345 | -0.086678 | 3.285461 |
| H | 1.380162 | -1.560047 | -2.630281 | H | -1.674662 | -1.387073 | -2.228830 |
| C | 3.445070 | -1.668789 | -1.793585 | H | -1.162839 | 0.357954 | -2.386043 |
| H | 4.045273 | -1.246052 | -2.587900 | H | 3.304789 | -0.796940 | 1.829991 |
| C | 3.927259 | -2.179311 | -0.554736 | Zr | 2.572469 | -0.207422 | 0.256939 |
| H | 4.961604 | -2.208433 | -0.238882 | C | 4.593225 | 1.255397 | 0.895510 |

1r'F2

SCF energy in gas phase: -1130.426372

Free energy in Et₂O : -1129.88685

Enthalpy in Et₂O : -1129.800504

| | | | |
|---|-----------|-----------|-----------|
| C | -2.360561 | -0.079192 | -0.545286 |
| C | -2.797099 | 1.355911 | -0.367384 |
| C | -2.966276 | 1.880304 | 0.924170 |
| C | -3.078940 | 2.184616 | -1.460987 |
| C | -3.393384 | 3.193407 | 1.114260 |
| H | -2.762064 | 1.249151 | 1.784153 |
| C | -3.508883 | 3.500898 | -1.274438 |
| H | -2.966156 | 1.795461 | -2.468819 |
| C | -3.665581 | 4.010935 | 0.014005 |
| H | -3.514457 | 3.579984 | 2.122574 |
| H | -3.724015 | 4.124581 | -2.137942 |
| H | -3.999160 | 5.034201 | 0.161492 |
| C | -3.401156 | -1.090499 | -0.114511 |
| C | -3.339619 | -1.717559 | 1.137064 |
| C | -4.478781 | -1.393571 | -0.959903 |
| C | -4.325761 | -2.623933 | 1.533619 |
| H | -2.511158 | -1.494857 | 1.804312 |
| C | -5.464126 | -2.299100 | -0.568366 |
| H | -4.540395 | -0.912010 | -1.932355 |
| C | -5.390825 | -2.918290 | 0.681981 |
| H | -4.259391 | -3.100482 | 2.507935 |
| H | -6.289192 | -2.522913 | -1.239144 |
| H | -6.156786 | -3.625273 | 0.987824 |
| C | -1.480712 | -0.444168 | -1.724692 |
| C | -0.881511 | -0.462218 | -0.339763 |
| H | -0.766437 | -1.450733 | 0.093202 |
| C | 0.126858 | 0.563108 | 0.084892 |
| H | -0.011312 | 1.514106 | -0.424800 |
| C | 0.528497 | 0.695070 | 1.445172 |
| H | 0.783900 | 1.702664 | 1.767913 |
| C | 0.926886 | -0.321696 | 2.299784 |
| H | 0.624733 | -1.353645 | 2.145763 |

| | | | |
|---|----------|-----------|-----------|
| H | 5.270155 | 0.893255 | 1.655270 |
| C | 3.454998 | 2.076657 | 1.114652 |
| H | 3.121015 | 2.443977 | 2.075591 |
| C | 2.854097 | 2.347259 | -0.142862 |
| H | 1.975886 | 2.954899 | -0.312241 |
| C | 3.597297 | 1.670611 | -1.139476 |
| H | 3.400167 | 1.689272 | -2.203117 |
| C | 4.679998 | 1.002205 | -0.495407 |
| H | 5.448846 | 0.423184 | -0.987829 |
| C | 3.100494 | -2.739277 | 0.187275 |
| H | 3.451266 | -3.226117 | 1.085224 |
| C | 1.747912 | -2.596471 | -0.216116 |
| H | 0.889391 | -2.987082 | 0.312480 |
| C | 1.724347 | -1.916657 | -1.467956 |
| H | 0.844128 | -1.672166 | -2.042339 |
| C | 3.060928 | -1.621425 | -1.823232 |
| H | 3.380685 | -1.112288 | -2.722787 |
| C | 3.911891 | -2.124183 | -0.797601 |
| H | 4.991670 | -2.066371 | -0.776918 |

1r'FTS6

SCF energy in gas phase: -1130.410173

Free energy in Et₂O : -1129.872408

Enthalpy in Et₂O : -1129.786426

| | | | |
|---|-----------|-----------|-----------|
| C | -2.348969 | -0.086235 | -0.541794 |
| C | -2.751259 | 1.358821 | -0.362357 |
| C | -2.880386 | 1.894967 | 0.929016 |
| C | -3.042179 | 2.186102 | -1.454765 |
| C | -3.278990 | 3.216892 | 1.119850 |
| H | -2.662826 | 1.266835 | 1.787707 |
| C | -3.443384 | 3.511353 | -1.267574 |
| H | -2.957374 | 1.788638 | -2.462125 |
| C | -3.561766 | 4.032253 | 0.020638 |
| H | -3.368750 | 3.612520 | 2.128017 |
| H | -3.665523 | 4.133851 | -2.130204 |
| H | -3.872763 | 5.062567 | 0.168832 |
| C | -3.414730 | -1.070038 | -0.109251 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.370455 | -1.694972 | 1.144025 | | | | |
| C | -4.498958 | -1.349638 | -0.954481 | 1r'F3 | | | |
| C | -4.378835 | -2.575607 | 1.542645 | SCF energy in gas phase: -1130.423967 | | | |
| H | -2.537419 | -1.489763 | 1.811085 | Free energy in Et ₂ O : -1129.892106 | | | |
| C | -5.506962 | -2.229046 | -0.561189 | Enthalpy in Et ₂ O : -1129.803932 | | | |
| H | -4.547511 | -0.869752 | -1.928500 | | | | |
| C | -5.450272 | -2.846144 | 0.691061 | C | -2.286487 | -0.052862 | -0.560390 |
| H | -4.325289 | -3.050794 | 2.518498 | C | -2.602217 | 1.387920 | -0.233101 |
| H | -6.336864 | -2.434207 | -1.232044 | C | -2.727287 | 1.793388 | 1.105267 |
| H | -6.233892 | -3.532893 | 0.998369 | C | -2.820021 | 2.341539 | -1.236140 |
| C | -1.486768 | -0.472607 | -1.728654 | C | -3.053091 | 3.109487 | 1.429096 |
| C | -0.878223 | -0.502656 | -0.348846 | H | -2.566575 | 1.065994 | 1.895663 |
| H | -0.780440 | -1.494424 | 0.083539 | C | -3.147982 | 3.661393 | -0.916270 |
| C | 0.167396 | 0.494414 | 0.058179 | H | -2.736013 | 2.046288 | -2.278238 |
| H | -0.015482 | 1.467493 | -0.392878 | C | -3.264493 | 4.050832 | 0.418008 |
| C | 0.612748 | 0.616407 | 1.427245 | H | -3.141402 | 3.402018 | 2.471993 |
| H | 0.818829 | 1.626389 | 1.769512 | H | -3.314895 | 4.383125 | -1.711496 |
| C | 1.143217 | -0.408415 | 2.285731 | H | -3.518645 | 5.076751 | 0.669379 |
| H | 0.728014 | -1.414587 | 2.217551 | C | -3.438984 | -0.998457 | -0.297645 |
| H | 1.321022 | -0.112748 | 3.317566 | C | -3.507509 | -1.764335 | 0.873804 |
| H | -1.707778 | -1.410709 | -2.230853 | C | -4.490697 | -1.100941 | -1.220931 |
| H | -1.152520 | 0.321087 | -2.392147 | C | -4.593457 | -2.608719 | 1.116879 |
| H | 2.524956 | -0.738038 | 2.050369 | H | -2.701269 | -1.700935 | 1.599222 |
| Zr | 2.505493 | -0.186987 | 0.198326 | C | -5.575934 | -1.943306 | -0.982734 |
| C | 4.598705 | 1.118182 | 0.834984 | H | -4.452859 | -0.512073 | -2.133771 |
| H | 5.304605 | 0.653144 | 1.509465 | C | -5.631449 | -2.701650 | 0.189406 |
| C | 3.527848 | 1.975057 | 1.204359 | H | -4.626002 | -3.194936 | 2.031395 |
| H | 3.266490 | 2.259489 | 2.215237 | H | -6.378660 | -2.009344 | -1.712346 |
| C | 2.868946 | 2.399576 | 0.020470 | H | -6.475516 | -3.359698 | 0.375844 |
| H | 2.006738 | 3.050577 | -0.029307 | C | -1.392997 | -0.358064 | -1.747445 |
| C | 3.514895 | 1.798629 | -1.083665 | C | -0.856801 | -0.588238 | -0.354019 |
| H | 3.249467 | 1.930781 | -2.124270 | H | -0.847097 | -1.630071 | -0.048451 |
| C | 4.590439 | 1.008764 | -0.582117 | C | 0.248826 | 0.263171 | 0.200019 |
| H | 5.297478 | 0.451100 | -1.180066 | H | 0.092136 | 1.309143 | -0.064586 |
| C | 3.089686 | -2.705684 | 0.243739 | C | 0.804176 | 0.072910 | 1.556591 |
| H | 3.425340 | -3.156733 | 1.167282 | H | 0.937787 | 1.006358 | 2.106963 |
| C | 1.741662 | -2.602257 | -0.203548 | C | 0.298945 | -1.020291 | 2.488875 |
| H | 0.875334 | -2.989784 | 0.314602 | H | -0.690461 | -0.771105 | 2.904573 |
| C | 1.742109 | -1.984176 | -1.485060 | H | 0.973594 | -1.158069 | 3.342151 |
| H | 0.874587 | -1.776902 | -2.092707 | H | -1.643258 | -1.216060 | -2.365912 |
| C | 3.083648 | -1.683561 | -1.815990 | H | -0.980295 | 0.484209 | -2.297417 |
| H | 3.421315 | -1.207361 | -2.727469 | H | 0.199372 | -1.994831 | 2.002379 |
| C | 3.916767 | -2.135248 | -0.749703 | Zr | 2.527286 | -0.151111 | 0.018436 |
| H | 4.994966 | -2.057100 | -0.705778 | C | 3.731892 | 1.902375 | 1.048811 |

| | | | | | | | |
|---|----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 3.883349 | 1.941069 | 2.119995 | C | -4.998209 | -3.003778 | -0.435621 |
| C | 2.634675 | 2.455356 | 0.344610 | H | -4.607928 | -3.389576 | 1.649306 |
| H | 1.790751 | 2.966075 | 0.788283 | H | -5.143537 | -2.398650 | -2.501150 |
| C | 2.811513 | 2.197674 | -1.036789 | H | -5.805056 | -3.727711 | -0.504594 |
| H | 2.141797 | 2.503934 | -1.829953 | C | -0.594666 | -0.305225 | -1.068305 |
| C | 4.027621 | 1.472994 | -1.194820 | C | -0.569288 | -0.481432 | 0.590194 |
| H | 4.465224 | 1.157866 | -2.133043 | H | -0.535143 | -1.540357 | 0.832766 |
| C | 4.598415 | 1.290500 | 0.099445 | C | 0.244998 | 0.417434 | 1.409081 |
| H | 5.542944 | 0.808456 | 0.314547 | H | -0.053916 | 1.460126 | 1.393019 |
| C | 2.866050 | -2.566233 | 0.803587 | C | 1.369963 | 0.014296 | 2.235119 |
| H | 2.761836 | -2.793413 | 1.855911 | H | 1.789049 | 0.862348 | 2.775466 |
| C | 1.844943 | -2.674547 | -0.176564 | C | 1.308576 | -1.214335 | 3.133386 |
| H | 0.827068 | -2.988442 | -0.000253 | H | 0.631602 | -1.042727 | 3.984413 |
| C | 2.387518 | -2.313407 | -1.432645 | H | 2.293308 | -1.454891 | 3.548856 |
| H | 1.850154 | -2.295042 | -2.372575 | H | -0.610332 | -1.182904 | -1.704064 |
| C | 3.754701 | -1.977211 | -1.240359 | H | -0.213581 | 0.600018 | -1.532429 |
| H | 4.453460 | -1.682857 | -2.012275 | H | 0.947669 | -2.111890 | 2.620934 |
| C | 4.053304 | -2.132652 | 0.145365 | Zr | 1.981229 | -0.066197 | -0.053327 |
| H | 5.022995 | -1.991720 | 0.605106 | C | 3.695330 | 1.836119 | 0.244933 |

1r'FTS7

SCF energy in gas phase: -1130.414774

Free energy in Et₂O : -1129.87433

Enthalpy in Et₂O : -1129.790938

| | | | |
|---|-----------|-----------|-----------|
| C | -1.802993 | -0.091325 | -0.169891 |
| C | -2.340666 | 1.317634 | -0.020627 |
| C | -2.853659 | 1.738459 | 1.215688 |
| C | -2.394343 | 2.205608 | -1.102654 |
| C | -3.397108 | 3.013761 | 1.366674 |
| H | -2.822539 | 1.059484 | 2.062637 |
| C | -2.940966 | 3.482863 | -0.955209 |
| H | -2.014802 | 1.894441 | -2.072138 |
| C | -3.441480 | 3.891940 | 0.281161 |
| H | -3.785312 | 3.322795 | 2.333174 |
| H | -2.977353 | 4.155118 | -1.807992 |
| H | -3.864072 | 4.885647 | 0.398491 |
| C | -2.902739 | -1.133533 | -0.259874 |
| C | -3.286403 | -1.885184 | 0.857933 |
| C | -3.588571 | -1.329980 | -1.466899 |
| C | -4.325857 | -2.814235 | 0.771897 |
| H | -2.767560 | -1.743335 | 1.802171 |
| C | -4.625897 | -2.257226 | -1.556405 |
| H | -3.303624 | -0.750610 | -2.341166 |

| | | | |
|---|----------|-----------|-----------|
| H | 4.472585 | 1.714402 | 0.987603 |
| C | 2.452584 | 2.483689 | 0.441520 |
| H | 2.102673 | 2.912929 | 1.370291 |
| C | 1.727353 | 2.437365 | -0.773880 |
| H | 0.736599 | 2.844181 | -0.931020 |
| C | 2.522680 | 1.759957 | -1.738347 |
| H | 2.267603 | 1.594584 | -2.777464 |
| C | 3.747481 | 1.397673 | -1.108643 |
| H | 4.584251 | 0.907937 | -1.585359 |
| C | 3.158406 | -2.256140 | 0.685956 |
| H | 3.405479 | -2.386954 | 1.728673 |
| C | 1.947643 | -2.652656 | 0.053082 |
| H | 1.119794 | -3.161897 | 0.526607 |
| C | 2.055115 | -2.349162 | -1.333915 |
| H | 1.312934 | -2.558097 | -2.093051 |
| C | 3.318463 | -1.761403 | -1.555803 |
| H | 3.698509 | -1.413934 | -2.507782 |
| C | 3.997878 | -1.695063 | -0.304279 |
| H | 4.991805 | -1.299314 | -0.140739 |

1r'F4

SCF energy in gas phase: -1130.437669

Free energy in Et₂O : -1129.890936

Enthalpy in Et₂O : -1129.807664

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | -1.440416 | -0.147328 | -0.110438 | H | 1.599013 | 1.690075 | -2.804090 |
| C | -2.139351 | 1.221632 | 0.027652 | C | 3.317465 | 1.562104 | -1.387775 |
| C | -2.668683 | 1.622927 | 1.265886 | H | 4.096800 | 1.124907 | -1.996436 |
| C | -2.365932 | 2.057485 | -1.074736 | C | 3.266417 | -2.045396 | 0.593023 |
| C | -3.368459 | 2.821175 | 1.402899 | H | 3.659681 | -2.075306 | 1.597802 |
| H | -2.533023 | 0.985661 | 2.134023 | C | 2.046955 | -2.629034 | 0.149583 |
| C | -3.069399 | 3.258106 | -0.943467 | H | 1.357510 | -3.201816 | 0.754409 |
| H | -2.001875 | 1.769311 | -2.055105 | C | 1.930272 | -2.398514 | -1.245250 |
| C | -3.569109 | 3.650321 | 0.297524 | H | 1.124239 | -2.736752 | -1.879336 |
| H | -3.761134 | 3.104741 | 2.375698 | C | 3.053181 | -1.648294 | -1.660563 |
| H | -3.226942 | 3.884121 | -1.817674 | H | 3.253721 | -1.313386 | -2.669829 |
| H | -4.113133 | 4.584656 | 0.401847 | C | 3.883868 | -1.433786 | -0.521527 |
| C | -2.565731 | -1.195380 | -0.230625 | H | 4.831143 | -0.912008 | -0.511984 |
| C | -3.040688 | -1.894944 | 0.886255 | | | | |
| C | -3.174296 | -1.441122 | -1.470162 | | | | |
| C | -4.083477 | -2.817540 | 0.770019 | | | | |
| H | -2.592980 | -1.718295 | 1.860666 | | | | |
| C | -4.217425 | -2.358151 | -1.590697 | | | | |
| H | -2.822639 | -0.908828 | -2.349103 | | | | |
| C | -4.676572 | -3.054076 | -0.469689 | Zr | -2.318327 | -0.212175 | 0.078788 |
| H | -4.430515 | -3.350477 | 1.651327 | C | -4.050060 | -2.050415 | -0.416919 |
| H | -4.671650 | -2.531672 | -2.562666 | H | -5.099990 | -1.805076 | -0.322380 |
| H | -5.486322 | -3.772171 | -0.563041 | C | -3.231747 | -2.589497 | 0.600954 |
| C | -0.379490 | -0.248316 | -1.239835 | H | -3.543967 | -2.821489 | 1.609806 |
| C | -0.496870 | -0.472349 | 1.052336 | C | -1.921566 | -2.750000 | 0.070471 |
| H | -0.318861 | -1.538155 | 1.180467 | H | -1.071007 | -3.163820 | 0.594737 |
| C | 0.247418 | 0.419109 | 1.796818 | C | -1.932280 | -2.318339 | -1.285777 |
| H | -0.013922 | 1.469878 | 1.689301 | H | -1.101074 | -2.356518 | -1.975932 |
| C | 1.528311 | 0.124092 | 2.390081 | C | -3.251683 | -1.881639 | -1.583453 |
| H | 1.993592 | 0.997234 | 2.846471 | H | -3.596129 | -1.507443 | -2.537685 |
| C | 1.715309 | -1.116726 | 3.253371 | C | -3.690936 | 1.962001 | 0.156036 |
| H | 1.205037 | -0.992882 | 4.220042 | H | -4.376549 | 2.111070 | 0.978206 |
| H | 2.772284 | -1.296573 | 3.473888 | C | -2.323510 | 2.359695 | 0.114976 |
| H | -0.458887 | -1.216336 | -1.733100 | H | -1.790477 | 2.880553 | 0.899353 |
| H | -0.466697 | 0.522968 | -2.006242 | C | -1.794228 | 2.009702 | -1.156929 |
| H | 1.315339 | -2.028234 | 2.801139 | H | -0.783894 | 2.192813 | -1.495680 |
| Zr | 1.775007 | -0.040230 | -0.095820 | C | -2.821495 | 1.376658 | -1.894070 |
| C | 3.436260 | 1.931555 | -0.019614 | H | -2.733057 | 0.990448 | -2.900908 |
| H | 4.318882 | 1.828367 | 0.597449 | C | -3.994881 | 1.350408 | -1.083447 |
| C | 2.201401 | 2.504377 | 0.377269 | H | -4.955403 | 0.943089 | -1.371417 |
| H | 1.977706 | 2.900288 | 1.358229 | C | 2.486045 | -0.042904 | 0.823118 |
| C | 1.311704 | 2.454294 | -0.721548 | C | 2.450950 | 1.353801 | 0.240196 |
| H | 0.285436 | 2.793690 | -0.726907 | C | 2.151776 | 1.527504 | -1.122025 |
| C | 2.001995 | 1.864809 | -1.815864 | C | 2.745339 | 2.492237 | 1.001685 |

1rBTS2

SCF energy in gas phase: -1130.41639

Free energy in Et₂O : -1129.877469

Enthalpy in Et₂O : -1129.792594

| | | | |
|---|-----------|-----------|-----------|
| H | -1.050471 | -1.378087 | 2.663933 |
| C | -2.396473 | 0.285176 | 2.396900 |
| H | -2.416092 | 1.370937 | 2.456036 |
| H | -3.153340 | -0.192649 | 3.011526 |
| H | 3.039198 | -1.017606 | 2.830574 |
| H | 2.339205 | 0.658572 | 3.005120 |
| H | -0.595348 | -0.365338 | -0.807375 |

1rB2

SCF energy in gas phase: -1130.430521

Free energy in Et₂O : -1129.890897

Enthalpy in Et₂O : -1129.804199

| | | | |
|----|-----------|-----------|-----------|
| Zr | -2.371111 | -0.230461 | 0.111553 |
| C | -3.633617 | -2.428288 | -0.324014 |
| H | -4.676268 | -2.492120 | -0.050667 |
| C | -2.530415 | -2.780845 | 0.498065 |
| H | -2.594344 | -3.164144 | 1.507157 |
| C | -1.337997 | -2.581458 | -0.250390 |
| H | -0.332495 | -2.783298 | 0.089159 |
| C | -1.698153 | -2.078646 | -1.522703 |
| H | -1.018440 | -1.839074 | -2.329728 |
| C | -3.119888 | -1.985297 | -1.568452 |
| H | -3.707209 | -1.660722 | -2.416239 |
| C | -3.621440 | 1.955231 | -0.471349 |
| H | -4.582725 | 2.140991 | -0.015219 |
| C | -2.358036 | 2.345059 | 0.042718 |
| H | -2.189480 | 2.903140 | 0.954314 |
| C | -1.352608 | 1.929068 | -0.876714 |
| H | -0.291239 | 2.105664 | -0.788064 |
| C | -1.996556 | 1.261469 | -1.944671 |
| H | -1.508774 | 0.834294 | -2.810907 |
| C | -3.397985 | 1.270747 | -1.692913 |
| H | -4.165014 | 0.850236 | -2.328984 |
| C | 2.334216 | 0.029322 | 0.894556 |
| C | 2.283034 | 1.415520 | 0.287150 |
| C | 2.380838 | 1.564197 | -1.108391 |
| C | 2.147772 | 2.582512 | 1.055291 |
| C | 2.333992 | 2.821681 | -1.709285 |
| H | 2.506994 | 0.682866 | -1.728500 |
| C | 2.094230 | 3.843217 | 0.455471 |
| H | 2.094251 | 2.519757 | 2.136702 |
| C | 2.185845 | 3.971059 | -0.929972 |
| H | 2.415024 | 2.902394 | -2.789794 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.990225 | 4.726992 | 1.078948 |
| H | 2.148777 | 4.951291 | -1.395958 |
| C | 3.294157 | -0.912921 | 0.198189 |
| C | 2.855101 | -1.892358 | -0.701719 |
| C | 4.672393 | -0.796182 | 0.434429 |
| C | 3.764474 | -2.736814 | -1.344394 |
| H | 1.792236 | -1.993239 | -0.902377 |
| C | 5.583072 | -1.636832 | -0.203619 |
| H | 5.026854 | -0.038711 | 1.128542 |
| C | 5.131330 | -2.612568 | -1.096290 |
| H | 3.402419 | -3.491678 | -2.037060 |
| H | 6.645894 | -1.532947 | -0.003068 |
| H | 5.839519 | -3.270310 | -1.592048 |
| C | 2.215416 | -0.156787 | 2.395600 |
| C | 1.073025 | -0.602361 | 1.504356 |
| H | 1.021373 | -1.680238 | 1.368960 |
| C | -0.262534 | 0.070093 | 1.576140 |
| H | -0.239471 | 1.154018 | 1.489332 |
| H | -4.060030 | -0.197307 | 0.808988 |
| C | -1.264856 | -0.481350 | 2.401693 |
| H | -1.129846 | -1.525252 | 2.688044 |
| C | -2.523871 | 0.068313 | 2.635519 |
| H | -2.677361 | 1.142714 | 2.596870 |
| H | -3.261721 | -0.488550 | 3.198350 |
| H | 2.844921 | -0.916737 | 2.849737 |
| H | 2.044759 | 0.709727 | 3.025575 |

1rBTS6

SCF energy in gas phase: -1130.415022

Free energy in Et₂O : -1129.875449

Enthalpy in Et₂O : -1129.790567

| | | | |
|----|-----------|-----------|-----------|
| Zr | -2.296634 | -0.246141 | 0.102864 |
| C | -3.645839 | -2.361492 | -0.279576 |
| H | -4.671144 | -2.400006 | 0.060509 |
| C | -2.499004 | -2.779063 | 0.453517 |
| H | -2.505154 | -3.187745 | 1.454540 |
| C | -1.355017 | -2.618950 | -0.377882 |
| H | -0.335779 | -2.861398 | -0.112532 |
| C | -1.787978 | -2.093030 | -1.616622 |
| H | -1.155567 | -1.856148 | -2.462611 |
| C | -3.200768 | -1.934839 | -1.559558 |
| H | -3.829801 | -1.573661 | -2.361257 |
| C | -3.669671 | 1.911312 | -0.253754 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -4.584190 | 2.054875 | 0.305234 | H | 1.954826 | 0.712145 | 2.996465 |
| C | -2.363886 | 2.316447 | 0.144438 | | | | |
| H | -2.113923 | 2.842728 | 1.056265 | 1rB3 | | | |
| C | -1.452208 | 1.975502 | -0.894542 | SCF energy in gas phase: -1130.426343 | | | |
| H | -0.390709 | 2.171320 | -0.906174 | Free energy in Et ₂ O : -1129.893077 | | | |
| C | -2.192107 | 1.338808 | -1.919004 | Enthalpy in Et ₂ O : -1129.806825 | | | |
| H | -1.790185 | 0.960254 | -2.850078 | | | | |
| C | -3.562051 | 1.302703 | -1.525669 | Zr | -1.946728 | -0.465669 | -0.135097 |
| H | -4.380555 | 0.888797 | -2.099171 | C | -2.263593 | -3.027700 | -0.522773 |
| C | 2.327320 | 0.025612 | 0.880335 | H | -3.013417 | -3.563629 | 0.045368 |
| C | 2.284374 | 1.407816 | 0.264874 | C | -0.901302 | -2.877955 | -0.167449 |
| C | 2.268371 | 1.538697 | -1.135470 | H | -0.434275 | -3.277997 | 0.721336 |
| C | 2.279207 | 2.584040 | 1.028467 | C | -0.256100 | -2.109422 | -1.168225 |
| C | 2.234768 | 2.791931 | -1.745320 | H | 0.793767 | -1.847916 | -1.184922 |
| H | 2.295098 | 0.645457 | -1.751312 | C | -1.229997 | -1.779483 | -2.157864 |
| C | 2.240509 | 3.841964 | 0.420650 | H | -1.049884 | -1.236336 | -3.076903 |
| H | 2.319549 | 2.526438 | 2.110853 | C | -2.469151 | -2.355307 | -1.757486 |
| C | 2.216108 | 3.953498 | -0.968874 | H | -3.400548 | -2.301683 | -2.305355 |
| H | 2.225212 | 2.861332 | -2.829707 | C | -3.017999 | 1.820485 | 0.522136 |
| H | 2.239450 | 4.735219 | 1.039434 | H | -2.615846 | 2.379651 | 1.354902 |
| H | 2.190285 | 4.930755 | -1.442091 | C | -2.618402 | 1.955117 | -0.827808 |
| C | 3.318692 | -0.903871 | 0.211454 | H | -1.845606 | 2.619285 | -1.192813 |
| C | 2.914500 | -1.896900 | -0.689940 | C | -3.378212 | 1.042224 | -1.606526 |
| C | 4.690262 | -0.759143 | 0.470333 | H | -3.319848 | 0.915525 | -2.679782 |
| C | 3.850912 | -2.726712 | -1.312494 | C | -4.257770 | 0.345953 | -0.726328 |
| H | 1.857051 | -2.018257 | -0.907359 | H | -4.989166 | -0.397348 | -1.016504 |
| C | 5.627857 | -1.585273 | -0.147342 | C | -4.033898 | 0.828383 | 0.593622 |
| H | 5.018071 | 0.009638 | 1.165150 | H | -4.556445 | 0.516696 | 1.487231 |
| C | 5.210691 | -2.574355 | -1.042252 | C | 2.184826 | 0.348497 | 0.895943 |
| H | 3.515610 | -3.491942 | -2.007388 | C | 1.886606 | 1.650259 | 0.197919 |
| H | 6.685009 | -1.459187 | 0.070142 | C | 1.276826 | 1.645726 | -1.068644 |
| H | 5.940100 | -3.220238 | -1.522729 | C | 2.225149 | 2.888744 | 0.758040 |
| C | 2.158430 | -0.156212 | 2.378180 | C | 1.014955 | 2.835873 | -1.749149 |
| C | 1.052992 | -0.610887 | 1.446328 | H | 1.034093 | 0.694133 | -1.534440 |
| H | 1.007160 | -1.689493 | 1.310107 | C | 1.955676 | 4.083945 | 0.086239 |
| C | -0.287348 | 0.058516 | 1.452421 | H | 2.711154 | 2.917030 | 1.728739 |
| H | -0.237758 | 1.146878 | 1.421544 | C | 1.348654 | 4.063083 | -1.170000 |
| H | -3.585643 | -0.134889 | 1.523933 | H | 0.556304 | 2.805538 | -2.734274 |
| C | -1.301325 | -0.517341 | 2.286204 | H | 2.229108 | 5.031220 | 0.542875 |
| H | -1.154521 | -1.561033 | 2.555650 | H | 1.144539 | 4.991082 | -1.696395 |
| C | -2.611507 | 0.004871 | 2.565567 | C | 3.295945 | -0.486315 | 0.294343 |
| H | -2.708851 | 1.080191 | 2.714784 | C | 4.083236 | -0.007006 | -0.766764 |
| H | -3.196024 | -0.561572 | 3.287719 | C | 3.606504 | -1.765020 | 0.796931 |
| H | 2.780036 | -0.906693 | 2.858699 | C | 5.118586 | -0.771178 | -1.308467 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 3.890400 | 0.979117 | -1.173041 | H | 3.916783 | 0.131598 | -2.186563 |
| C | 4.639884 | -2.528963 | 0.256815 | C | 3.881497 | -0.337126 | 0.000123 |
| H | 3.043084 | -2.176002 | 1.628787 | H | 4.632846 | 0.323122 | 0.410290 |
| C | 5.403450 | -2.038939 | -0.803886 | C | -1.879916 | -0.528292 | 1.017189 |
| H | 5.705477 | -0.365806 | -2.128428 | C | -1.448892 | -1.817604 | 0.405330 |
| H | 4.848500 | -3.511931 | 0.670681 | C | -1.165413 | -1.940789 | -0.975213 |
| H | 6.208262 | -2.634155 | -1.225316 | C | -1.344671 | -2.997964 | 1.170592 |
| C | 2.031256 | 0.288640 | 2.413717 | C | -0.821403 | -3.160068 | -1.552921 |
| C | 1.000148 | -0.393555 | 1.554164 | H | -1.214580 | -1.058263 | -1.604420 |
| H | 1.087138 | -1.475838 | 1.497663 | C | -0.977195 | -4.218134 | 0.598854 |
| C | -0.421371 | 0.096920 | 1.503518 | H | -1.580971 | -2.974902 | 2.228871 |
| H | -0.488203 | 1.162986 | 1.732129 | C | -0.719006 | -4.313392 | -0.768421 |
| H | -3.226397 | -0.727991 | 3.454845 | H | -0.621494 | -3.208302 | -2.620205 |
| C | -1.490193 | -0.713164 | 2.124913 | H | -0.911393 | -5.101966 | 1.227934 |
| H | -1.185735 | -1.741439 | 2.332870 | H | -0.443522 | -5.263831 | -1.215324 |
| C | -2.303446 | -0.158639 | 3.287546 | C | -2.978409 | 0.261845 | 0.416776 |
| H | -2.588016 | 0.887453 | 3.135195 | C | -3.661601 | -0.141228 | -0.757399 |
| H | -1.729643 | -0.194343 | 4.226316 | C | -3.449205 | 1.455746 | 1.023111 |
| H | 2.761003 | -0.302252 | 2.961061 | C | -4.700954 | 0.610212 | -1.301655 |
| H | 1.717717 | 1.194480 | 2.925182 | H | -3.402988 | -1.078400 | -1.233032 |

1rBTS7

SCF energy in gas phase: -1130.403376

Free energy in Et₂O : -1129.868437

Enthalpy in Et₂O : -1129.784514

| | | | |
|----|-----------|-----------|-----------|
| Zr | 1.479493 | 0.486338 | -0.199686 |
| C | 1.530237 | 2.962287 | -0.930021 |
| H | 2.163247 | 3.655113 | -0.393348 |
| C | 0.158280 | 2.690487 | -0.659182 |
| H | -0.437653 | 3.141953 | 0.121245 |
| C | -0.310292 | 1.764986 | -1.622747 |
| H | -1.318338 | 1.373209 | -1.677835 |
| C | 0.765471 | 1.446166 | -2.489090 |
| H | 0.724681 | 0.778190 | -3.339662 |
| C | 1.899884 | 2.199596 | -2.065053 |
| H | 2.869674 | 2.209922 | -2.543109 |
| C | 3.132960 | -1.304649 | 0.722314 |
| H | 3.195297 | -1.489643 | 1.785070 |
| C | 2.282804 | -1.982661 | -0.182282 |
| H | 1.571047 | -2.756974 | 0.071807 |
| C | 2.498300 | -1.445114 | -1.477394 |
| H | 2.008299 | -1.765917 | -2.386575 |
| C | 3.494365 | -0.432320 | -1.367552 |

| | | | |
|---|-----------|-----------|-----------|
| C | -4.484324 | 2.207179 | 0.471494 |
| H | -3.006909 | 1.811894 | 1.946568 |
| C | -5.117873 | 1.800103 | -0.703016 |
| H | -5.196869 | 0.249752 | -2.199412 |
| H | -4.800930 | 3.117890 | 0.973509 |
| H | -5.924981 | 2.386238 | -1.131746 |
| C | -1.615056 | -0.315026 | 2.488341 |
| C | -0.589303 | 0.611988 | 1.970804 |
| H | -0.940288 | 1.602351 | 1.701273 |
| C | 0.825904 | 0.425883 | 2.078488 |
| H | 1.151388 | -0.467544 | 2.608800 |
| H | 3.824761 | 2.171808 | 2.326002 |
| C | 1.817011 | 1.484149 | 1.860557 |
| H | 1.378354 | 2.481153 | 1.783254 |
| C | 3.057021 | 1.505747 | 2.736907 |
| H | 3.508369 | 0.514077 | 2.843290 |
| H | 2.827538 | 1.861132 | 3.752529 |
| H | -2.437706 | 0.117378 | 3.063222 |
| H | -1.194732 | -1.166577 | 3.021414 |

1rB4

SCF energy in gas phase: -1130.436791

Free energy in Et₂O : -1129.894195

Enthalpy in Et₂O : -1129.811614

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Zr | -1.335590 | -0.074552 | -0.196154 | H | 4.295974 | -4.383872 | -0.342103 |
| C | -2.132862 | -2.376456 | -1.136536 | C | 0.731482 | 0.034728 | 2.178347 |
| H | -2.861302 | -2.964512 | -0.596556 | C | -0.518946 | -0.794747 | 2.044026 |
| C | -0.724320 | -2.455059 | -1.002073 | H | -0.386078 | -1.820423 | 1.706594 |
| H | -0.170172 | -3.113756 | -0.347915 | C | -1.817375 | -0.364449 | 2.268383 |
| C | -0.144238 | -1.544434 | -1.931100 | H | -1.956824 | 0.590825 | 2.772349 |
| H | 0.914939 | -1.403627 | -2.083445 | H | -5.012681 | -0.664596 | 1.029938 |
| C | -1.195071 | -0.899172 | -2.621406 | C | -2.927933 | -0.919900 | 1.577996 |
| H | -1.079421 | -0.154603 | -3.397549 | H | -2.834778 | -1.979157 | 1.344916 |
| C | -2.430343 | -1.394113 | -2.113674 | C | -4.343606 | -0.481735 | 1.877982 |
| H | -3.420427 | -1.104866 | -2.440940 | H | -4.395239 | 0.586056 | 2.116516 |
| C | -2.243273 | 2.249178 | 0.670728 | H | -4.762462 | -1.023904 | 2.737744 |
| H | -2.490011 | 2.410011 | 1.710046 | H | 1.442310 | -0.336897 | 2.935421 |
| C | -0.992070 | 2.504102 | 0.068566 | H | 0.448059 | 1.046575 | 2.486242 |
| H | -0.102946 | 2.865039 | 0.563447 | | | | |
| C | -1.104346 | 2.199376 | -1.315046 | 1r'BTS2 | | | |
| H | -0.324624 | 2.323706 | -2.051608 | SCF energy in gas phase: -1130.409299 | | | |
| C | -2.442015 | 1.786821 | -1.562850 | Free energy in Et ₂ O : -1129.871778 | | | |
| H | -2.855258 | 1.513589 | -2.523744 | Enthalpy in Et ₂ O : -1129.787312 | | | |
| C | -3.141026 | 1.786464 | -0.333187 | Zr | -2.227626 | -0.226977 | 0.051503 |
| H | -4.179554 | 1.522898 | -0.189196 | C | -1.111007 | -2.584339 | -0.057840 |
| C | 1.285085 | 0.053745 | 0.735952 | H | -0.505046 | -2.944890 | 0.761711 |
| C | 1.983653 | 1.337333 | 0.353611 | C | -0.638820 | -1.898562 | -1.202575 |
| C | 2.139828 | 1.753915 | -0.984820 | H | 0.387622 | -1.616857 | -1.395311 |
| C | 2.549408 | 2.174697 | 1.336592 | C | -1.746347 | -1.647710 | -2.050303 |
| C | 2.817898 | 2.924004 | -1.323283 | H | -1.712392 | -1.147945 | -3.009245 |
| H | 1.695041 | 1.157096 | -1.774877 | C | -2.902137 | -2.207338 | -1.432556 |
| C | 3.217325 | 3.356286 | 1.004983 | H | -3.904406 | -2.198726 | -1.840187 |
| H | 2.484852 | 1.893304 | 2.382857 | C | -2.516029 | -2.775436 | -0.193865 |
| C | 3.359551 | 3.740280 | -0.327845 | H | -3.160945 | -3.292888 | 0.502523 |
| H | 2.912164 | 3.205367 | -2.369197 | C | -4.241335 | 1.275492 | 0.714014 |
| H | 3.638229 | 3.971275 | 1.796455 | H | -4.628028 | 1.218697 | 1.722230 |
| H | 3.879638 | 4.657607 | -0.587652 | C | -3.209394 | 2.141627 | 0.256458 |
| C | 2.108809 | -1.173125 | 0.427876 | H | -2.695592 | 2.888377 | 0.846142 |
| C | 2.971678 | -1.257452 | -0.693460 | C | -2.996656 | 1.892479 | -1.127751 |
| C | 2.119419 | -2.308913 | 1.275801 | H | -2.302424 | 2.415711 | -1.770174 |
| C | 3.739470 | -2.386944 | -0.966447 | C | -3.897160 | 0.865848 | -1.519534 |
| H | 3.071087 | -0.408996 | -1.358054 | H | -3.994391 | 0.454557 | -2.514907 |
| C | 2.884702 | -3.444406 | 1.000296 | C | -4.661798 | 0.486152 | -0.381071 |
| H | 1.544775 | -2.315709 | 2.193311 | H | -5.427782 | -0.278163 | -0.353131 |
| C | 3.697776 | -3.502986 | -0.129120 | C | 2.353570 | 0.206842 | 0.830831 |
| H | 4.385331 | -2.386295 | -1.841099 | C | 2.497287 | 1.555415 | 0.164501 |
| H | 2.851020 | -4.282281 | 1.692522 | C | 1.910578 | 1.804623 | -1.087197 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.255698 | 2.575149 | 0.755798 | C | -2.043241 | -1.720464 | -1.969948 |
| C | 2.066840 | 3.039276 | -1.718253 | H | -2.267554 | -1.344807 | -2.959176 |
| H | 1.324527 | 1.025281 | -1.564250 | C | -2.973398 | -2.293724 | -1.056819 |
| C | 3.414684 | 3.811735 | 0.126816 | H | -4.033137 | -2.426500 | -1.229032 |
| H | 3.729304 | 2.395712 | 1.716692 | C | -2.271599 | -2.657294 | 0.116781 |
| C | 2.818239 | 4.048690 | -1.112170 | H | -2.696645 | -3.119314 | 0.997273 |
| H | 1.600785 | 3.212766 | -2.684342 | C | -4.221053 | 1.321706 | 0.819912 |
| H | 4.006574 | 4.587379 | 0.604794 | H | -4.439132 | 1.340422 | 1.878648 |
| H | 2.938881 | 5.010341 | -1.602826 | C | -3.384545 | 2.230481 | 0.120155 |
| C | 3.209400 | -0.909729 | 0.264704 | H | -2.851489 | 3.069050 | 0.547047 |
| C | 3.168104 | -2.208563 | 0.805741 | C | -3.377872 | 1.863700 | -1.251852 |
| C | 4.089619 | -0.684544 | -0.805621 | H | -2.842266 | 2.370380 | -2.041210 |
| C | 3.960985 | -3.234401 | 0.294253 | C | -4.196636 | 0.717372 | -1.395705 |
| H | 2.516311 | -2.432282 | 1.644964 | H | -4.407387 | 0.201364 | -2.322394 |
| C | 4.884913 | -1.711438 | -1.318599 | C | -4.712299 | 0.374415 | -0.111604 |
| H | 4.159127 | 0.304538 | -1.242887 | H | -5.385876 | -0.443127 | 0.108788 |
| C | 4.825496 | -2.993247 | -0.774827 | C | 2.460276 | 0.222429 | 0.884243 |
| H | 3.902495 | -4.225234 | 0.736370 | C | 2.755620 | 1.490381 | 0.116071 |
| H | 5.554987 | -1.501166 | -2.147775 | C | 1.947294 | 1.920157 | -0.945956 |
| H | 5.443659 | -3.792026 | -1.173951 | C | 3.901083 | 2.237449 | 0.430493 |
| C | 2.105608 | 0.197484 | 2.334435 | C | 2.274029 | 3.071704 | -1.666513 |
| C | 0.983938 | -0.184933 | 1.410380 | H | 1.046538 | 1.365494 | -1.191513 |
| H | 0.764660 | -1.244020 | 1.352636 | C | 4.230509 | 3.385058 | -0.290876 |
| C | -0.227457 | 0.714031 | 1.326061 | H | 4.539343 | 1.911499 | 1.247491 |
| H | 0.059254 | 1.764657 | 1.299486 | C | 3.415439 | 3.806994 | -1.343480 |
| C | -1.376810 | 0.491596 | 2.171126 | H | 1.630728 | 3.393953 | -2.480926 |
| H | -1.879671 | 1.404819 | 2.474045 | H | 5.122096 | 3.949109 | -0.030825 |
| C | -2.120412 | -0.713718 | 2.391741 | H | 3.667464 | 4.702419 | -1.904884 |
| H | -1.601212 | -1.669076 | 2.439209 | C | 3.036653 | -1.052161 | 0.300688 |
| H | -2.947911 | -0.642921 | 3.091108 | C | 3.052541 | -2.254072 | 1.032403 |
| H | 2.587216 | -0.574693 | 2.926756 | C | 3.558095 | -1.081288 | -1.002879 |
| H | 2.028644 | 1.158960 | 2.833847 | C | 3.560779 | -3.431122 | 0.484233 |
| H | -0.536768 | 0.683305 | -0.101816 | H | 2.668551 | -2.282874 | 2.047812 |
| | | | | C | 4.068110 | -2.259421 | -1.552240 |
| | | | | H | 3.569035 | -0.172724 | -1.593825 |
| | | | | C | 4.072915 | -3.442049 | -0.814098 |
| | | | | H | 3.559884 | -4.341016 | 1.078277 |
| | | | | H | 4.464938 | -2.246562 | -2.563750 |
| | | | | H | 4.470646 | -4.357968 | -1.241189 |
| Zr | -2.209231 | -0.081724 | -0.019927 | C | 2.399948 | 0.362837 | 2.391786 |
| C | -0.901854 | -2.324351 | -0.078885 | C | 1.119509 | 0.066558 | 1.635168 |
| H | -0.096164 | -2.515433 | 0.615070 | H | 0.796810 | -0.964849 | 1.713054 |
| C | -0.758516 | -1.759426 | -1.369087 | C | 0.023569 | 1.064027 | 1.628137 |
| H | 0.165603 | -1.418197 | -1.812503 | H | 0.318850 | 2.084427 | 1.401191 |

1r'B1

SCF energy in gas phase: -1130.427003

Free energy in Et₂O : -1129.889446

Enthalpy in Et₂O : -1129.802796

| | | | |
|---|-----------|-----------|-----------|
| C | -1.229412 | 0.882101 | 2.172291 |
| H | -1.798188 | 1.800529 | 2.305581 |
| C | -1.966744 | -0.337375 | 2.363777 |
| H | -1.399639 | -1.249285 | 2.542135 |
| H | -2.854444 | -0.270165 | 2.987420 |
| H | 2.827084 | -0.414060 | 3.018734 |
| H | 2.514504 | 1.367341 | 2.788125 |
| H | -0.956115 | 0.852121 | -0.985518 |

1r'B2

SCF energy in gas phase: -1130.42381

Free energy in Et₂O : -1129.884584

Enthalpy in Et₂O : -1129.800069

| | | | |
|----|-----------|-----------|-----------|
| Zr | -2.277754 | -0.415544 | 0.102862 |
| C | -0.927130 | -2.592171 | -0.191175 |
| H | -0.445297 | -3.057675 | 0.657621 |
| C | -0.333317 | -1.647252 | -1.074840 |
| H | 0.674166 | -1.264927 | -1.008929 |
| C | -1.283666 | -1.336943 | -2.075788 |
| H | -1.135266 | -0.657187 | -2.904563 |
| C | -2.459461 | -2.098977 | -1.819605 |
| H | -3.363722 | -2.097611 | -2.412749 |
| C | -2.233701 | -2.883979 | -0.662408 |
| H | -2.931793 | -3.579316 | -0.220388 |
| C | -3.864260 | 1.550532 | 0.678139 |
| H | -4.147445 | 1.718021 | 1.708342 |
| C | -2.760731 | 2.136512 | 0.003164 |
| H | -2.043358 | 2.824787 | 0.427822 |
| C | -2.750869 | 1.648988 | -1.325486 |
| H | -2.040796 | 1.918681 | -2.095767 |
| C | -3.871341 | 0.779864 | -1.479109 |
| H | -4.159938 | 0.274622 | -2.390217 |
| C | -4.560625 | 0.722875 | -0.243202 |
| H | -5.456538 | 0.156379 | -0.036139 |
| H | -3.614136 | -1.403594 | 0.869762 |
| C | 2.247033 | 0.244294 | 0.879163 |
| C | 2.283995 | 1.601954 | 0.217105 |
| C | 1.503398 | 1.886952 | -0.913920 |
| C | 3.147667 | 2.598540 | 0.693747 |
| C | 1.577913 | 3.131566 | -1.542068 |
| H | 0.825934 | 1.129288 | -1.294492 |
| C | 3.226708 | 3.843440 | 0.067519 |
| H | 3.764758 | 2.391356 | 1.563547 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.439897 | 4.115187 | -1.053037 |
| H | 0.962537 | 3.333361 | -2.414855 |
| H | 3.903355 | 4.600197 | 0.454847 |
| H | 2.497878 | 5.083942 | -1.541081 |
| C | 3.142718 | -0.810069 | 0.259887 |
| C | 3.281329 | -2.086055 | 0.838474 |
| C | 3.870246 | -0.552392 | -0.913653 |
| C | 4.102576 | -3.057179 | 0.268505 |
| H | 2.747634 | -2.334344 | 1.751045 |
| C | 4.693247 | -1.524899 | -1.485690 |
| H | 3.797879 | 0.420733 | -1.385315 |
| C | 4.815082 | -2.783727 | -0.900459 |
| H | 4.186176 | -4.031054 | 0.743251 |
| H | 5.241805 | -1.290092 | -2.393865 |
| H | 5.455387 | -3.540105 | -1.344758 |
| C | 2.084643 | 0.226768 | 2.393752 |
| C | 0.936794 | -0.238023 | 1.528338 |
| H | 0.817061 | -1.315889 | 1.490985 |
| C | -0.335616 | 0.560965 | 1.484749 |
| H | -0.156136 | 1.621054 | 1.328512 |
| C | -1.414265 | 0.291379 | 2.375732 |
| H | -2.007565 | 1.156335 | 2.668498 |
| C | -1.987071 | -0.938012 | 2.660258 |
| H | -1.444550 | -1.869259 | 2.528253 |
| H | -2.872857 | -0.993972 | 3.279630 |
| H | 2.656302 | -0.501457 | 2.962465 |
| H | 1.971509 | 1.188649 | 2.885520 |

1r'BTS6

SCF energy in gas phase: -1130.408024

Free energy in Et₂O : -1129.871305

Enthalpy in Et₂O : -1129.786537

| | | | |
|----|-----------|-----------|-----------|
| Zr | -2.224331 | -0.373044 | 0.087545 |
| C | -0.937212 | -2.576109 | -0.223516 |
| H | -0.441175 | -3.043929 | 0.615920 |
| C | -0.344345 | -1.666159 | -1.140796 |
| H | 0.672304 | -1.304104 | -1.106849 |
| C | -1.314452 | -1.349571 | -2.120049 |
| H | -1.174365 | -0.683666 | -2.961890 |
| C | -2.500401 | -2.084376 | -1.823790 |
| H | -3.420993 | -2.064295 | -2.391747 |
| C | -2.269060 | -2.843126 | -0.654350 |
| H | -2.969688 | -3.521772 | -0.188127 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.131801 | 1.300307 | 0.664633 | H | 2.601928 | -0.526965 | 2.962225 |
| H | -4.579488 | 1.264920 | 1.649439 | H | 1.898960 | 1.155574 | 2.883035 |
| C | -3.035843 | 2.112358 | 0.273774 | | | | |
| H | -2.494135 | 2.800401 | 0.908310 | 1r'B3 | | | |
| C | -2.749668 | 1.848740 | -1.085932 | SCF energy in gas phase: -1130.424133 | | | |
| H | -1.973630 | 2.320650 | -1.673245 | Free energy in Et ₂ O : -1129.891852 | | | |
| C | -3.689959 | 0.880255 | -1.545489 | Enthalpy in Et ₂ O : -1129.805309 | | | |
| H | -3.761380 | 0.497328 | -2.553834 | | | | |
| C | -4.542529 | 0.538976 | -0.461044 | Zr | -1.995558 | -0.359052 | -0.116638 |
| H | -5.366471 | -0.161166 | -0.489718 | C | -2.005640 | -2.888661 | -0.449615 |
| H | -3.102286 | -1.375544 | 1.482678 | H | -2.315338 | -3.521675 | 0.369797 |
| C | 2.246338 | 0.235778 | 0.874824 | C | -0.668743 | -2.508770 | -0.755706 |
| C | 2.287995 | 1.599288 | 0.226270 | H | 0.218233 | -2.792409 | -0.209087 |
| C | 1.552870 | 1.876668 | -0.936958 | C | -0.689456 | -1.717934 | -1.929722 |
| C | 3.111580 | 2.608285 | 0.745690 | H | 0.177367 | -1.287705 | -2.416324 |
| C | 1.633954 | 3.125741 | -1.555285 | C | -2.036424 | -1.593041 | -2.357641 |
| H | 0.904865 | 1.109756 | -1.348114 | H | -2.380320 | -1.060766 | -3.234802 |
| C | 3.196275 | 3.858017 | 0.129693 | C | -2.852172 | -2.319308 | -1.442201 |
| H | 3.693583 | 2.407213 | 1.640776 | H | -3.924861 | -2.445312 | -1.512151 |
| C | 2.455895 | 4.121747 | -1.023939 | C | -3.103398 | 1.726083 | 1.033019 |
| H | 1.055680 | 3.321008 | -2.454675 | H | -2.767178 | 2.024837 | 2.016678 |
| H | 3.841798 | 4.624253 | 0.550255 | C | -2.560908 | 2.173145 | -0.193363 |
| H | 2.519094 | 5.093786 | -1.504935 | H | -1.745286 | 2.875108 | -0.308447 |
| C | 3.170407 | -0.803650 | 0.273055 | C | -3.255047 | 1.512362 | -1.247598 |
| C | 3.295276 | -2.088084 | 0.836312 | H | -3.102588 | 1.666191 | -2.307892 |
| C | 3.940910 | -0.524209 | -0.867842 | C | -4.237481 | 0.664655 | -0.655558 |
| C | 4.142644 | -3.046137 | 0.282683 | H | -4.953770 | 0.054666 | -1.189795 |
| H | 2.729648 | -2.352811 | 1.724675 | C | -4.137974 | 0.795257 | 0.757535 |
| C | 4.790190 | -1.483461 | -1.423591 | H | -4.745696 | 0.283254 | 1.491990 |
| H | 3.881057 | 0.455825 | -1.326727 | C | 2.208521 | 0.286590 | 0.885290 |
| C | 4.896950 | -2.751008 | -0.854325 | C | 1.891072 | 1.642659 | 0.309756 |
| H | 4.213806 | -4.026978 | 0.745120 | C | 1.245084 | 1.743357 | -0.934515 |
| H | 5.371145 | -1.231500 | -2.306755 | C | 2.239808 | 2.829898 | 0.965970 |
| H | 5.557436 | -3.497199 | -1.286267 | C | 0.952826 | 2.985764 | -1.499275 |
| C | 2.037244 | 0.200331 | 2.384811 | H | 0.996310 | 0.832953 | -1.473182 |
| C | 0.922635 | -0.265145 | 1.479617 | C | 1.941898 | 4.076826 | 0.409995 |
| H | 0.818504 | -1.344638 | 1.426810 | H | 2.753930 | 2.776800 | 1.921005 |
| C | -0.362881 | 0.512195 | 1.393990 | C | 1.295500 | 4.160438 | -0.824028 |
| H | -0.183582 | 1.580943 | 1.301880 | H | 0.461894 | 3.037754 | -2.467637 |
| C | -1.469932 | 0.230176 | 2.279322 | H | 2.223052 | 4.983020 | 0.939499 |
| H | -2.033262 | 1.094214 | 2.620719 | H | 1.068257 | 5.129217 | -1.259672 |
| C | -2.140654 | -1.019645 | 2.503781 | C | 3.306019 | -0.489004 | 0.187491 |
| H | -1.553416 | -1.937834 | 2.495141 | C | 4.060993 | 0.081671 | -0.851038 |
| H | -2.887255 | -1.020817 | 3.294819 | C | 3.633332 | -1.803732 | 0.571418 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 5.080006 | -0.630419 | -1.486720 | C | -3.541667 | 0.498025 | -1.284401 |
| H | 3.855086 | 1.097891 | -1.166538 | H | -3.939474 | -0.033706 | -2.136881 |
| C | 4.650235 | -2.516057 | -0.062521 | C | -3.946340 | 0.329579 | 0.070324 |
| H | 3.096326 | -2.285710 | 1.382644 | H | -4.688906 | -0.366757 | 0.435467 |
| C | 5.380360 | -1.935629 | -1.100937 | C | 1.868027 | 0.552127 | 0.979894 |
| H | 5.641881 | -0.155038 | -2.286404 | C | 1.418167 | 1.867140 | 0.439840 |
| H | 4.872288 | -3.529741 | 0.260256 | C | 1.055022 | 2.044919 | -0.915469 |
| H | 6.172126 | -2.490515 | -1.595777 | C | 1.369468 | 3.019519 | 1.252196 |
| C | 2.084869 | 0.095684 | 2.393836 | C | 0.686004 | 3.286864 | -1.426052 |
| C | 1.038430 | -0.515005 | 1.496756 | H | 1.061098 | 1.187442 | -1.580321 |
| H | 1.136930 | -1.585620 | 1.349142 | C | 0.977597 | 4.262088 | 0.749675 |
| C | -0.377026 | -0.010318 | 1.505174 | H | 1.667975 | 2.956796 | 2.292888 |
| H | -0.410299 | 1.049350 | 1.764505 | C | 0.638022 | 4.410325 | -0.594891 |
| C | -1.466114 | -0.809046 | 2.106120 | H | 0.424144 | 3.375939 | -2.477224 |
| H | 2.824478 | -0.539736 | 2.874099 | H | 0.956402 | 5.121754 | 1.414328 |
| H | 1.779798 | 0.952454 | 2.988146 | H | 0.342463 | 5.378064 | -0.988650 |
| C | -1.209547 | -2.178462 | 2.718875 | C | 2.916008 | -0.231123 | 0.290374 |
| H | -0.659310 | -2.095698 | 3.668820 | C | 3.543362 | 0.209818 | -0.901384 |
| H | -2.151462 | -2.695187 | 2.937596 | C | 3.393831 | -1.458376 | 0.819380 |
| H | -0.623765 | -2.841356 | 2.075333 | C | 4.537233 | -0.535915 | -1.531793 |
| H | -2.129922 | -0.228943 | 2.748959 | H | 3.278510 | 1.170935 | -1.323235 |

1r'BTS7

SCF energy in gas phase: -1130.400199

Free energy in Et₂O : -1129.865015

Enthalpy in Et₂O : -1129.781626

| | | | |
|----|-----------|-----------|-----------|
| Zr | -1.512753 | -0.443255 | -0.134594 |
| C | -1.483285 | -2.924390 | -0.843814 |
| H | -2.003651 | -3.654075 | -0.241382 |
| C | -0.113523 | -2.555350 | -0.721705 |
| H | 0.599840 | -2.959746 | -0.018710 |
| C | 0.184242 | -1.614493 | -1.740121 |
| H | 1.153860 | -1.162813 | -1.909322 |
| C | -0.993858 | -1.390160 | -2.491952 |
| H | -1.091398 | -0.731406 | -3.345148 |
| C | -2.024492 | -2.205356 | -1.937671 |
| H | -3.039810 | -2.283138 | -2.302462 |
| C | -3.224106 | 1.268288 | 0.852052 |
| H | -3.296667 | 1.385190 | 1.924557 |
| C | -2.369660 | 2.002463 | -0.002961 |
| H | -1.671246 | 2.771866 | 0.299417 |
| C | -2.557830 | 1.526595 | -1.327983 |
| H | -2.062426 | 1.901818 | -2.213010 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.541667 | 0.498025 | -1.284401 |
| H | -3.939474 | -0.033706 | -2.136881 |
| C | -3.946340 | 0.329579 | 0.070324 |
| H | -4.688906 | -0.366757 | 0.435467 |
| C | 1.868027 | 0.552127 | 0.979894 |
| C | 1.418167 | 1.867140 | 0.439840 |
| C | 1.055022 | 2.044919 | -0.915469 |
| C | 1.369468 | 3.019519 | 1.252196 |
| C | 0.686004 | 3.286864 | -1.426052 |
| H | 1.061098 | 1.187442 | -1.580321 |
| C | 0.977597 | 4.262088 | 0.749675 |
| H | 1.667975 | 2.956796 | 2.292888 |
| C | 0.638022 | 4.410325 | -0.594891 |
| H | 0.424144 | 3.375939 | -2.477224 |
| H | 0.956402 | 5.121754 | 1.414328 |
| H | 0.342463 | 5.378064 | -0.988650 |
| C | 2.916008 | -0.231123 | 0.290374 |
| C | 3.543362 | 0.209818 | -0.901384 |
| C | 3.393831 | -1.458376 | 0.819380 |
| C | 4.537233 | -0.535915 | -1.531793 |
| H | 3.278510 | 1.170935 | -1.323235 |
| C | 4.383831 | -2.203100 | 0.182411 |
| H | 2.993124 | -1.846842 | 1.749201 |
| C | 4.962201 | -1.757208 | -1.006664 |
| H | 4.991873 | -0.146202 | -2.439178 |
| H | 4.708489 | -3.139917 | 0.628110 |
| H | 5.733714 | -2.338457 | -1.502296 |
| C | 1.678863 | 0.296281 | 2.456787 |
| C | 0.601074 | -0.585925 | 1.969203 |
| H | 0.909301 | -1.584743 | 1.683610 |
| C | -0.801054 | -0.337521 | 2.116330 |
| H | -1.058797 | 0.601063 | 2.604038 |
| C | -1.856308 | -1.354254 | 1.976082 |
| H | 2.519635 | -0.180121 | 2.966586 |
| H | 1.317047 | 1.139957 | 3.042284 |
| C | -1.609089 | -2.800258 | 2.387342 |
| H | -1.501176 | -2.884744 | 3.479079 |
| H | -2.448448 | -3.441464 | 2.095268 |
| H | -0.705351 | -3.231761 | 1.946979 |
| H | -2.790458 | -0.998333 | 2.409587 |

1r'B4

SCF energy in gas phase: -1130.4294

Free energy in Et₂O : -1129.888031

Enthalpy in Et₂O : -1129.805648

| | | | |
|----|-----------|-----------|-----------|
| Zr | -1.388782 | 0.173547 | -0.156902 |
| C | -2.585522 | -1.861142 | -1.209245 |
| H | -3.454559 | -2.282829 | -0.730148 |
| C | -1.235213 | -2.247862 | -0.997366 |
| H | -0.879766 | -3.026832 | -0.337362 |
| C | -0.416165 | -1.478278 | -1.869790 |
| H | 0.656099 | -1.564594 | -1.959813 |
| C | -1.256212 | -0.606999 | -2.599060 |
| H | -0.933599 | 0.105658 | -3.346641 |
| C | -2.599440 | -0.833164 | -2.181579 |
| H | -3.481742 | -0.334734 | -2.560254 |
| C | -2.085535 | 2.545795 | 0.772030 |
| H | -2.383456 | 2.675842 | 1.802541 |
| C | -0.774324 | 2.671200 | 0.260637 |
| H | 0.119367 | 2.900672 | 0.822449 |
| C | -0.834402 | 2.452569 | -1.143371 |
| H | 0.000563 | 2.514640 | -1.824196 |
| C | -2.190181 | 2.213486 | -1.490013 |
| H | -2.567859 | 2.040230 | -2.487830 |
| C | -2.962799 | 2.236708 | -0.303049 |
| H | -4.030839 | 2.083030 | -0.230286 |
| C | 1.302928 | -0.104131 | 0.727197 |
| C | 2.121394 | 1.120202 | 0.396573 |
| C | 2.300390 | 1.583590 | -0.924008 |
| C | 2.793325 | 1.842971 | 1.404223 |
| C | 3.096052 | 2.688635 | -1.222456 |
| H | 1.784888 | 1.073600 | -1.731790 |
| C | 3.580237 | 2.960152 | 1.113465 |
| H | 2.723108 | 1.517704 | 2.437164 |
| C | 3.740439 | 3.392174 | -0.202366 |
| H | 3.203768 | 3.007748 | -2.256162 |
| H | 4.080563 | 3.484856 | 1.923494 |
| H | 4.353537 | 4.259078 | -0.430407 |
| C | 1.960092 | -1.394058 | 0.308776 |
| C | 2.826817 | -1.492135 | -0.809076 |
| C | 1.794509 | -2.596296 | 1.041757 |
| C | 3.432983 | -2.688549 | -1.185721 |
| H | 3.056236 | -0.607776 | -1.388722 |
| C | 2.397441 | -3.796883 | 0.662002 |
| H | 1.205726 | -2.610093 | 1.949988 |
| C | 3.216942 | -3.862643 | -0.462621 |
| H | 4.090552 | -2.695581 | -2.051602 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.231278 | -4.684056 | 1.268372 |
| H | 3.687823 | -4.795562 | -0.757590 |
| C | 0.798213 | -0.153558 | 2.185462 |
| C | -0.571823 | -0.764122 | 2.065724 |
| H | -0.624550 | -1.789331 | 1.708305 |
| C | -1.749374 | -0.087766 | 2.306071 |
| H | -1.645806 | 0.896484 | 2.758050 |
| C | -3.007256 | -0.415439 | 1.694065 |
| H | 1.468616 | -0.689171 | 2.876980 |
| H | 0.684014 | 0.861336 | 2.579200 |
| C | -3.566567 | -1.828023 | 1.801006 |
| H | -3.908177 | -2.021645 | 2.828080 |
| H | -4.433056 | -1.969086 | 1.147442 |
| H | -2.836263 | -2.605428 | 1.559010 |
| H | -3.776872 | 0.335367 | 1.872194 |

2r

SCF energy in gas phase: -391.873697

Free energy in Et₂O : -391.424545

Enthalpy in Et₂O : -391.372022

| | | | |
|---|-----------|-----------|-----------|
| C | 0.544025 | 0.625020 | -0.018409 |
| C | 1.189172 | 0.196267 | 1.320807 |
| H | 1.541958 | 0.978417 | 1.992271 |
| H | 0.767873 | -0.666420 | 1.836459 |
| C | 1.873612 | -0.005456 | 0.031715 |
| C | 2.943900 | -0.452942 | -0.609534 |
| H | 2.976508 | -0.367072 | -1.696718 |
| C | 4.139141 | -1.081268 | 0.053375 |
| H | 4.303614 | -2.104020 | -0.309809 |
| H | 4.013526 | -1.120526 | 1.138929 |
| C | 0.468969 | 2.118018 | -0.315392 |
| H | 0.397901 | 2.295879 | -1.395167 |
| H | -0.403908 | 2.581088 | 0.158145 |
| H | 1.362584 | 2.634355 | 0.047506 |
| C | -0.627877 | -0.215647 | -0.529302 |
| H | -0.700036 | -0.094539 | -1.619944 |
| H | -0.399166 | -1.275469 | -0.358418 |
| C | -1.983956 | 0.116152 | 0.111169 |
| H | -2.253727 | 1.159422 | -0.100158 |
| H | -1.894697 | 0.039633 | 1.203792 |
| C | -3.116701 | -0.798984 | -0.372528 |
| H | -3.197913 | -0.728007 | -1.465900 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.854381 | -1.843829 | -0.156671 |
| C | -4.471774 | -0.470814 | 0.262339 |
| H | -4.779366 | 0.555732 | 0.031926 |
| H | -5.257586 | -1.141979 | -0.099774 |
| H | -4.431000 | -0.564702 | 1.353612 |
| H | 5.056746 | -0.520035 | -0.165519 |

2rTS1

SCF energy in gas phase: -982.815434

Free energy in Et₂O : -982.279531

Enthalpy in Et₂O : -982.188594

| | | | |
|----|-----------|-----------|-----------|
| C | -2.528932 | 1.185366 | -0.459201 |
| C | -2.087739 | 1.753343 | 0.880350 |
| H | -2.100888 | 2.836289 | 1.007930 |
| H | -2.397816 | 1.216028 | 1.777098 |
| C | -1.068673 | 1.155916 | -0.048411 |
| C | 0.064379 | 1.881412 | -0.617860 |
| H | 0.084702 | 1.889049 | -1.714441 |
| C | 0.482037 | 3.233069 | -0.051422 |
| H | 1.452313 | 3.564689 | -0.439288 |
| H | 0.554869 | 3.222155 | 1.040968 |
| C | -2.935916 | 2.161655 | -1.553353 |
| H | -2.828407 | 1.708827 | -2.548682 |
| H | -3.980561 | 2.479757 | -1.453276 |
| H | -2.310874 | 3.058602 | -1.533557 |
| C | -3.368592 | -0.089345 | -0.400303 |
| H | -3.323536 | -0.607682 | -1.370176 |
| H | -2.916796 | -0.769693 | 0.332930 |
| C | -4.843459 | 0.129424 | -0.024725 |
| H | -5.334707 | 0.757222 | -0.779825 |
| H | -4.894882 | 0.691705 | 0.917966 |
| C | -5.632686 | -1.178486 | 0.120840 |
| H | -5.575920 | -1.743524 | -0.819877 |
| H | -5.151331 | -1.809099 | 0.881502 |
| C | -7.101885 | -0.959498 | 0.496569 |
| H | -7.620409 | -0.364316 | -0.263947 |
| H | -7.638134 | -1.909040 | 0.597860 |
| H | -7.190382 | -0.423928 | 1.448882 |
| H | -0.239657 | 4.025560 | -0.307920 |
| Zr | 0.744772 | -0.247596 | 0.091628 |
| C | -0.114361 | -0.527789 | 2.492084 |
| H | -1.181821 | -0.602133 | 2.643704 |
| C | 0.653594 | 0.668522 | 2.538227 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.260694 | 1.662022 | 2.696492 |
| C | 2.004980 | 0.333907 | 2.308581 |
| H | 2.831985 | 1.030547 | 2.280227 |
| C | 2.090439 | -1.072493 | 2.105321 |
| H | 2.994521 | -1.642364 | 1.940169 |
| C | 0.775553 | -1.603033 | 2.238322 |
| H | 0.504133 | -2.648067 | 2.177061 |
| C | -0.606292 | -2.070496 | -1.183765 |
| H | -1.573377 | -2.363514 | -0.801210 |
| C | -0.364027 | -1.051000 | -2.139769 |
| H | -1.112514 | -0.409875 | -2.582159 |
| C | 1.028682 | -0.979935 | -2.368160 |
| H | 1.524032 | -0.301082 | -3.050113 |
| C | 1.659874 | -1.974038 | -1.558952 |
| H | 2.713680 | -2.213943 | -1.540089 |
| C | 0.643331 | -2.650487 | -0.839077 |
| H | 0.795328 | -3.472307 | -0.152622 |
| C | 6.417334 | -0.018381 | -0.408752 |
| H | 6.675867 | 1.020069 | -0.637503 |
| H | 6.547684 | -0.604514 | -1.324976 |
| H | 7.130565 | -0.393193 | 0.332016 |
| C | 4.974596 | -0.124639 | 0.119849 |
| H | 4.773677 | -1.172521 | 0.379109 |
| H | 4.874023 | 0.457754 | 1.042359 |
| C | 3.973022 | 0.346698 | -0.898716 |
| H | 3.941942 | -0.230583 | -1.822371 |
| C | 3.225495 | 1.459959 | -0.818058 |
| H | 3.260805 | 2.111046 | 0.050198 |
| H | 2.615806 | 1.795981 | -1.647275 |

2rIM1

SCF energy in gas phase: -825.586355

Free energy in Et₂O : -825.246946

Enthalpy in Et₂O : -825.169302

| | | | |
|---|-----------|----------|-----------|
| C | -1.920842 | 0.976531 | -0.685057 |
| C | -1.376304 | 2.014423 | 0.280144 |
| H | -1.407977 | 3.059347 | -0.030271 |
| H | -1.573186 | 1.876380 | 1.343829 |
| C | -0.430007 | 1.083801 | -0.433511 |
| C | 0.647824 | 1.476540 | -1.366761 |
| H | 0.518050 | 1.086882 | -2.381089 |
| C | 1.157531 | 2.911343 | -1.400966 |

| | | | | | | | |
|--------------------------------------|-----------|-----------|-----------|--|-----------|-----------|-----------|
| H | 2.121464 | 2.990157 | -1.918744 | Free energy in Et ₂ O : -825.224603 | | | |
| H | 1.285452 | 3.331178 | -0.398599 | Enthalpy in Et ₂ O : -825.149665 | | | |
| C | -2.455308 | 1.462853 | -2.023749 | | | | |
| H | -2.423458 | 0.663295 | -2.776488 | C | 2.009060 | -0.931423 | 0.876265 |
| H | -3.495903 | 1.801090 | -1.952991 | C | 1.467620 | -0.029346 | 1.973927 |
| H | -1.858450 | 2.295822 | -2.405555 | H | 1.515660 | -0.392700 | 3.000205 |
| C | -2.684139 | -0.198251 | -0.076324 | H | 1.632445 | 1.042516 | 1.882656 |
| H | -2.651322 | -1.052001 | -0.770871 | C | 0.526143 | -0.726758 | 1.017392 |
| H | -2.152524 | -0.522429 | 0.829212 | C | -0.434451 | -1.756793 | 1.331666 |
| C | -4.148767 | 0.091199 | 0.288018 | H | -0.337957 | -2.695345 | 0.788705 |
| H | -4.715709 | 0.350464 | -0.615862 | C | -1.695362 | -1.555924 | 1.979041 |
| H | -4.190262 | 0.976474 | 0.937790 | H | -2.721013 | -0.925363 | 1.156900 |
| C | -4.841596 | -1.086147 | 0.987051 | H | -1.738627 | -0.850639 | 2.809679 |
| H | -4.786528 | -1.974020 | 0.341763 | C | 2.596863 | -2.273993 | 1.287699 |
| H | -4.286278 | -1.341975 | 1.900344 | H | 2.571515 | -2.989003 | 0.454661 |
| C | -6.305076 | -0.804823 | 1.342475 | H | 3.641501 | -2.181545 | 1.605861 |
| H | -6.894754 | -0.583674 | 0.445386 | H | 2.031434 | -2.710829 | 2.116146 |
| H | -6.769658 | -1.661374 | 1.842399 | C | 2.721940 | -0.248633 | -0.291170 |
| H | -6.390705 | 0.058200 | 2.012749 | H | 2.687187 | -0.913082 | -1.168317 |
| H | 0.458738 | 3.577882 | -1.931373 | H | 2.152800 | 0.647022 | -0.568623 |
| Zr | 1.338423 | -0.220973 | 0.034507 | C | 4.182215 | 0.145003 | -0.020163 |
| C | 1.558188 | 0.381241 | 2.553089 | H | 4.779101 | -0.750710 | 0.197357 |
| H | 0.734349 | 0.164803 | 3.222493 | H | 4.226730 | 0.766583 | 0.885242 |
| C | 1.752130 | 1.589249 | 1.840061 | C | 4.830289 | 0.900065 | -1.188080 |
| H | 1.093042 | 2.444806 | 1.861014 | H | 4.771433 | 0.282907 | -2.095353 |
| C | 2.943089 | 1.467518 | 1.074772 | H | 4.246815 | 1.806465 | -1.401880 |
| H | 3.369005 | 2.230342 | 0.437790 | C | 6.290376 | 1.283369 | -0.926418 |
| C | 3.484135 | 0.171541 | 1.315858 | H | 6.907320 | 0.394875 | -0.749110 |
| H | 4.402890 | -0.224102 | 0.901771 | H | 6.722638 | 1.823624 | -1.775308 |
| C | 2.626353 | -0.498689 | 2.232596 | H | 6.378886 | 1.926298 | -0.043108 |
| H | 2.771342 | -1.495300 | 2.628362 | H | -2.294258 | -2.446298 | 2.157923 |
| C | 0.217936 | -2.486295 | -0.598333 | Zr | -1.463793 | -0.017169 | 0.014438 |
| H | -0.696996 | -2.774067 | -0.096340 | C | -0.604685 | 2.324446 | 0.604201 |
| C | 0.304023 | -1.751471 | -1.805390 | H | 0.456159 | 2.515633 | 0.528147 |
| H | -0.532651 | -1.372704 | -2.375244 | C | -1.296080 | 1.864860 | 1.761235 |
| C | 1.676684 | -1.573595 | -2.122091 | H | -0.842846 | 1.634501 | 2.715345 |
| H | 2.067090 | -1.066421 | -2.993991 | C | -2.676694 | 1.783346 | 1.447824 |
| C | 2.443898 | -2.198410 | -1.098301 | H | -3.467385 | 1.473085 | 2.117757 |
| H | 3.523695 | -2.263506 | -1.059423 | C | -2.843717 | 2.169378 | 0.095358 |
| C | 1.539293 | -2.763185 | -0.154519 | H | -3.781810 | 2.208264 | -0.442447 |
| H | 1.810057 | -3.328879 | 0.727261 | C | -1.562182 | 2.514708 | -0.421413 |
| | | | | H | -1.357253 | 2.866718 | -1.424160 |
| 2rTS2 | | | | C | -0.602648 | -1.417180 | -1.997559 |
| SCF energy in gas phase: -825.572246 | | | | H | 0.409584 | -1.794564 | -1.970933 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.759142 | -2.079690 | -1.502672 |
| H | -1.787558 | -3.068458 | -1.065964 |
| C | -2.884779 | -1.236529 | -1.717915 |
| H | -3.912878 | -1.471701 | -1.479818 |
| C | -2.416468 | -0.048530 | -2.338415 |
| H | -3.026476 | 0.790373 | -2.644214 |
| C | -1.007309 | -0.160963 | -2.506446 |
| H | -0.357356 | 0.581653 | -2.950999 |

2rIM2

SCF energy in gas phase: -825.585828

Free energy in Et₂O : -825.239409

Enthalpy in Et₂O : -825.163162

| | | | |
|----|-----------|-----------|-----------|
| C | -1.973958 | -1.196853 | -0.605632 |
| C | -1.444001 | -0.615296 | -1.908994 |
| H | -1.529809 | -1.223046 | -2.809441 |
| H | -1.587496 | 0.447750 | -2.089796 |
| C | -0.492316 | -1.073395 | -0.830666 |
| C | 0.441838 | -2.157436 | -0.933689 |
| H | 0.371760 | -2.952175 | -0.188686 |
| C | 1.601040 | -2.104066 | -1.671990 |
| H | 3.164694 | -0.681710 | -0.490879 |
| H | 1.701279 | -1.425548 | -2.515017 |
| C | -2.597262 | -2.585161 | -0.654428 |
| H | -2.532089 | -3.083760 | 0.321639 |
| H | -3.657114 | -2.546205 | -0.929979 |
| H | -2.087691 | -3.220450 | -1.385752 |
| C | -2.651191 | -0.224482 | 0.361160 |
| H | -2.658579 | -0.666997 | 1.368971 |
| H | -2.036412 | 0.681172 | 0.434493 |
| C | -4.086153 | 0.173128 | -0.018132 |
| H | -4.727906 | -0.717295 | -0.049652 |
| H | -4.088961 | 0.585187 | -1.036938 |
| C | -4.703732 | 1.194963 | 0.945746 |
| H | -4.695693 | 0.782582 | 1.964170 |
| H | -4.069215 | 2.091648 | 0.978525 |
| C | -6.133723 | 1.595456 | 0.569243 |
| H | -6.799916 | 0.725082 | 0.562284 |
| H | -6.546123 | 2.323603 | 1.275564 |
| H | -6.169277 | 2.044521 | -0.429966 |
| H | 2.362601 | -2.868619 | -1.579965 |
| Zr | 1.516075 | -0.013114 | -0.027113 |
| C | 0.503771 | 2.081925 | -1.119079 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.568650 | 2.214612 | -1.095372 |
| C | 1.249793 | 1.432704 | -2.144376 |
| H | 0.833909 | 0.970417 | -3.029058 |
| C | 2.622773 | 1.510220 | -1.808219 |
| H | 3.446542 | 1.111037 | -2.382446 |
| C | 2.730468 | 2.187521 | -0.565108 |
| H | 3.651322 | 2.395420 | -0.036845 |
| C | 1.421771 | 2.556921 | -0.152161 |
| H | 1.169908 | 3.103525 | 0.747019 |
| C | 0.542761 | -0.965398 | 2.178661 |
| H | -0.440235 | -1.412861 | 2.158488 |
| C | 1.774705 | -1.640231 | 1.973451 |
| H | 1.900084 | -2.698123 | 1.786934 |
| C | 2.826847 | -0.691087 | 2.083894 |
| H | 3.882637 | -0.900584 | 1.994414 |
| C | 2.240920 | 0.573784 | 2.332536 |
| H | 2.776021 | 1.502457 | 2.477359 |
| C | 0.824862 | 0.406742 | 2.382799 |
| H | 0.096128 | 1.183173 | 2.574361 |

2rTS3

SCF energy in gas phase: -825.567243

Free energy in Et₂O : -825.224724

Enthalpy in Et₂O : -825.146644

| | | | |
|---|-----------|-----------|-----------|
| C | -2.936980 | -1.149658 | -0.732233 |
| C | -2.333791 | -0.381269 | -1.932743 |
| H | -2.527903 | -0.755878 | -2.938573 |
| H | -2.328226 | 0.708150 | -1.876281 |
| C | -1.494538 | -1.181708 | -1.025421 |
| C | -0.313271 | -1.766706 | -0.783195 |
| H | -0.291445 | -2.465183 | 0.056547 |
| C | 0.973665 | -1.558680 | -1.489056 |
| H | 3.652547 | -0.395052 | -1.079799 |
| H | 0.836384 | -1.177164 | -2.503955 |
| C | -3.760473 | -2.397846 | -1.030678 |
| H | -3.784198 | -3.066294 | -0.161161 |
| H | -4.796450 | -2.150289 | -1.288501 |
| H | -3.328347 | -2.956509 | -1.865920 |
| C | -3.418671 | -0.309708 | 0.454149 |
| H | -3.378357 | -0.927801 | 1.363475 |
| H | -2.704810 | 0.509163 | 0.615116 |
| C | -4.830071 | 0.277831 | 0.304148 |
| H | -5.564339 | -0.533127 | 0.210839 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -4.886197 | 0.849216 | -0.632932 | H | 3.684476 | -0.049169 | -1.536003 |
| C | -5.233870 | 1.181842 | 1.476472 | H | 0.543081 | -0.952837 | -2.177189 |
| H | -5.162082 | 0.613005 | 2.413759 | C | -3.991209 | -2.518045 | -0.819785 |
| H | -4.509900 | 2.003672 | 1.565958 | H | -4.008832 | -3.129971 | 0.090606 |
| C | -6.646078 | 1.759125 | 1.336879 | H | -5.029864 | -2.333668 | -1.116959 |
| H | -7.396714 | 0.962140 | 1.285675 | H | -3.514625 | -3.109899 | -1.606695 |
| H | -6.902321 | 2.402386 | 2.185236 | C | -3.778811 | -0.324583 | 0.530838 |
| H | -6.740455 | 2.358972 | 0.424413 | H | -3.744957 | -0.881065 | 1.479245 |
| H | 1.568589 | -2.476807 | -1.524996 | H | -3.100951 | 0.529676 | 0.659501 |
| Zr | 2.096868 | -0.014375 | -0.171086 | C | -5.204841 | 0.198256 | 0.301362 |
| C | 0.579047 | 1.891296 | -0.991263 | H | -5.906500 | -0.643757 | 0.235891 |
| H | -0.482397 | 1.691740 | -1.033015 | H | -5.250020 | 0.709187 | -0.670536 |
| C | 1.509409 | 1.656969 | -2.034862 | C | -5.678269 | 1.155796 | 1.403070 |
| H | 1.277690 | 1.269574 | -3.017044 | H | -5.619221 | 0.646531 | 2.374924 |
| C | 2.799794 | 2.029786 | -1.566850 | H | -4.985223 | 2.006174 | 1.465557 |
| H | 3.718929 | 1.983928 | -2.132109 | C | -7.103323 | 1.673840 | 1.184368 |
| C | 2.662941 | 2.482014 | -0.229100 | H | -7.824926 | 0.849286 | 1.156605 |
| H | 3.464101 | 2.835514 | 0.406984 | H | -7.409618 | 2.356167 | 1.984276 |
| C | 1.289453 | 2.392965 | 0.130298 | H | -7.186534 | 2.215601 | 0.235191 |
| H | 0.856354 | 2.684296 | 1.077931 | H | 1.304728 | -2.286036 | -1.278062 |
| C | 1.467513 | -1.098226 | 2.064920 | Zr | 2.320780 | 0.053306 | -0.282629 |
| H | 0.416238 | -1.238922 | 2.279296 | C | 0.446703 | 1.765854 | -0.641467 |
| C | 2.318937 | -2.024542 | 1.399944 | H | -0.562671 | 1.379458 | -0.626464 |
| H | 2.033352 | -2.999970 | 1.031396 | C | 1.279147 | 1.875337 | -1.782329 |
| C | 3.616801 | -1.453373 | 1.328528 | H | 1.006491 | 1.605422 | -2.794182 |
| H | 4.491179 | -1.909991 | 0.888446 | C | 2.540466 | 2.383471 | -1.370338 |
| C | 3.564347 | -0.172970 | 1.940385 | H | 3.385885 | 2.583619 | -2.012594 |
| H | 4.392728 | 0.516734 | 2.037799 | C | 2.492568 | 2.572351 | 0.033953 |
| C | 2.239253 | 0.042642 | 2.401777 | H | 3.292928 | 2.961137 | 0.649385 |
| H | 1.880820 | 0.920778 | 2.922259 | C | 1.198059 | 2.185323 | 0.487930 |

2rIM3

SCF energy in gas phase: -825.568152

Free energy in Et₂O : -825.22803

Enthalpy in Et₂O : -825.146471

| | | | |
|---|-----------|-----------|-----------|
| C | -3.229366 | -1.218620 | -0.583685 |
| C | -2.624610 | -0.509872 | -1.819979 |
| H | -2.781815 | -0.962366 | -2.799654 |
| H | -2.653648 | 0.580480 | -1.839590 |
| C | -1.778767 | -1.208369 | -0.835860 |
| C | -0.566475 | -1.637494 | -0.483624 |
| H | -0.507203 | -2.252444 | 0.417797 |
| C | 0.720297 | -1.358053 | -1.171792 |

| | | | |
|----|-----------|-----------|-----------|
| H | 3.684476 | -0.049169 | -1.536003 |
| H | 0.543081 | -0.952837 | -2.177189 |
| C | -3.991209 | -2.518045 | -0.819785 |
| H | -4.008832 | -3.129971 | 0.090606 |
| H | -5.029864 | -2.333668 | -1.116959 |
| H | -3.514625 | -3.109899 | -1.606695 |
| C | -3.778811 | -0.324583 | 0.530838 |
| H | -3.744957 | -0.881065 | 1.479245 |
| H | -3.100951 | 0.529676 | 0.659501 |
| C | -5.204841 | 0.198256 | 0.301362 |
| H | -5.906500 | -0.643757 | 0.235891 |
| H | -5.250020 | 0.709187 | -0.670536 |
| C | -5.678269 | 1.155796 | 1.403070 |
| H | -5.619221 | 0.646531 | 2.374924 |
| H | -4.985223 | 2.006174 | 1.465557 |
| C | -7.103323 | 1.673840 | 1.184368 |
| H | -7.824926 | 0.849286 | 1.156605 |
| H | -7.409618 | 2.356167 | 1.984276 |
| H | -7.186534 | 2.215601 | 0.235191 |
| H | 1.304728 | -2.286036 | -1.278062 |
| Zr | 2.320780 | 0.053306 | -0.282629 |
| C | 0.446703 | 1.765854 | -0.641467 |
| H | -0.562671 | 1.379458 | -0.626464 |
| C | 1.279147 | 1.875337 | -1.782329 |
| H | 1.006491 | 1.605422 | -2.794182 |
| C | 2.540466 | 2.383471 | -1.370338 |
| H | 3.385885 | 2.583619 | -2.012594 |
| C | 2.492568 | 2.572351 | 0.033953 |
| H | 3.292928 | 2.961137 | 0.649385 |
| C | 1.198059 | 2.185323 | 0.487930 |
| H | 0.838845 | 2.238607 | 1.507203 |
| C | 2.334488 | -1.787414 | 1.523408 |
| H | 1.487466 | -2.456066 | 1.584894 |
| C | 3.509700 | -1.997981 | 0.761511 |
| H | 3.711831 | -2.849815 | 0.125172 |
| C | 4.378146 | -0.892129 | 0.965445 |
| H | 5.354493 | -0.762698 | 0.520525 |
| C | 3.728707 | 0.013155 | 1.840439 |
| H | 4.134088 | 0.948449 | 2.202372 |
| C | 2.456737 | -0.533427 | 2.179380 |
| H | 1.735013 | -0.096616 | 2.856878 |

2rIM4

SCF energy in gas phase: -825.567713

| | | | | | | | |
|--|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Free energy in Et ₂ O : -825.225818 | | | | C | 3.816743 | -1.756020 | -0.564008 |
| Enthalpy in Et ₂ O : -825.145485 | | | | H | 3.461670 | -2.718118 | -0.909312 |
| C | -3.236986 | -1.446147 | 0.130058 | C | 4.234468 | -0.678081 | -1.390235 |
| C | -2.409208 | -1.471748 | -1.177975 | H | 4.267681 | -0.679231 | -2.469846 |
| H | -2.420512 | -2.383916 | -1.775313 | C | 4.598584 | 0.400120 | -0.543563 |
| H | -2.385253 | -0.562303 | -1.780008 | H | 4.963233 | 1.365850 | -0.867515 |
| C | -1.765209 | -1.486225 | 0.146884 | C | 4.417681 | -0.016799 | 0.805958 |
| C | -0.638302 | -1.585604 | 0.852252 | H | 4.637036 | 0.570098 | 1.687904 |
| H | -0.731415 | -1.614823 | 1.941212 | 2rTS4 | | | |
| C | 0.745353 | -1.661665 | 0.328417 | SCF energy in gas phase: -825.567676 | | | |
| H | 1.828902 | 0.223066 | -2.051914 | Free energy in Et ₂ O : -825.22389 | | | |
| H | 0.734159 | -1.934084 | -0.752554 | Enthalpy in Et ₂ O : -825.146767 | | | |
| C | -3.991066 | -2.717054 | 0.506959 | C | 3.234162 | 1.433145 | 0.195419 |
| H | -4.179857 | -2.751245 | 1.587078 | C | 2.395084 | 1.575043 | -1.097741 |
| H | -4.959035 | -2.783275 | -0.002721 | H | 2.411553 | 2.534135 | -1.616388 |
| H | -3.409712 | -3.605861 | 0.244669 | H | 2.353374 | 0.719517 | -1.773108 |
| C | -3.940836 | -0.134568 | 0.487042 | C | 1.762946 | 1.483984 | 0.229497 |
| H | -4.099759 | -0.102009 | 1.575089 | C | 0.643069 | 1.524956 | 0.951994 |
| H | -3.266429 | 0.700908 | 0.257510 | H | 0.747049 | 1.457190 | 2.038208 |
| C | -5.280506 | 0.094516 | -0.228797 | C | -0.743975 | 1.652297 | 0.446199 |
| H | -5.989634 | -0.699267 | 0.040757 | H | -1.636624 | -0.255531 | -2.005950 |
| H | -5.127305 | 0.010841 | -1.313816 | H | -0.737644 | 2.034415 | -0.597841 |
| C | -5.912663 | 1.455396 | 0.093151 | C | 4.002975 | 2.662033 | 0.669326 |
| H | -6.054526 | 1.541353 | 1.179328 | H | 4.200701 | 2.605733 | 1.746943 |
| H | -5.211909 | 2.255055 | -0.183756 | H | 4.967493 | 2.761679 | 0.158426 |
| C | -7.251755 | 1.682356 | -0.615580 | H | 3.427763 | 3.574334 | 0.486120 |
| H | -7.985819 | 0.920397 | -0.329214 | C | 3.927098 | 0.090606 | 0.439673 |
| H | -7.675726 | 2.661376 | -0.368657 | H | 4.082193 | -0.036406 | 1.521372 |
| H | -7.136437 | 1.634787 | -1.704515 | H | 3.246597 | -0.716449 | 0.137477 |
| H | 1.311707 | -2.442247 | 0.846804 | C | 5.267318 | -0.091223 | -0.288953 |
| Zr | 2.085011 | 0.122510 | -0.221212 | H | 5.982223 | 0.671808 | 0.046212 |
| C | 0.497438 | 1.454648 | 1.288055 | H | 5.119395 | 0.080455 | -1.364266 |
| H | -0.040228 | 0.916772 | 2.055786 | C | 5.884825 | -1.479378 | -0.073898 |
| C | 0.046750 | 1.667575 | -0.038526 | H | 6.018989 | -1.652794 | 1.002740 |
| H | -0.882583 | 1.301661 | -0.452131 | H | 5.178179 | -2.247451 | -0.417284 |
| C | 1.036984 | 2.412719 | -0.733216 | C | 7.226029 | -1.662772 | -0.791331 |
| H | 0.981733 | 2.739120 | -1.761645 | H | 7.965499 | -0.933161 | -0.441575 |
| C | 2.114765 | 2.637956 | 0.159881 | H | 7.639305 | -2.662411 | -0.620554 |
| H | 3.022038 | 3.183990 | -0.062526 | H | 7.117864 | -1.528082 | -1.873701 |
| C | 1.783731 | 2.041506 | 1.411639 | H | -1.313339 | 2.371659 | 1.044747 |
| H | 2.388466 | 2.068613 | 2.308600 | Zr | -2.053685 | -0.125485 | -0.206730 |
| C | 3.942906 | -1.353499 | 0.790146 | C | -0.640844 | -1.470347 | 1.462146 |
| H | 3.705848 | -1.954177 | 1.657933 | | | | |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -0.165283 | -0.937541 | 2.273393 | H | 4.284627 | 1.011987 | 0.603368 |
| C | -0.073238 | -1.711633 | 0.186622 | C | 4.958156 | 0.724853 | -1.430816 |
| H | 0.898155 | -1.369979 | -0.141942 | H | 5.004176 | -0.088979 | -2.167489 |
| C | -1.011290 | -2.444089 | -0.589066 | H | 4.292930 | 1.485076 | -1.862536 |
| H | -0.867003 | -2.786713 | -1.603498 | C | 6.357050 | 1.319454 | -1.238504 |
| C | -2.171903 | -2.635980 | 0.202715 | H | 7.054600 | 0.572396 | -0.842390 |
| H | -3.066071 | -3.166321 | -0.097147 | H | 6.769390 | 1.690867 | -2.182640 |
| C | -1.946218 | -2.028489 | 1.471941 | H | 6.337403 | 2.157403 | -0.532063 |
| H | -2.630731 | -2.032992 | 2.309890 | H | -2.207842 | -2.053684 | 2.197913 |
| C | -3.967402 | 1.392336 | 0.631023 | Zr | -1.363331 | 0.051879 | -0.062024 |
| H | -3.798313 | 1.994874 | 1.513284 | C | -3.249858 | -1.088803 | -1.349382 |
| C | -3.717414 | 1.785109 | -0.708453 | H | -4.268197 | -0.920976 | -1.024612 |
| H | -3.319574 | 2.740210 | -1.025124 | C | -2.411228 | -2.152609 | -0.940018 |
| C | -4.077051 | 0.708360 | -1.563146 | H | -2.671830 | -2.927368 | -0.232297 |
| H | -4.015288 | 0.703311 | -2.641500 | C | -1.164522 | -2.012050 | -1.607098 |
| C | -4.531969 | -0.358801 | -0.746442 | H | -0.309027 | -2.665674 | -1.508182 |
| H | -4.883020 | -1.320379 | -1.096639 | C | -1.241351 | -0.874727 | -2.455517 |
| C | -4.463659 | 0.063407 | 0.611372 | H | -0.460659 | -0.517892 | -3.110839 |
| H | -4.767308 | -0.515081 | 1.473544 | C | -2.526402 | -0.300358 | -2.291996 |

2rIM5

SCF energy in gas phase: -825.584092

Free energy in Et₂O : -825.234951

Enthalpy in Et₂O : -825.158033

| | | | |
|---|-----------|-----------|-----------|
| C | 2.246460 | -0.850516 | 0.955543 |
| C | 1.625648 | 0.241583 | 1.835694 |
| H | 1.699612 | 0.143996 | 2.918989 |
| H | 1.699063 | 1.265514 | 1.477366 |
| C | 0.767094 | -0.735190 | 1.096743 |
| C | -0.225021 | -1.643343 | 1.465812 |
| H | -0.162856 | -2.633177 | 1.009982 |
| C | -1.455262 | -1.286610 | 2.047119 |
| H | 0.184304 | 0.572233 | -0.879446 |
| H | -1.480922 | -0.469377 | 2.761509 |
| C | 2.911442 | -2.026784 | 1.660775 |
| H | 2.913528 | -2.916931 | 1.019152 |
| H | 3.953285 | -1.807326 | 1.919448 |
| H | 2.382386 | -2.283353 | 2.583955 |
| C | 2.937357 | -0.398297 | -0.331061 |
| H | 3.001289 | -1.256813 | -1.016709 |
| H | 2.295100 | 0.337809 | -0.825284 |
| C | 4.340200 | 0.195045 | -0.129964 |
| H | 5.014551 | -0.556026 | 0.303138 |

| | | | |
|----|-----------|-----------|-----------|
| H | 4.284627 | 1.011987 | 0.603368 |
| C | 4.958156 | 0.724853 | -1.430816 |
| H | 5.004176 | -0.088979 | -2.167489 |
| H | 4.292930 | 1.485076 | -1.862536 |
| C | 6.357050 | 1.319454 | -1.238504 |
| H | 7.054600 | 0.572396 | -0.842390 |
| H | 6.769390 | 1.690867 | -2.182640 |
| H | 6.337403 | 2.157403 | -0.532063 |
| H | -2.207842 | -2.053684 | 2.197913 |
| Zr | -1.363331 | 0.051879 | -0.062024 |
| C | -3.249858 | -1.088803 | -1.349382 |
| H | -4.268197 | -0.920976 | -1.024612 |
| C | -2.411228 | -2.152609 | -0.940018 |
| H | -2.671830 | -2.927368 | -0.232297 |
| C | -1.164522 | -2.012050 | -1.607098 |
| H | -0.309027 | -2.665674 | -1.508182 |
| C | -1.241351 | -0.874727 | -2.455517 |
| H | -0.460659 | -0.517892 | -3.110839 |
| C | -2.526402 | -0.300358 | -2.291996 |
| H | -2.901331 | 0.572101 | -2.809446 |
| C | -2.693011 | 1.636391 | 1.483046 |
| H | -3.288824 | 1.212289 | 2.279497 |
| C | -1.329577 | 2.041144 | 1.574973 |
| H | -0.703392 | 1.968896 | 2.453396 |
| C | -0.942225 | 2.574970 | 0.321883 |
| H | 0.028209 | 2.977253 | 0.070055 |
| C | -2.053656 | 2.478473 | -0.555615 |
| H | -2.073131 | 2.801150 | -1.587870 |
| C | -3.138331 | 1.912460 | 0.168853 |
| H | -4.130972 | 1.722915 | -0.217845 |

2rTS5

SCF energy in gas phase: -825.573021

Free energy in Et₂O : -825.224227

Enthalpy in Et₂O : -825.148928

| | | | |
|---|-----------|-----------|----------|
| C | 2.225079 | -0.582082 | 1.040437 |
| C | 1.620974 | 0.668002 | 1.668570 |
| H | 1.626244 | 0.768532 | 2.751665 |
| H | 1.742683 | 1.604151 | 1.129496 |
| C | 0.728787 | -0.394240 | 1.083346 |
| C | -0.252137 | -1.213276 | 1.707667 |
| H | -0.178393 | -2.276659 | 1.482331 |
| C | -1.496524 | -0.767453 | 2.251181 |

| | | | | | | | |
|--------------------------------------|-----------|-----------|-----------|--|-----------|-----------|-----------|
| H | 0.418093 | 0.127489 | -0.343011 | Free energy in Et ₂ O : -825.246215 | | | |
| H | -1.519042 | 0.164126 | 2.813284 | Enthalpy in Et ₂ O : -825.168324 | | | |
| C | 2.801758 | -1.639176 | 1.971149 | | | | |
| H | 2.817334 | -2.622409 | 1.484895 | C | 2.812295 | -0.481425 | 0.404496 |
| H | 3.830541 | -1.397398 | 2.259223 | C | 2.202270 | 0.813394 | 0.897643 |
| H | 2.206079 | -1.727258 | 2.883806 | H | 1.872981 | 0.842918 | 1.932936 |
| C | 2.977456 | -0.408646 | -0.278025 | H | 2.618071 | 1.754193 | 0.542661 |
| H | 3.014869 | -1.379433 | -0.794226 | C | 1.422374 | -0.049550 | -0.072586 |
| H | 2.400728 | 0.259260 | -0.929300 | C | 0.154981 | -0.793964 | 0.284414 |
| C | 4.403180 | 0.144148 | -0.131630 | H | 0.177937 | -1.806024 | -0.126942 |
| H | 5.014681 | -0.540618 | 0.470543 | C | -0.497900 | -0.707965 | 1.601564 |
| H | 4.367975 | 1.090720 | 0.425910 | H | 1.444903 | 0.318374 | -1.099131 |
| C | 5.098555 | 0.375392 | -1.479916 | H | -0.127660 | 0.042018 | 2.299182 |
| H | 5.126637 | -0.569432 | -2.039934 | C | 2.926802 | -1.638969 | 1.381603 |
| H | 4.495272 | 1.066746 | -2.084233 | H | 3.014655 | -2.593585 | 0.846713 |
| C | 6.520547 | 0.927540 | -1.339022 | H | 3.810452 | -1.538216 | 2.022282 |
| H | 7.158140 | 0.240600 | -0.770718 | H | 2.048669 | -1.700875 | 2.028286 |
| H | 6.988912 | 1.083458 | -2.316429 | C | 3.946482 | -0.377917 | -0.611641 |
| H | 6.521822 | 1.888964 | -0.812584 | H | 3.994761 | -1.311049 | -1.193515 |
| H | -2.164876 | -1.530128 | 2.639089 | H | 3.705335 | 0.415788 | -1.332476 |
| Zr | -1.432664 | 0.013263 | -0.019506 | C | 5.331577 | -0.088376 | -0.011676 |
| C | -3.261292 | -1.387429 | -1.164785 | H | 5.623541 | -0.903006 | 0.664088 |
| H | -4.296058 | -1.169820 | -0.934168 | H | 5.274237 | 0.816585 | 0.609368 |
| C | -2.446082 | -2.333886 | -0.502876 | C | 6.423736 | 0.091791 | -1.074362 |
| H | -2.745523 | -2.955864 | 0.329318 | H | 6.467157 | -0.807234 | -1.704573 |
| C | -1.160073 | -2.304565 | -1.108668 | H | 6.144114 | 0.916521 | -1.744448 |
| H | -0.314369 | -2.921964 | -0.839306 | C | 7.808844 | 0.365060 | -0.479232 |
| C | -1.183510 | -1.345938 | -2.159418 | H | 8.132730 | -0.460255 | 0.165326 |
| H | -0.368307 | -1.115453 | -2.830585 | H | 8.564994 | 0.491954 | -1.261270 |
| C | -2.484032 | -0.776789 | -2.189958 | H | 7.805211 | 1.275894 | 0.130586 |
| H | -2.831782 | -0.025563 | -2.885593 | H | -0.754402 | -1.638142 | 2.108596 |
| C | -2.699385 | 1.979739 | 1.070541 | Zr | -1.997530 | 0.042006 | 0.041422 |
| H | -3.312586 | 1.780413 | 1.938268 | C | -4.276722 | -0.985440 | -0.343076 |
| C | -1.322070 | 2.337484 | 1.077852 | H | -5.150931 | -0.379549 | -0.144178 |
| H | -0.701163 | 2.457064 | 1.954953 | C | -3.656783 | -1.887403 | 0.566298 |
| C | -0.908199 | 2.537139 | -0.266817 | H | -3.952360 | -2.063349 | 1.592915 |
| H | 0.076746 | 2.837204 | -0.596295 | C | -2.577142 | -2.510955 | -0.103689 |
| C | -2.020473 | 2.285780 | -1.105379 | H | -1.894767 | -3.228876 | 0.330411 |
| H | -2.027756 | 2.355577 | -2.184890 | C | -2.521262 | -2.010212 | -1.428673 |
| C | -3.128184 | 1.943613 | -0.277694 | H | -1.810546 | -2.305760 | -2.189369 |
| H | -4.126588 | 1.705021 | -0.620590 | C | -3.572887 | -1.061224 | -1.581369 |
| | | | | H | -3.825112 | -0.527880 | -2.488686 |
| | | | | C | -2.285452 | 2.374792 | 1.156486 |
| 2rIM6 | | | | H | -2.568237 | 2.435773 | 2.200064 |
| SCF energy in gas phase: -825.589349 | | | | | | | |

| | | | | | | | |
|---|-----------|----------|-----------|---|-----------|-----------|-----------|
| C | -0.962078 | 2.362516 | 0.655606 | H | 1.646783 | -2.726365 | -1.924714 |
| H | -0.058602 | 2.393799 | 1.246265 | C | -0.295876 | -2.058355 | -1.056280 |
| C | -1.019405 | 2.268784 | -0.758669 | H | -0.839855 | -1.727435 | -1.929712 |
| H | -0.167872 | 2.254455 | -1.425545 | C | -0.769339 | -2.073104 | 0.283261 |
| C | -2.392508 | 2.221097 | -1.137819 | H | -1.747604 | -1.764724 | 0.620079 |
| H | -2.775891 | 2.188860 | -2.149451 | C | 0.249921 | -2.610559 | 1.110524 |
| C | -3.176382 | 2.285451 | 0.051629 | H | 0.189309 | -2.765626 | 2.177808 |
| H | -4.257217 | 2.299498 | 0.101338 | C | 1.353920 | -2.929179 | 0.282936 |

2rTS6

SCF energy in gas phase: -825.557399

Free energy in Et₂O : -825.215574

Enthalpy in Et₂O : -825.142369

| | | | |
|----|-----------|-----------|-----------|
| C | -1.759604 | 1.559597 | -0.129376 |
| C | -0.961836 | 1.277119 | 1.134005 |
| H | -0.886171 | 2.054791 | 1.891050 |
| H | -1.051981 | 0.281790 | 1.572457 |
| C | -0.232366 | 1.456245 | -0.224719 |
| C | 0.427213 | 2.763562 | -0.485985 |
| H | 0.473235 | 3.017333 | -1.548044 |
| C | 0.928282 | 3.654513 | 0.381515 |
| H | 1.319895 | -0.415465 | 2.042252 |
| H | 0.904482 | 3.490699 | 1.456198 |
| C | -2.399692 | 2.947824 | -0.214447 |
| H | -2.538747 | 3.246946 | -1.260872 |
| H | -3.388455 | 2.940791 | 0.256730 |
| H | -1.800642 | 3.715913 | 0.274152 |
| C | -2.695675 | 0.504463 | -0.722796 |
| H | -3.063523 | 0.892721 | -1.683758 |
| H | -2.142102 | -0.398679 | -0.966685 |
| C | -3.902498 | 0.136801 | 0.156855 |
| H | -4.483141 | 1.036374 | 0.397951 |
| H | -3.547186 | -0.253276 | 1.121948 |
| C | -4.834050 | -0.895023 | -0.494049 |
| H | -5.188276 | -0.503530 | -1.457452 |
| H | -4.263538 | -1.804196 | -0.729888 |
| C | -6.036792 | -1.259717 | 0.382050 |
| H | -6.646504 | -0.376410 | 0.604077 |
| H | -6.683013 | -1.994710 | -0.109035 |
| H | -5.715608 | -1.686432 | 1.339241 |
| H | 1.379698 | 4.581975 | 0.040884 |
| Zr | 1.197960 | -0.356897 | 0.207409 |
| C | 1.020110 | -2.585096 | -1.054793 |

| | | | |
|---|----------|-----------|-----------|
| H | 2.284134 | -3.366461 | 0.617281 |
| C | 3.259045 | -0.218153 | -1.306849 |
| H | 3.212791 | -0.646067 | -2.299534 |
| C | 2.961262 | 1.124922 | -0.963336 |
| H | 2.616371 | 1.892368 | -1.639478 |
| C | 3.183534 | 1.280615 | 0.427002 |
| H | 3.015187 | 2.184024 | 0.993338 |
| C | 3.650082 | 0.043171 | 0.944359 |
| H | 3.919021 | -0.154924 | 1.971833 |
| C | 3.700801 | -0.880778 | -0.126771 |
| H | 4.028404 | -1.908768 | -0.063127 |

2rIM7

SCF energy in gas phase: -825.571763

Free energy in Et₂O : -825.234327

Enthalpy in Et₂O : -825.15645

| | | | |
|---|-----------|-----------|-----------|
| C | 1.826450 | 1.278610 | 0.379215 |
| C | 1.218927 | 1.870081 | -0.874126 |
| H | 1.334819 | 2.940449 | -1.040974 |
| H | 1.290302 | 1.284021 | -1.790552 |
| C | 0.294124 | 1.403311 | 0.236124 |
| C | -0.398539 | 2.430063 | 1.050452 |
| H | -0.565719 | 2.161037 | 2.096427 |
| C | -0.859064 | 3.628560 | 0.653859 |
| H | -0.071331 | -1.727574 | -1.057515 |
| H | -0.720129 | 3.990576 | -0.361880 |
| C | 2.558336 | 2.226245 | 1.320544 |
| H | 2.651141 | 1.791966 | 2.324963 |
| H | 3.572454 | 2.438840 | 0.963679 |
| H | 2.032167 | 3.178977 | 1.416653 |
| C | 2.476054 | -0.098968 | 0.259026 |
| H | 2.520887 | -0.567422 | 1.253762 |
| H | 1.837630 | -0.752453 | -0.353774 |
| C | 3.886733 | -0.098071 | -0.353011 |
| H | 4.569937 | 0.487911 | 0.275635 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 3.856543 | 0.409817 | -1.326969 | H | 0.019825 | -1.471370 | 1.027353 |
| C | 4.463699 | -1.508689 | -0.533216 | H | 0.923877 | 3.749513 | 0.202335 |
| H | 4.482149 | -2.019002 | 0.439840 | C | -2.627235 | 2.077525 | -1.468382 |
| H | 3.789197 | -2.096519 | -1.170543 | H | -2.677918 | 1.584701 | -2.448663 |
| C | 5.871750 | -1.513231 | -1.137131 | H | -3.655122 | 2.313063 | -1.170465 |
| H | 6.577100 | -0.964428 | -0.502387 | H | -2.095318 | 3.023722 | -1.599034 |
| H | 6.254909 | -2.532238 | -1.255747 | C | -2.621542 | -0.166655 | -0.238789 |
| H | 5.879927 | -1.037904 | -2.124757 | H | -2.647097 | -0.704331 | -1.199667 |
| H | -1.380098 | 4.291099 | 1.338980 | H | -2.005304 | -0.774916 | 0.433493 |
| Zr | -1.060331 | -0.458136 | -0.148699 | C | -4.049411 | -0.091892 | 0.325990 |
| C | -1.878784 | -0.548107 | 2.258208 | H | -4.705058 | 0.453739 | -0.365496 |
| H | -2.387009 | 0.321553 | 2.653457 | H | -4.037586 | 0.490655 | 1.258089 |
| C | -0.481765 | -0.806426 | 2.326942 | C | -4.660373 | -1.472754 | 0.600057 |
| H | 0.262319 | -0.159243 | 2.768390 | H | -4.663722 | -2.058560 | -0.329776 |
| C | -0.237958 | -2.055382 | 1.703481 | H | -4.015310 | -2.021017 | 1.300138 |
| H | 0.725631 | -2.527720 | 1.573884 | C | -6.083711 | -1.403588 | 1.162692 |
| C | -1.482833 | -2.580360 | 1.263129 | H | -6.760247 | -0.892808 | 0.467598 |
| H | -1.624275 | -3.515848 | 0.738626 | H | -6.491746 | -2.402646 | 1.349447 |
| C | -2.495587 | -1.656309 | 1.615400 | H | -6.108244 | -0.852023 | 2.109666 |
| H | -3.554441 | -1.768138 | 1.424477 | H | 1.482136 | 3.972793 | -1.548493 |
| C | -3.288831 | 0.414958 | -0.957211 | Zr | 1.162616 | -0.351553 | 0.122478 |
| H | -4.015617 | 0.719150 | -0.215355 | C | 1.836619 | -0.631381 | -2.329503 |
| C | -2.332384 | 1.257552 | -1.582662 | H | 2.191755 | 0.239450 | -2.864923 |
| H | -2.163993 | 2.298918 | -1.350477 | C | 0.484720 | -1.069332 | -2.239840 |
| C | -1.600221 | 0.475017 | -2.506334 | H | -0.371547 | -0.587954 | -2.690037 |
| H | -0.781696 | 0.822416 | -3.122402 | C | 0.460658 | -2.254355 | -1.461224 |
| C | -2.117163 | -0.849913 | -2.480346 | H | -0.415818 | -2.831901 | -1.205859 |
| H | -1.770321 | -1.679615 | -3.079095 | C | 1.794154 | -2.548411 | -1.068189 |
| C | -3.161343 | -0.887225 | -1.524872 | H | 2.103256 | -3.385856 | -0.456537 |
| H | -3.758875 | -1.753460 | -1.273194 | C | 2.643717 | -1.553572 | -1.614327 |

2rTS7

SCF energy in gas phase: -825.570978

Free energy in Et₂O : -825.231401

Enthalpy in Et₂O : -825.154545

| | | | |
|---|-----------|----------|-----------|
| C | -1.941094 | 1.186218 | -0.440007 |
| C | -1.348738 | 1.866094 | 0.776180 |
| H | -1.450738 | 2.948575 | 0.852219 |
| H | -1.435494 | 1.353044 | 1.732503 |
| C | -0.417003 | 1.299721 | -0.281074 |
| C | 0.312268 | 2.237372 | -1.165494 |
| H | 0.359661 | 1.952298 | -2.219370 |
| C | 0.946480 | 3.373800 | -0.817620 |

2rIM8

SCF energy in gas phase: -825.571763

| | | | |
|----|-----------|-----------|-----------|
| H | 0.019825 | -1.471370 | 1.027353 |
| H | 0.923877 | 3.749513 | 0.202335 |
| C | -2.627235 | 2.077525 | -1.468382 |
| H | -2.677918 | 1.584701 | -2.448663 |
| H | -3.655122 | 2.313063 | -1.170465 |
| H | -2.095318 | 3.023722 | -1.599034 |
| C | -2.621542 | -0.166655 | -0.238789 |
| H | -2.647097 | -0.704331 | -1.199667 |
| H | -2.005304 | -0.774916 | 0.433493 |
| C | -4.049411 | -0.091892 | 0.325990 |
| H | -4.705058 | 0.453739 | -0.365496 |
| H | -4.037586 | 0.490655 | 1.258089 |
| C | -4.660373 | -1.472754 | 0.600057 |
| H | -4.663722 | -2.058560 | -0.329776 |
| H | -4.015310 | -2.021017 | 1.300138 |
| C | -6.083711 | -1.403588 | 1.162692 |
| H | -6.760247 | -0.892808 | 0.467598 |
| H | -6.491746 | -2.402646 | 1.349447 |
| H | -6.108244 | -0.852023 | 2.109666 |
| H | 1.482136 | 3.972793 | -1.548493 |
| Zr | 1.162616 | -0.351553 | 0.122478 |
| C | 1.836619 | -0.631381 | -2.329503 |
| H | 2.191755 | 0.239450 | -2.864923 |
| C | 0.484720 | -1.069332 | -2.239840 |
| H | -0.371547 | -0.587954 | -2.690037 |
| C | 0.460658 | -2.254355 | -1.461224 |
| H | -0.415818 | -2.831901 | -1.205859 |
| C | 1.794154 | -2.548411 | -1.068189 |
| H | 2.103256 | -3.385856 | -0.456537 |
| C | 2.643717 | -1.553572 | -1.614327 |
| H | 3.718684 | -1.503257 | -1.504546 |
| C | 3.455730 | 0.206524 | 1.120070 |
| H | 4.317899 | 0.237484 | 0.467240 |
| C | 2.624633 | 1.308123 | 1.452821 |
| H | 2.715525 | 2.309849 | 1.057595 |
| C | 1.629414 | 0.853472 | 2.352401 |
| H | 0.838413 | 1.453620 | 2.779704 |
| C | 1.855525 | -0.530423 | 2.597990 |
| H | 1.277295 | -1.162749 | 3.255587 |
| C | 2.984292 | -0.927830 | 1.837415 |
| H | 3.408689 | -1.922921 | 1.803787 |

Free energy in Et₂O : -825.234327

Enthalpy in Et₂O : -825.15645

| | | | |
|----|-----------|-----------|-----------|
| C | 1.826450 | 1.278610 | 0.379215 |
| C | 1.218927 | 1.870081 | -0.874126 |
| H | 1.334819 | 2.940449 | -1.040974 |
| H | 1.290302 | 1.284021 | -1.790552 |
| C | 0.294124 | 1.403311 | 0.236124 |
| C | -0.398539 | 2.430063 | 1.050452 |
| H | -0.565719 | 2.161037 | 2.096427 |
| C | -0.859064 | 3.628560 | 0.653859 |
| H | -0.071331 | -1.727574 | -1.057515 |
| H | -0.720129 | 3.990576 | -0.361880 |
| C | 2.558336 | 2.226245 | 1.320544 |
| H | 2.651141 | 1.791966 | 2.324963 |
| H | 3.572454 | 2.438840 | 0.963679 |
| H | 2.032167 | 3.178977 | 1.416653 |
| C | 2.476054 | -0.098968 | 0.259026 |
| H | 2.520887 | -0.567422 | 1.253762 |
| H | 1.837630 | -0.752453 | -0.353774 |
| C | 3.886733 | -0.098071 | -0.353011 |
| H | 4.569937 | 0.487911 | 0.275635 |
| H | 3.856543 | 0.409817 | -1.326969 |
| C | 4.463699 | -1.508689 | -0.533216 |
| H | 4.482149 | -2.019002 | 0.439840 |
| H | 3.789197 | -2.096519 | -1.170543 |
| C | 5.871750 | -1.513231 | -1.137131 |
| H | 6.577100 | -0.964428 | -0.502387 |
| H | 6.254909 | -2.532238 | -1.255747 |
| H | 5.879927 | -1.037904 | -2.124757 |
| H | -1.380098 | 4.291099 | 1.338980 |
| Zr | -1.060331 | -0.458136 | -0.148699 |
| C | -1.878784 | -0.548107 | 2.258208 |
| H | -2.387009 | 0.321553 | 2.653457 |
| C | -0.481765 | -0.806426 | 2.326942 |
| H | 0.262319 | -0.159243 | 2.768390 |
| C | -0.237958 | -2.055382 | 1.703481 |
| H | 0.725631 | -2.527720 | 1.573884 |
| C | -1.482833 | -2.580360 | 1.263129 |
| H | -1.624275 | -3.515848 | 0.738626 |
| C | -2.495587 | -1.656309 | 1.615400 |
| H | -3.554441 | -1.768138 | 1.424477 |
| C | -3.288831 | 0.414958 | -0.957211 |
| H | -4.015617 | 0.719150 | -0.215355 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.332384 | 1.257552 | -1.582662 |
| H | -2.163993 | 2.298918 | -1.350477 |
| C | -1.600221 | 0.475017 | -2.506334 |
| H | -0.781696 | 0.822416 | -3.122402 |
| C | -2.117163 | -0.849913 | -2.480346 |
| H | -1.770321 | -1.679615 | -3.079095 |
| C | -3.161343 | -0.887225 | -1.524872 |
| H | -3.758875 | -1.753460 | -1.273194 |

2rTS8

SCF energy in gas phase: -825.563209

Free energy in Et₂O : -825.225987

Enthalpy in Et₂O : -825.14949

| | | | |
|----|-----------|-----------|-----------|
| C | -1.807351 | 1.455952 | -0.029621 |
| C | -1.236856 | 1.627544 | 1.345031 |
| H | -1.346403 | 2.594359 | 1.835180 |
| H | -1.301033 | 0.789651 | 2.040123 |
| C | -0.261961 | 1.525866 | 0.154524 |
| C | 0.389072 | 2.808322 | -0.236525 |
| H | -0.267981 | 3.596332 | -0.609586 |
| C | 1.691456 | 3.129498 | -0.199613 |
| H | -0.106875 | -1.914553 | 0.364443 |
| H | 2.461292 | 2.444081 | 0.138878 |
| C | -2.568715 | 2.624184 | -0.646193 |
| H | -2.451593 | 2.649284 | -1.737532 |
| H | -3.639927 | 2.539885 | -0.435453 |
| H | -2.250401 | 3.592178 | -0.253064 |
| C | -2.436532 | 0.098847 | -0.357696 |
| H | -2.515247 | -0.015046 | -1.448797 |
| H | -1.772135 | -0.711592 | -0.021843 |
| C | -3.817640 | -0.145804 | 0.273454 |
| H | -4.537535 | 0.601696 | -0.084592 |
| H | -3.745774 | -0.002863 | 1.360500 |
| C | -4.373826 | -1.546273 | -0.018684 |
| H | -4.437539 | -1.691432 | -1.106086 |
| H | -3.664314 | -2.300920 | 0.346704 |
| C | -5.749940 | -1.791309 | 0.608540 |
| H | -6.490472 | -1.075523 | 0.233117 |
| H | -6.118740 | -2.798086 | 0.385935 |
| H | -5.712594 | -1.684450 | 1.698765 |
| H | 2.029580 | 4.115004 | -0.507623 |
| Zr | 0.975734 | -0.460440 | 0.027585 |
| C | 1.734028 | 0.310190 | -2.302016 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 2.008993 | 1.350368 | -2.405183 | H | 4.279155 | 0.881164 | -1.107075 |
| C | 0.429928 | -0.222903 | -2.471688 | C | 4.843574 | -1.189637 | -0.843506 |
| H | -0.448351 | 0.341765 | -2.749514 | H | 4.773917 | -1.961290 | -0.064259 |
| C | 0.485127 | -1.618571 | -2.213611 | H | 4.250585 | -1.560614 | -1.690683 |
| H | -0.341634 | -2.312522 | -2.262945 | C | 6.305341 | -1.031100 | -1.273924 |
| C | 1.824466 | -1.945860 | -1.875348 | H | 6.930548 | -0.695295 | -0.438546 |
| H | 2.188491 | -2.930902 | -1.614591 | H | 6.720700 | -1.975772 | -1.640483 |
| C | 2.596394 | -0.755240 | -1.935036 | H | 6.403828 | -0.291101 | -2.076469 |
| H | 3.658137 | -0.675068 | -1.742388 | H | -2.056296 | 1.912425 | 2.359340 |
| C | 3.080539 | 0.043636 | 1.342590 | Zr | -1.310630 | -0.124441 | -0.033482 |
| H | 3.862219 | 0.622148 | 0.867762 | C | -1.466022 | -1.735218 | 1.980066 |
| C | 2.034567 | 0.555723 | 2.157342 | H | -1.852092 | -1.361567 | 2.918399 |
| H | 1.839241 | 1.598251 | 2.363161 | C | -0.100374 | -1.735049 | 1.570279 |
| C | 1.264139 | -0.540396 | 2.610673 | H | 0.735726 | -1.361559 | 2.144954 |
| H | 0.382061 | -0.482496 | 3.234472 | C | -0.023692 | -2.348697 | 0.295096 |
| C | 1.847321 | -1.738119 | 2.111761 | H | 0.874757 | -2.516764 | -0.279061 |
| H | 1.488509 | -2.741015 | 2.293007 | C | -1.339563 | -2.701089 | -0.098899 |
| C | 2.970384 | -1.378421 | 1.331438 | H | -1.611494 | -3.187715 | -1.025882 |
| H | 3.633057 | -2.062129 | 0.817826 | C | -2.227657 | -2.332700 | 0.949411 |

2rIM9

SCF energy in gas phase: -825.581838

Free energy in Et₂O : -825.234511

Enthalpy in Et₂O : -825.157893

| | | | |
|---|-----------|-----------|-----------|
| C | 2.068142 | 1.237677 | 0.533296 |
| C | 1.651472 | 2.187370 | -0.591274 |
| H | 1.805529 | 3.257072 | -0.447762 |
| H | 1.828173 | 1.845068 | -1.608871 |
| C | 0.612519 | 1.501713 | 0.221669 |
| C | -0.453838 | 2.069438 | 0.933353 |
| H | -0.941790 | 2.922609 | 0.458066 |
| C | -1.169427 | 1.434971 | 1.955676 |
| H | -0.011738 | -0.297884 | -1.309418 |
| H | -0.652824 | 0.760373 | 2.630305 |
| C | 2.603314 | 1.846356 | 1.822465 |
| H | 2.418405 | 1.183378 | 2.677247 |
| H | 3.684682 | 2.015339 | 1.766736 |
| H | 2.121204 | 2.804017 | 2.037941 |
| C | 2.752465 | -0.058033 | 0.103049 |
| H | 2.704290 | -0.786566 | 0.925730 |
| H | 2.183134 | -0.486266 | -0.728082 |
| C | 4.219174 | 0.112556 | -0.324261 |
| H | 4.821462 | 0.484801 | 0.515227 |

| | | | |
|----|-----------|-----------|-----------|
| H | 4.279155 | 0.881164 | -1.107075 |
| C | 4.843574 | -1.189637 | -0.843506 |
| H | 4.773917 | -1.961290 | -0.064259 |
| H | 4.250585 | -1.560614 | -1.690683 |
| C | 6.305341 | -1.031100 | -1.273924 |
| H | 6.930548 | -0.695295 | -0.438546 |
| H | 6.720700 | -1.975772 | -1.640483 |
| H | 6.403828 | -0.291101 | -2.076469 |
| H | -2.056296 | 1.912425 | 2.359340 |
| Zr | -1.310630 | -0.124441 | -0.033482 |
| C | -1.466022 | -1.735218 | 1.980066 |
| H | -1.852092 | -1.361567 | 2.918399 |
| C | -0.100374 | -1.735049 | 1.570279 |
| H | 0.735726 | -1.361559 | 2.144954 |
| C | -0.023692 | -2.348697 | 0.295096 |
| H | 0.874757 | -2.516764 | -0.279061 |
| C | -1.339563 | -2.701089 | -0.098899 |
| H | -1.611494 | -3.187715 | -1.025882 |
| C | -2.227657 | -2.332700 | 0.949411 |
| H | -3.298771 | -2.485144 | 0.958842 |
| C | -3.774396 | 0.170251 | -0.646976 |
| H | -4.522885 | -0.243528 | 0.015569 |
| C | -3.261036 | 1.487708 | -0.600401 |
| H | -3.535886 | 2.248229 | 0.117686 |
| C | -2.311463 | 1.628481 | -1.648620 |
| H | -1.739733 | 2.516704 | -1.879154 |
| C | -2.256695 | 0.402344 | -2.363569 |
| H | -1.643962 | 0.199055 | -3.229276 |
| C | -3.153773 | -0.501503 | -1.740518 |
| H | -3.351828 | -1.516569 | -2.056214 |

2rTS9

SCF energy in gas phase: -825.570971

Free energy in Et₂O : -825.223098

Enthalpy in Et₂O : -825.147911

| | | | |
|---|-----------|-----------|-----------|
| C | -2.063589 | -1.137827 | 0.573294 |
| C | -1.665142 | -2.178500 | -0.464694 |
| H | -1.742163 | -3.232870 | -0.208004 |
| H | -1.896790 | -1.950933 | -1.502956 |
| C | -0.601593 | -1.381857 | 0.227452 |
| C | 0.468206 | -1.936787 | 0.985623 |
| H | 0.914734 | -2.830203 | 0.549824 |
| C | 1.243886 | -1.279602 | 1.988336 |

| | | | | | | | |
|--------------------------------------|-----------|-----------|-----------|--|-----------|-----------|-----------|
| H | -0.254487 | -0.304137 | -0.838555 | Free energy in Et ₂ O : -825.247789 | | | |
| H | 0.743828 | -0.618537 | 2.692788 | Enthalpy in Et ₂ O : -825.16945 | | | |
| C | -2.519139 | -1.618403 | 1.942538 | | | | |
| H | -2.365953 | -0.841744 | 2.701847 | C | -2.794864 | -0.753524 | -0.007126 |
| H | -3.585372 | -1.870400 | 1.937909 | C | -2.137031 | -0.338118 | -1.309363 |
| H | -1.960000 | -2.503410 | 2.255466 | H | -1.740914 | -1.125341 | -1.947782 |
| C | -2.797577 | 0.090512 | 0.043241 | H | -2.554699 | 0.502346 | -1.860303 |
| H | -2.725909 | 0.904012 | 0.778693 | C | -1.415932 | -0.086221 | -0.001567 |
| H | -2.285112 | 0.441329 | -0.860216 | C | -0.138876 | -0.794711 | 0.351115 |
| C | -4.278082 | -0.153034 | -0.290746 | H | -0.123774 | -1.819835 | -0.019299 |
| H | -4.828177 | -0.441191 | 0.614558 | C | 0.464610 | -0.617841 | 1.686524 |
| H | -4.358183 | -1.004520 | -0.980489 | H | -1.456202 | 0.945132 | 0.345853 |
| C | -4.957291 | 1.072827 | -0.916024 | H | 0.007035 | 0.134950 | 2.328662 |
| H | -4.864924 | 1.927246 | -0.231448 | C | -2.920255 | -2.234522 | 0.307174 |
| H | -4.417451 | 1.357494 | -1.829596 | H | -3.024068 | -2.397865 | 1.387121 |
| C | -6.435148 | 0.841627 | -1.246854 | H | -3.796821 | -2.674535 | -0.181924 |
| H | -7.008289 | 0.591225 | -0.346761 | H | -2.045351 | -2.797859 | -0.026946 |
| H | -6.890159 | 1.731978 | -1.693180 | C | -3.963145 | 0.101917 | 0.477788 |
| H | -6.557811 | 0.014622 | -1.955649 | H | -4.068764 | -0.017075 | 1.566589 |
| H | 2.066012 | -1.842024 | 2.420245 | H | -3.719200 | 1.160586 | 0.311498 |
| Zr | 1.375851 | 0.094829 | 0.022835 | C | -5.311541 | -0.198083 | -0.196242 |
| C | 1.482986 | 1.900439 | 1.862738 | H | -5.612781 | -1.233107 | 0.012830 |
| H | 1.897466 | 1.630574 | 2.823851 | H | -5.191781 | -0.130445 | -1.286653 |
| C | 0.117402 | 1.796414 | 1.474999 | C | -6.434874 | 0.746143 | 0.251833 |
| H | -0.693650 | 1.446757 | 2.099325 | H | -6.544433 | 0.686728 | 1.343506 |
| C | -0.003428 | 2.284872 | 0.144545 | H | -6.144453 | 1.783310 | 0.034064 |
| H | -0.916934 | 2.365352 | -0.425817 | C | -7.781586 | 0.443351 | -0.413021 |
| C | 1.285169 | 2.664361 | -0.296730 | H | -8.117438 | -0.574130 | -0.181811 |
| H | 1.524938 | 3.076587 | -1.267785 | H | -8.561098 | 1.134909 | -0.076121 |
| C | 2.204233 | 2.427485 | 0.766019 | H | -7.712190 | 0.526316 | -1.503823 |
| H | 3.267887 | 2.625826 | 0.741856 | H | 0.736112 | -1.512134 | 2.247645 |
| C | 3.816013 | -0.225129 | -0.723381 | Zr | 1.991976 | 0.102362 | 0.143971 |
| H | 4.598971 | 0.209137 | -0.115452 | C | 2.295704 | 2.534117 | 1.039583 |
| C | 3.305190 | -1.537694 | -0.602944 | H | 2.659126 | 2.690665 | 2.047907 |
| H | 3.619742 | -2.275650 | 0.122242 | C | 0.937646 | 2.422296 | 0.655733 |
| C | 2.288251 | -1.705044 | -1.582076 | H | 0.088609 | 2.483737 | 1.321538 |
| H | 1.706808 | -2.600977 | -1.751066 | C | 0.884875 | 2.215716 | -0.749804 |
| C | 2.178906 | -0.495933 | -2.322275 | H | -0.012312 | 2.106722 | -1.342823 |
| H | 1.517203 | -0.317524 | -3.158103 | C | 2.225271 | 2.193562 | -1.233294 |
| C | 3.123461 | 0.420147 | -1.787251 | H | 2.528982 | 2.086419 | -2.266869 |
| H | 3.303440 | 1.425588 | -2.141802 | C | 3.096738 | 2.393057 | -0.124157 |
| | | | | H | 4.176760 | 2.446741 | -0.164387 |
| 2rIM10 | | | | C | 3.695067 | -1.746274 | 0.810811 |
| SCF energy in gas phase: -825.590154 | | | | H | 3.966041 | -1.859511 | 1.852989 |

| | | | | | | | |
|---|----------|-----------|-----------|---|----------|----------|-----------|
| C | 2.653268 | -2.435421 | 0.145889 | H | 2.759340 | 2.302672 | 2.059961 |
| H | 1.981528 | -3.152383 | 0.598026 | C | 0.999299 | 2.498307 | 0.686668 |
| C | 2.619012 | -2.003404 | -1.204421 | H | 0.178794 | 2.670376 | 1.369078 |
| H | 1.940548 | -2.359540 | -1.968292 | C | 0.916506 | 2.476769 | -0.727314 |
| C | 3.645922 | -1.031563 | -1.376805 | H | 0.015142 | 2.599187 | -1.314086 |
| H | 3.905203 | -0.533621 | -2.302008 | C | 2.215001 | 2.256311 | -1.246656 |
| C | 4.312432 | -0.871467 | -0.126071 | H | 2.481907 | 2.201186 | -2.293862 |
| H | 5.162661 | -0.229731 | 0.064508 | C | 3.110125 | 2.157449 | -0.139974 |

2rTS10

SCF energy in gas phase: -825.579965

Free energy in Et₂O : -825.236441

Enthalpy in Et₂O : -825.16092

| | | | |
|----|-----------|-----------|-----------|
| C | -2.435153 | -0.738726 | 0.369851 |
| C | -1.517006 | -0.047997 | -0.618805 |
| H | -0.979211 | -0.696148 | -1.310806 |
| H | -1.833382 | 0.898305 | -1.048528 |
| C | -1.165070 | -0.117243 | 0.909237 |
| C | 0.022006 | -0.886616 | 1.384603 |
| H | -0.058242 | -1.966452 | 1.301650 |
| C | 1.047493 | -0.375056 | 2.258332 |
| H | -1.322353 | 0.833596 | 1.416124 |
| H | 0.875727 | 0.562438 | 2.785206 |
| C | -2.551244 | -2.252713 | 0.300278 |
| H | -2.842636 | -2.667794 | 1.272451 |
| H | -3.304570 | -2.556436 | -0.434002 |
| H | -1.608597 | -2.722482 | 0.008444 |
| C | -3.737833 | -0.011766 | 0.707530 |
| H | -4.109867 | -0.382084 | 1.673833 |
| H | -3.519538 | 1.054268 | 0.856869 |
| C | -4.846323 | -0.140693 | -0.348939 |
| H | -5.133981 | -1.193630 | -0.466022 |
| H | -4.454715 | 0.178862 | -1.324862 |
| C | -6.097750 | 0.679837 | -0.009552 |
| H | -6.481355 | 0.365962 | 0.970867 |
| H | -5.819362 | 1.737076 | 0.099486 |
| C | -7.207692 | 0.549818 | -1.057565 |
| H | -7.532511 | -0.491612 | -1.163643 |
| H | -8.085856 | 1.145636 | -0.787785 |
| H | -6.865305 | 0.889427 | -2.041869 |
| H | 1.604593 | -1.094374 | 2.852881 |
| Zr | 1.626213 | 0.058247 | 0.016845 |
| C | 2.363562 | 2.303585 | 1.054338 |

| | | | |
|---|----------|-----------|-----------|
| H | 4.179931 | 2.005725 | -0.202366 |
| C | 3.767288 | -1.380642 | 0.002436 |
| H | 4.575209 | -1.125898 | 0.676012 |
| C | 2.726018 | -2.298279 | 0.269492 |
| H | 2.590514 | -2.850585 | 1.189093 |
| C | 1.863906 | -2.333555 | -0.857159 |
| H | 0.985864 | -2.956784 | -0.963326 |
| C | 2.377834 | -1.434143 | -1.838427 |
| H | 1.982714 | -1.276254 | -2.833498 |
| C | 3.560737 | -0.847055 | -1.300791 |
| H | 4.203018 | -0.139621 | -1.806603 |

2rIM11

SCF energy in gas phase: -825.607574

Free energy in Et₂O : -825.255285

Enthalpy in Et₂O : -825.180451

| | | | |
|---|-----------|-----------|-----------|
| C | -1.799143 | -0.760537 | 0.505426 |
| C | -1.025707 | -0.306544 | -0.761789 |
| H | -1.028841 | -1.079177 | -1.536034 |
| H | -1.455516 | 0.599185 | -1.198429 |
| C | -0.774394 | -0.328377 | 1.553097 |
| C | 0.305431 | -1.037303 | 2.037993 |
| H | 0.332579 | -2.109725 | 1.847390 |
| C | 1.545850 | -0.413608 | 2.409736 |
| H | -0.847848 | 0.722393 | 1.834135 |
| H | 1.491726 | 0.552803 | 2.906497 |
| C | -2.061971 | -2.273428 | 0.526351 |
| H | -2.524738 | -2.585932 | 1.470181 |
| H | -2.727682 | -2.560416 | -0.292817 |
| H | -1.140138 | -2.847901 | 0.400367 |
| C | -3.118694 | 0.016322 | 0.738032 |
| H | -3.505030 | -0.231917 | 1.738357 |
| H | -2.877113 | 1.089481 | 0.765713 |
| C | -4.224144 | -0.204291 | -0.302303 |
| H | -4.570408 | -1.245490 | -0.268828 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -3.813564 | -0.050551 | -1.309290 | H | -0.774462 | 0.415497 | 1.918183 |
| C | -5.431158 | 0.722146 | -0.100144 | H | 0.993077 | -0.275942 | 3.677408 |
| H | -5.829176 | 0.583247 | 0.914554 | C | -1.785526 | -2.209332 | -0.098745 |
| H | -5.097923 | 1.767902 | -0.152488 | H | -2.226939 | -2.732148 | 0.758041 |
| C | -6.548739 | 0.490814 | -1.122104 | H | -2.454199 | -2.340874 | -0.954967 |
| H | -6.927627 | -0.536375 | -1.068778 | H | -0.847515 | -2.712719 | -0.346436 |
| H | -7.394435 | 1.165683 | -0.952661 | C | -2.934200 | -0.088631 | 0.638113 |
| H | -6.190983 | 0.656312 | -2.144932 | H | -3.253836 | -0.567223 | 1.575856 |
| H | 2.330777 | -1.052631 | 2.803504 | H | -2.747873 | 0.966742 | 0.886939 |
| Zr | 1.264650 | 0.085153 | 0.033766 | C | -4.078574 | -0.149520 | -0.383399 |
| C | 2.370549 | 2.302973 | 0.806717 | H | -4.377015 | -1.192272 | -0.554077 |
| H | 3.096403 | 2.252517 | 1.606454 | H | -3.725946 | 0.230300 | -1.351845 |
| C | 0.974596 | 2.528471 | 0.953388 | C | -5.313756 | 0.651705 | 0.050849 |
| H | 0.456073 | 2.693233 | 1.888322 | H | -5.661285 | 0.284867 | 1.026529 |
| C | 0.388118 | 2.533747 | -0.335494 | H | -5.027116 | 1.700790 | 0.208339 |
| H | -0.658607 | 2.684525 | -0.555924 | C | -6.464582 | 0.584616 | -0.958513 |
| C | 1.410784 | 2.288759 | -1.283748 | H | -6.799965 | -0.448026 | -1.109262 |
| H | 1.282706 | 2.233108 | -2.356897 | H | -7.328536 | 1.168463 | -0.623421 |
| C | 2.640732 | 2.163043 | -0.574666 | H | -6.157434 | 0.975856 | -1.935415 |
| H | 3.615084 | 2.000893 | -1.014506 | H | 1.400594 | -2.078932 | 3.748530 |
| C | 3.463299 | -1.069919 | -0.628421 | Zr | 1.174349 | 0.165415 | -0.090938 |
| H | 4.384892 | -0.645268 | -0.253162 | C | 1.508664 | 2.245268 | 1.430281 |
| C | 2.707815 | -2.095688 | -0.011180 | H | 1.442227 | 2.104865 | 2.501380 |
| H | 2.946006 | -2.577969 | 0.926457 | C | 0.440958 | 2.590299 | 0.567938 |
| C | 1.577200 | -2.361113 | -0.823089 | H | -0.586747 | 2.750995 | 0.862491 |
| H | 0.810278 | -3.097178 | -0.628046 | C | 0.944991 | 2.655849 | -0.756594 |
| C | 1.647008 | -1.517634 | -1.965687 | H | 0.373572 | 2.892831 | -1.643553 |
| H | 0.936635 | -1.487304 | -2.779487 | C | 2.331340 | 2.355241 | -0.710753 |
| C | 2.813411 | -0.728296 | -1.850504 | H | 3.005009 | 2.337757 | -1.556940 |
| H | 3.155406 | 0.003209 | -2.569966 | C | 2.681470 | 2.091853 | 0.643027 |

2rTS11

SCF energy in gas phase: -825.585156

Free energy in Et₂O : -825.241556

Enthalpy in Et₂O : -825.166456

| | | | |
|---|-----------|-----------|-----------|
| C | -1.579969 | -0.715678 | 0.204133 |
| C | -0.959451 | 0.035986 | -1.020117 |
| H | -1.086971 | -0.483784 | -1.973959 |
| H | -1.401977 | 1.030875 | -1.129041 |
| C | -0.529496 | -0.471798 | 1.329459 |
| C | 0.127615 | -1.488250 | 2.139829 |
| H | 0.063286 | -2.519204 | 1.791742 |
| C | 0.899407 | -1.265111 | 3.235031 |

| | | | |
|---|----------|-----------|-----------|
| C | 3.368085 | -0.706060 | -1.209222 |
| H | 4.214378 | -0.032822 | -1.241358 |
| C | 3.058387 | -1.597216 | -0.153874 |
| H | 3.634183 | -1.740092 | 0.751416 |
| C | 1.873025 | -2.303085 | -0.511858 |
| H | 1.412831 | -3.091658 | 0.063948 |
| C | 1.447447 | -1.828345 | -1.776696 |
| H | 0.582241 | -2.169236 | -2.325834 |
| C | 2.361929 | -0.831378 | -2.203623 |
| H | 2.307423 | -0.273927 | -3.130127 |

2rIM12

SCF energy in gas phase: -825.591829

Free energy in Et₂O : -825.244094

Enthalpy in Et₂O : -825.166866

| | | | |
|----|-----------|-----------|-----------|
| C | -1.383350 | -0.819494 | -0.179131 |
| C | -0.793654 | 0.147621 | -1.295442 |
| H | -0.796224 | -0.328971 | -2.277782 |
| H | -1.366228 | 1.074957 | -1.366641 |
| C | -0.359194 | -0.972638 | 1.054125 |
| C | -0.073008 | -2.318860 | 1.583396 |
| H | 0.146255 | -3.100394 | 0.855622 |
| C | -0.019050 | -2.667074 | 2.880640 |
| H | -0.711559 | -0.340521 | 1.874607 |
| H | -0.233678 | -1.954317 | 3.674215 |
| C | -1.698741 | -2.187182 | -0.816433 |
| H | -2.146331 | -2.872442 | -0.088374 |
| H | -2.398266 | -2.063795 | -1.648283 |
| H | -0.805919 | -2.668527 | -1.221267 |
| C | -2.693060 | -0.224633 | 0.419113 |
| H | -3.001207 | -0.866203 | 1.256532 |
| H | -2.454288 | 0.751629 | 0.861262 |
| C | -3.885506 | -0.045507 | -0.532395 |
| H | -4.242412 | -1.023735 | -0.878397 |
| H | -3.571029 | 0.501881 | -1.430563 |
| C | -5.055907 | 0.697887 | 0.127885 |
| H | -5.356389 | 0.164064 | 1.039878 |
| H | -4.715807 | 1.689624 | 0.457186 |
| C | -6.269602 | 0.855332 | -0.793780 |
| H | -6.656823 | -0.120582 | -1.108573 |
| H | -7.084986 | 1.391329 | -0.296540 |
| H | -6.009121 | 1.413415 | -1.700573 |
| H | 0.250143 | -3.672859 | 3.188694 |
| Zr | 1.129013 | 0.281709 | -0.141114 |
| C | 1.038814 | 1.882978 | 1.908263 |
| H | 0.840882 | 1.453927 | 2.881216 |
| C | 0.070401 | 2.378536 | 0.998899 |
| H | -0.999112 | 2.390235 | 1.155485 |
| C | 0.744848 | 2.857020 | -0.153574 |
| H | 0.280912 | 3.296782 | -1.026098 |
| C | 2.134320 | 2.651629 | 0.039380 |
| H | 2.919678 | 2.920860 | -0.654164 |
| C | 2.316349 | 2.045583 | 1.313974 |
| H | 3.263965 | 1.778337 | 1.762521 |
| C | 3.548013 | -0.547829 | -0.392628 |
| H | 4.299232 | -0.102377 | 0.245709 |

| | | | |
|---|----------|-----------|-----------|
| C | 2.795448 | -1.713329 | -0.105273 |
| H | 2.844752 | -2.303111 | 0.800457 |
| C | 1.942724 | -1.961625 | -1.211761 |
| H | 1.258315 | -2.791672 | -1.304566 |
| C | 2.164200 | -0.954100 | -2.183602 |
| H | 1.669797 | -0.871689 | -3.141533 |
| C | 3.152483 | -0.072164 | -1.675048 |
| H | 3.555742 | 0.792883 | -2.185117 |

2rTS12

SCF energy in gas phase: -825.557872

Free energy in Et₂O : -825.21049

Enthalpy in Et₂O : -825.135276

| | | | |
|----|-----------|-----------|-----------|
| C | -2.205215 | -0.045054 | 0.764899 |
| C | -1.271512 | -0.188248 | -0.434537 |
| H | -0.922396 | -1.203493 | -0.569208 |
| H | -1.572533 | 0.303586 | -1.354855 |
| C | -1.030429 | 0.846683 | 0.968172 |
| C | 0.124161 | 0.872668 | 1.844556 |
| H | 0.409840 | 1.887884 | 2.090199 |
| C | 1.022462 | -0.136203 | 2.346366 |
| H | -1.237293 | 1.848521 | 0.594569 |
| H | 0.674985 | -1.160193 | 2.485437 |
| C | -2.330862 | -1.262611 | 1.671052 |
| H | -2.742788 | -0.974135 | 2.644661 |
| H | -2.992698 | -2.016979 | 1.232380 |
| H | -1.364400 | -1.736010 | 1.856391 |
| C | -3.533658 | 0.673157 | 0.503592 |
| H | -3.959457 | 0.995766 | 1.464899 |
| H | -3.328661 | 1.592935 | -0.061870 |
| C | -4.575662 | -0.150451 | -0.266745 |
| H | -4.860793 | -1.036291 | 0.315684 |
| H | -4.126420 | -0.527649 | -1.196230 |
| C | -5.841013 | 0.649795 | -0.603985 |
| H | -6.282418 | 1.037331 | 0.324410 |
| H | -5.563969 | 1.531823 | -1.197681 |
| C | -6.888864 | -0.168741 | -1.364723 |
| H | -7.215446 | -1.036251 | -0.779869 |
| H | -7.776380 | 0.430242 | -1.593790 |
| H | -6.486957 | -0.543610 | -2.313074 |
| H | 1.690283 | 0.180804 | 3.142695 |
| Zr | 1.412744 | 0.036155 | 0.041445 |
| C | 3.576436 | 1.377875 | -0.487788 |

| | | | | | | | |
|---|----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 4.531572 | 0.883572 | -0.374224 | H | 3.600820 | 0.533691 | -1.266646 |
| C | 2.888021 | 2.090079 | 0.529186 | C | 5.486584 | -0.354686 | -0.703805 |
| H | 3.239203 | 2.259914 | 1.537455 | H | 6.019072 | -0.625744 | 0.218253 |
| C | 1.680385 | 2.588863 | -0.040874 | H | 5.316772 | -1.297318 | -1.242115 |
| H | 0.958332 | 3.225121 | 0.449873 | C | 6.371420 | 0.564907 | -1.551641 |
| C | 1.611020 | 2.152191 | -1.390548 | H | 6.590004 | 1.500741 | -1.024282 |
| H | 0.827090 | 2.386095 | -2.098654 | H | 7.327842 | 0.090298 | -1.795461 |
| C | 2.795655 | 1.413787 | -1.665745 | H | 5.880045 | 0.827084 | -2.495795 |
| H | 3.047864 | 0.958328 | -2.612650 | H | -2.020836 | -0.601873 | 2.768072 |
| C | 2.325589 | -2.356308 | 0.594382 | Zr | -1.306206 | 0.040133 | -0.053723 |
| H | 2.564771 | -2.566026 | 1.627173 | C | -3.179592 | -1.669662 | -0.579258 |
| C | 1.070394 | -2.555721 | -0.032466 | H | -4.175683 | -1.454635 | -0.214192 |
| H | 0.189724 | -2.977556 | 0.434017 | C | -2.181496 | -2.408597 | 0.108592 |
| C | 1.198903 | -2.184064 | -1.406075 | H | -2.283625 | -2.856252 | 1.086719 |
| H | 0.426940 | -2.249388 | -2.162733 | C | -1.031348 | -2.465253 | -0.720177 |
| C | 2.525128 | -1.760407 | -1.616388 | H | -0.092822 | -2.936507 | -0.467229 |
| H | 2.942412 | -1.428461 | -2.557130 | C | -1.316666 | -1.763744 | -1.918828 |
| C | 3.218926 | -1.842178 | -0.375024 | H | -0.639435 | -1.625288 | -2.751620 |
| H | 4.260647 | -1.602752 | -0.209549 | C | -2.648677 | -1.279496 | -1.836034 |

2rIM13

SCF energy in gas phase: -825.603131

Free energy in Et₂O : -825.253004

Enthalpy in Et₂O : -825.176668

| | | | |
|---|-----------|-----------|-----------|
| C | 1.839588 | -0.135298 | 0.904928 |
| C | 1.000027 | 0.151010 | -0.380971 |
| H | 1.337365 | 1.092551 | -0.829142 |
| H | 1.240260 | -0.628408 | -1.117333 |
| C | 1.192472 | -1.252098 | 1.738293 |
| C | -0.045433 | -1.298494 | 2.276216 |
| H | -0.305121 | -2.236597 | 2.770605 |
| C | -1.135037 | -0.285120 | 2.212110 |
| H | 1.823738 | -2.123650 | 1.913344 |
| H | -0.829728 | 0.692048 | 2.599999 |
| C | 2.001955 | 1.136226 | 1.771818 |
| H | 2.650496 | 0.938295 | 2.632726 |
| H | 2.444628 | 1.955775 | 1.195533 |
| H | 1.044784 | 1.488547 | 2.160951 |
| C | 3.260100 | -0.652301 | 0.513271 |
| H | 3.805317 | -0.894255 | 1.438722 |
| H | 3.133342 | -1.605855 | -0.019839 |
| C | 4.132602 | 0.272944 | -0.342683 |
| H | 4.313637 | 1.218697 | 0.184824 |

| | | | |
|----|-----------|-----------|-----------|
| H | 3.600820 | 0.533691 | -1.266646 |
| C | 5.486584 | -0.354686 | -0.703805 |
| H | 6.019072 | -0.625744 | 0.218253 |
| H | 5.316772 | -1.297318 | -1.242115 |
| C | 6.371420 | 0.564907 | -1.551641 |
| H | 6.590004 | 1.500741 | -1.024282 |
| H | 7.327842 | 0.090298 | -1.795461 |
| H | 5.880045 | 0.827084 | -2.495795 |
| H | -2.020836 | -0.601873 | 2.768072 |
| Zr | -1.306206 | 0.040133 | -0.053723 |
| C | -3.179592 | -1.669662 | -0.579258 |
| H | -4.175683 | -1.454635 | -0.214192 |
| C | -2.181496 | -2.408597 | 0.108592 |
| H | -2.283625 | -2.856252 | 1.086719 |
| C | -1.031348 | -2.465253 | -0.720177 |
| H | -0.092822 | -2.936507 | -0.467229 |
| C | -1.316666 | -1.763744 | -1.918828 |
| H | -0.639435 | -1.625288 | -2.751620 |
| C | -2.648677 | -1.279496 | -1.836034 |
| H | -3.168725 | -0.715241 | -2.598217 |
| C | -2.603202 | 2.119443 | 0.809028 |
| H | -3.056759 | 2.063305 | 1.789320 |
| C | -1.299459 | 2.599691 | 0.518110 |
| H | -0.583003 | 2.969257 | 1.239011 |
| C | -1.095643 | 2.509182 | -0.879823 |
| H | -0.201965 | 2.802114 | -1.412323 |
| C | -2.263202 | 1.950702 | -1.457973 |
| H | -2.427179 | 1.773338 | -2.512333 |
| C | -3.200942 | 1.716250 | -0.410172 |
| H | -4.199304 | 1.316919 | -0.528633 |

2rTS13

SCF energy in gas phase: -825.573211

Free energy in Et₂O : -825.228606

Enthalpy in Et₂O : -825.153791

| | | | |
|---|-----------|-----------|-----------|
| C | -1.608297 | -0.534565 | 0.319854 |
| C | -0.960342 | 0.139731 | -0.929769 |
| H | -1.135680 | -0.382801 | -1.874117 |
| H | -1.335996 | 1.161925 | -1.039511 |
| C | -0.620853 | -0.104725 | 1.449809 |
| C | 0.094440 | -0.852373 | 2.471643 |
| H | 0.446316 | -0.204764 | 3.280115 |
| C | 0.515676 | -2.143373 | 2.572562 |

| | | | | | | |
|--------------------------|-------------|-----------|-----------|--|-----------|---------------------|
| H | -0.931073 | 0.860483 | 1.846154 | Free energy in Et ₂ O : -825.238719 | | |
| H | 0.204982 | -2.925285 | 1.891352 | Enthalpy in Et ₂ O : -825.162663 | | |
| C | -1.770063 | -2.055225 | 0.146662 | | | |
| H | -2.179278 | -2.513552 | 1.053358 | C | 1.423106 | 0.685314 -0.043562 |
| H | -2.454329 | -2.272391 | -0.679765 | C | 0.812951 | -0.259071 -1.170944 |
| H | -0.830104 | -2.557312 | -0.086270 | H | 0.917861 | 0.179733 -2.164715 |
| C | -3.002958 | 0.079292 | 0.646259 | H | 1.310499 | -1.232234 -1.179945 |
| H | -3.350308 | -0.339048 | 1.602905 | C | 0.421482 | 0.751059 1.195660 |
| H | -2.858353 | 1.154946 | 0.821108 | C | 0.218923 | 1.909850 2.088227 |
| C | -4.098300 | -0.089813 | -0.415531 | H | -0.140859 | 1.589290 3.070205 |
| H | -4.358307 | -1.150218 | -0.528716 | C | 0.343900 | 3.244961 1.950679 |
| H | -3.716148 | 0.239422 | -1.391151 | H | 0.677923 | -0.094498 1.842935 |
| C | -5.375493 | 0.695055 | -0.083661 | H | 0.693895 | 3.737804 1.052583 |
| H | -5.749706 | 0.380479 | 0.900313 | C | 1.728626 | 2.065369 -0.656217 |
| H | -5.129709 | 1.761516 | 0.014094 | H | 2.270091 | 2.699905 0.050595 |
| C | -6.481687 | 0.520494 | -1.129356 | H | 2.350780 | 1.948270 -1.548613 |
| H | -6.774850 | -0.531498 | -1.223889 | H | 0.823214 | 2.594922 -0.959085 |
| H | -7.378007 | 1.092441 | -0.866530 | C | 2.747109 | 0.064384 0.501195 |
| H | -6.149407 | 0.858718 | -2.117711 | H | 3.071816 | 0.666007 1.361828 |
| H | 1.124967 | -2.450372 | 3.416444 | H | 2.513930 | -0.933424 0.898649 |
| Zr | 1.174502 | 0.131986 | -0.000877 | C | 3.916003 | -0.067215 -0.485594 |
| C | 1.832374 | 2.213098 | 1.434599 | H | 4.251997 | 0.927283 -0.805526 |
| H | 1.836817 | 2.114788 | 2.512735 | H | 3.582243 | -0.586545 -1.393551 |
| C | 0.743162 | 2.653102 | 0.643582 | C | 5.111890 | -0.819614 0.116149 |
| H | -0.232722 | 2.938125 | 1.009519 | H | 5.429650 | -0.315815 1.039264 |
| C | 1.140380 | 2.620320 | -0.715003 | H | 4.792586 | -1.827149 0.416943 |
| H | 0.532127 | 2.899168 | -1.564248 | C | 6.302629 | -0.926705 -0.842007 |
| C | 2.488709 | 2.171720 | -0.763739 | H | 6.669171 | 0.065331 -1.130019 |
| H | 3.088697 | 2.071058 | -1.656728 | H | 7.137553 | -1.469877 -0.386695 |
| C | 2.916541 | 1.915598 | 0.566835 | H | 6.025071 | -1.454148 -1.762007 |
| H | 3.897566 | 1.571679 | 0.867487 | H | 0.097281 | 3.894974 2.785029 |
| C | 3.312723 | -0.807241 | -1.339501 | Zr | -1.168826 | -0.269989 -0.114430 |
| H | 4.188172 | -0.176241 | -1.416377 | C | -1.357496 | -2.008441 1.824942 |
| C | 3.012696 | -1.672394 | -0.258891 | H | -1.187488 | -1.668918 2.838141 |
| H | 3.643796 | -1.869609 | 0.598403 | C | -0.379320 | -2.538165 0.945527 |
| C | 1.776101 | -2.321708 | -0.554615 | H | 0.672958 | -2.659397 1.165105 |
| H | 1.313825 | -3.088781 | 0.046828 | C | -1.013623 | -2.868573 -0.278653 |
| C | 1.301727 | -1.816602 | -1.784810 | H | -0.533963 | -3.294821 -1.149419 |
| H | 0.392044 | -2.113130 | -2.285768 | C | -2.387750 | -2.537097 -0.160476 |
| C | 2.242811 | -0.862878 | -2.262760 | H | -3.143699 | -2.678515 -0.921862 |
| H | 2.158506 | -0.294268 | -3.179978 | C | -2.600582 | -2.001258 1.140403 |
| | | | | H | -3.547228 | -1.666324 1.544039 |
| | | | | C | -3.499377 | 0.512406 -0.923675 |
| 2rIM14 | | | | H | -4.335705 | -0.163905 -0.806247 |
| SCF energy in gas phase: | -825.586345 | | | | | |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| C | -3.054657 | 1.462721 | 0.030877 | H | 0.959889 | 1.655179 | 2.862568 |
| H | -3.495622 | 1.646729 | 1.002502 | C | 0.213622 | 2.493788 | 0.932020 |
| C | -1.934970 | 2.145573 | -0.515753 | H | -0.852590 | 2.569694 | 1.096474 |
| H | -1.377162 | 2.922951 | -0.012646 | C | 0.896374 | 2.854173 | -0.258952 |
| C | -1.682852 | 1.607054 | -1.804263 | H | 0.444519 | 3.261056 | -1.153614 |
| H | -0.902045 | 1.914810 | -2.484532 | C | 2.275164 | 2.588775 | -0.066171 |
| C | -2.642050 | 0.589050 | -2.051938 | H | 3.063275 | 2.761769 | -0.787073 |
| H | -2.715379 | -0.012481 | -2.949231 | C | 2.442116 | 2.054237 | 1.241134 |

2rTS14

SCF energy in gas phase: -825.580441

Free energy in Et₂O : -825.232504

Enthalpy in Et₂O : -825.157386

| | | | |
|----|-----------|-----------|-----------|
| C | -1.423776 | -0.740174 | -0.046556 |
| C | -0.821555 | 0.177674 | -1.188913 |
| H | -0.877062 | -0.307134 | -2.165118 |
| H | -1.349056 | 1.132236 | -1.255045 |
| C | -0.397321 | -0.802184 | 1.209054 |
| C | -0.441845 | -2.024562 | 2.070474 |
| H | -1.179115 | -1.989180 | 2.880206 |
| C | 0.279584 | -3.150484 | 2.003146 |
| H | -0.717437 | 0.022083 | 1.857021 |
| H | 1.056654 | -3.307302 | 1.263728 |
| C | -1.698880 | -2.146563 | -0.607217 |
| H | -2.172472 | -2.789713 | 0.140668 |
| H | -2.358753 | -2.083479 | -1.477659 |
| H | -0.782945 | -2.647138 | -0.926981 |
| C | -2.751227 | -0.124144 | 0.489342 |
| H | -3.073211 | -0.708169 | 1.363481 |
| H | -2.529507 | 0.884421 | 0.864832 |
| C | -3.923889 | -0.027289 | -0.497859 |
| H | -4.255447 | -1.032801 | -0.786516 |
| H | -3.593450 | 0.464892 | -1.421963 |
| C | -5.121462 | 0.739870 | 0.081331 |
| H | -5.438727 | 0.263733 | 1.019302 |
| H | -4.804093 | 1.756629 | 0.351737 |
| C | -6.312203 | 0.816574 | -0.879734 |
| H | -6.677555 | -0.183993 | -1.138117 |
| H | -7.147821 | 1.372317 | -0.441152 |
| H | -6.034838 | 1.316603 | -1.814970 |
| H | 0.108307 | -3.964892 | 2.701987 |
| Zr | 1.138635 | 0.263765 | -0.087948 |
| C | 1.166343 | 2.006479 | 1.860613 |

| | | | |
|---|----------|-----------|-----------|
| H | 3.379771 | 1.762536 | 1.695929 |
| C | 3.550514 | -0.480834 | -0.617169 |
| H | 4.355682 | 0.086252 | -0.169692 |
| C | 2.927856 | -1.624735 | -0.059487 |
| H | 3.166296 | -2.081342 | 0.892290 |
| C | 1.935028 | -2.067712 | -0.972553 |
| H | 1.305295 | -2.935111 | -0.847553 |
| C | 1.937281 | -1.195415 | -2.089423 |
| H | 1.302900 | -1.273834 | -2.960648 |
| C | 2.930348 | -0.207040 | -1.867307 |
| H | 3.183662 | 0.601478 | -2.540834 |

CH₃CHO

SCF energy in gas phase: -153.832735

Free energy in Et₂O : -153.75308

Enthalpy in Et₂O : -153.723285

| | | | |
|---|-----------|-----------|-----------|
| C | 1.170591 | -0.149175 | -0.000056 |
| H | 1.712659 | 0.219149 | -0.879683 |
| H | 1.155394 | -1.240286 | 0.000761 |
| H | 1.712259 | 0.220469 | 0.879521 |
| C | -0.233765 | 0.399651 | -0.000007 |
| H | -0.299151 | 1.512163 | -0.000155 |
| O | -1.237765 | -0.276794 | -0.000009 |

2rIM15

SCF energy in gas phase: -825.589446

Free energy in Et₂O : -825.24882

Enthalpy in Et₂O : -825.170459

| | | | |
|---|-----------|-----------|----------|
| C | 2.456705 | -0.869762 | 0.216977 |
| C | 2.449298 | -1.499317 | 1.595937 |
| H | 2.205070 | -2.556411 | 1.670736 |
| H | 3.181402 | -1.163449 | 2.327359 |
| C | 1.326941 | -0.554362 | 1.187237 |
| C | -0.089445 | -1.040263 | 1.040009 |

| | | | | | | | |
|----|-----------|-----------|-----------|--|-----------|-----------|-----------|
| H | -0.131424 | -2.077590 | 0.707032 | 2rTS15 | | | |
| C | -1.084650 | -0.709455 | 2.080237 | SCF energy in gas phase: -825.564685 | | | |
| H | 1.402154 | 0.434499 | 1.638466 | Free energy in Et ₂ O : -825.217022 | | | |
| H | -0.771661 | 0.001930 | 2.844422 | Enthalpy in Et ₂ O : -825.143284 | | | |
| C | 2.181938 | -1.759872 | -0.985024 | | | | |
| H | 1.814580 | -1.171832 | -1.836276 | C | 1.706773 | -0.942580 | 0.288738 |
| H | 3.089122 | -2.280271 | -1.312053 | C | 1.886594 | -1.535864 | 1.664896 |
| H | 1.432689 | -2.523748 | -0.763004 | H | 1.741860 | -2.614335 | 1.741984 |
| C | 3.485275 | 0.232085 | -0.032804 | H | 2.745789 | -1.205082 | 2.250141 |
| H | 3.154518 | 0.854057 | -0.879457 | C | 0.651372 | -0.721340 | 1.785715 |
| H | 3.510408 | 0.898062 | 0.840642 | C | -0.680027 | -1.239081 | 1.953211 |
| C | 4.913704 | -0.264392 | -0.307901 | H | -0.802050 | -2.313426 | 1.842735 |
| H | 4.926769 | -0.886981 | -1.212420 | C | -1.831632 | -0.423514 | 2.269870 |
| H | 5.230023 | -0.918551 | 0.516314 | H | 0.827871 | 0.296804 | 2.125612 |
| C | 5.928598 | 0.874199 | -0.473215 | H | -1.681123 | 0.454744 | 2.897521 |
| H | 5.606275 | 1.531700 | -1.292559 | C | 1.497983 | -1.987395 | -0.794376 |
| H | 5.924789 | 1.496964 | 0.432107 | H | 1.320138 | -1.534129 | -1.773281 |
| C | 7.353215 | 0.380979 | -0.746118 | H | 2.392127 | -2.625067 | -0.876547 |
| H | 7.398046 | -0.212576 | -1.666513 | H | 0.661866 | -2.653836 | -0.568996 |
| H | 8.053196 | 1.216096 | -0.855274 | C | 2.688849 | 0.167691 | -0.062550 |
| H | 7.716266 | -0.252457 | 0.071377 | H | 2.360639 | 0.680591 | -0.975243 |
| H | -1.664789 | -1.526841 | 2.508280 | H | 2.689560 | 0.923349 | 0.735054 |
| Zr | -1.851006 | 0.148017 | 0.104311 | C | 4.141307 | -0.313130 | -0.267439 |
| C | -4.064138 | -0.488667 | -0.949195 | H | 4.183077 | -1.014953 | -1.110719 |
| H | -4.818333 | 0.278791 | -1.064000 | H | 4.473755 | -0.876387 | 0.615126 |
| C | -3.946739 | -1.392013 | 0.143557 | C | 5.118657 | 0.841067 | -0.527628 |
| H | -4.570863 | -1.408612 | 1.028131 | H | 4.780459 | 1.412163 | -1.403264 |
| C | -2.860551 | -2.259773 | -0.121023 | H | 5.086346 | 1.540164 | 0.319481 |
| H | -2.502497 | -3.041053 | 0.535504 | C | 6.561124 | 0.375008 | -0.749442 |
| C | -2.302075 | -1.910542 | -1.376785 | H | 6.632783 | -0.295736 | -1.613224 |
| H | -1.466844 | -2.400466 | -1.859421 | H | 7.231985 | 1.221459 | -0.929823 |
| C | -3.044668 | -0.810163 | -1.893375 | H | 6.940317 | -0.169666 | 0.122824 |
| H | -2.893561 | -0.331657 | -2.852395 | H | -2.735160 | -0.964229 | 2.535448 |
| C | -2.111371 | 2.613031 | 0.920329 | Zr | -1.255289 | 0.079053 | 0.070729 |
| H | -2.774765 | 2.833240 | 1.747745 | C | -3.501269 | -0.454506 | -1.109651 |
| C | -0.731637 | 2.312892 | 1.020903 | H | -4.326315 | 0.231170 | -0.969287 |
| H | -0.162412 | 2.267245 | 1.938489 | C | -3.214792 | -1.574890 | -0.295283 |
| C | -0.228317 | 2.074357 | -0.286124 | H | -3.792319 | -1.903436 | 0.556390 |
| H | 0.796505 | 1.841238 | -0.538338 | C | -2.038866 | -2.194320 | -0.801075 |
| C | -1.311709 | 2.224358 | -1.200935 | H | -1.593779 | -3.103294 | -0.422349 |
| H | -1.253010 | 2.142871 | -2.278805 | C | -1.603356 | -1.451719 | -1.937858 |
| C | -2.475758 | 2.559587 | -0.451270 | H | -0.769782 | -1.693276 | -2.580834 |
| H | -3.459127 | 2.757656 | -0.857024 | C | -2.511133 | -0.377732 | -2.123229 |
| | | | | H | -2.455472 | 0.369542 | -2.903254 |

| | | | | | | | |
|---|-----------|----------|-----------|----|-----------|-----------|-----------|
| C | -2.070682 | 2.414237 | 0.794011 | Zr | -1.093104 | 0.138265 | 0.101564 |
| H | -2.922446 | 2.464707 | 1.457685 | C | -3.449146 | -0.666663 | -0.599837 |
| C | -0.699915 | 2.399745 | 1.182741 | H | -4.301455 | -0.069840 | -0.303869 |
| H | -0.331194 | 2.427558 | 2.199427 | C | -2.909960 | -1.760427 | 0.119012 |
| C | 0.090765 | 2.368663 | 0.012290 | H | -3.274732 | -2.130725 | 1.066765 |
| H | 1.169647 | 2.361128 | -0.024301 | C | -1.801603 | -2.264317 | -0.603202 |
| C | -0.772563 | 2.351196 | -1.111254 | H | -1.182273 | -3.100745 | -0.312489 |
| H | -0.468722 | 2.353599 | -2.149770 | C | -1.666411 | -1.495571 | -1.793006 |
| C | -2.109912 | 2.403513 | -0.621527 | H | -0.927808 | -1.642715 | -2.566493 |
| H | -3.003964 | 2.437458 | -1.228643 | C | -2.693880 | -0.522373 | -1.796172 |

2rIM16

SCF energy in gas phase: -825.591255

Free energy in Et₂O : -825.237752

Enthalpy in Et₂O : -825.164276

| | | | |
|---|-----------|-----------|-----------|
| C | 1.327709 | -0.931086 | -0.211732 |
| C | 1.320281 | -1.634949 | 1.164312 |
| H | 0.831686 | -2.615660 | 1.096098 |
| H | 2.313307 | -1.811141 | 1.605728 |
| C | 0.453096 | -0.697864 | 1.959497 |
| C | -0.847101 | -0.954958 | 2.343947 |
| H | -1.184764 | -1.987724 | 2.261121 |
| C | -1.844199 | 0.064079 | 2.445811 |
| H | 0.864217 | 0.293769 | 2.150661 |
| H | -1.534262 | 1.020944 | 2.858759 |
| C | 1.486959 | -1.928139 | -1.363750 |
| H | 1.442728 | -1.430902 | -2.341625 |
| H | 2.457025 | -2.449761 | -1.319001 |
| H | 0.726976 | -2.713462 | -1.357350 |
| C | 2.471488 | 0.106174 | -0.286407 |
| H | 2.428731 | 0.603880 | -1.264312 |
| H | 2.328581 | 0.899022 | 0.460348 |
| C | 3.919617 | -0.413528 | -0.120668 |
| H | 4.139814 | -1.176396 | -0.878009 |
| H | 4.043319 | -0.906822 | 0.852122 |
| C | 4.959657 | 0.709903 | -0.236568 |
| H | 4.848248 | 1.208375 | -1.209659 |
| H | 4.750655 | 1.478565 | 0.520831 |
| C | 6.402901 | 0.219838 | -0.078638 |
| H | 6.655030 | -0.522000 | -0.845223 |
| H | 7.119797 | 1.043506 | -0.164890 |
| H | 6.555841 | -0.252982 | 0.898423 |
| H | -2.849274 | -0.227920 | 2.736134 |

| | | | |
|---|-----------|----------|-----------|
| C | -1.507135 | 2.636671 | 0.713819 |
| H | -2.029917 | 2.871539 | 1.629536 |
| C | -0.101757 | 2.493420 | 0.558700 |
| H | 0.641348 | 2.627538 | 1.333280 |
| C | 0.161650 | 2.228395 | -0.813372 |
| H | 1.133589 | 2.108362 | -1.262338 |
| C | -1.074718 | 2.174147 | -1.492894 |
| H | -1.204901 | 1.999427 | -2.552305 |
| C | -2.110495 | 2.419716 | -0.546094 |
| H | -3.171389 | 2.456297 | -0.754506 |

2rTS16

SCF energy in gas phase: -979.429508

Free energy in Et₂O : -978.976687

Enthalpy in Et₂O : -978.888749

| | | | |
|---|-----------|-----------|-----------|
| C | -1.706079 | 0.496527 | 0.763985 |
| C | -1.414180 | -1.045944 | 0.770048 |
| H | -1.572218 | -1.483263 | 1.758655 |
| H | -2.052875 | -1.587552 | 0.068208 |
| C | -0.426072 | 1.246568 | 0.175998 |
| C | 0.083773 | 2.428887 | 0.882969 |
| H | 0.293261 | 2.309621 | 1.947307 |
| C | 0.348562 | 3.640771 | 0.353159 |
| H | -0.632549 | 1.519000 | -0.867117 |
| H | 0.116625 | 3.873160 | -0.684311 |
| C | -2.035913 | 0.969287 | 2.192928 |
| H | -2.254792 | 2.042798 | 2.219827 |
| H | -2.905972 | 0.430235 | 2.579822 |
| H | -1.212415 | 0.780273 | 2.885952 |
| C | -2.901690 | 0.847258 | -0.168672 |
| H | -2.983240 | 1.942735 | -0.217201 |
| H | -2.646133 | 0.521356 | -1.186506 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | -4.273107 | 0.258822 | 0.195027 | | | | |
| H | -4.628819 | 0.684932 | 1.141936 | C | -2.010090 | 0.803595 | 0.445656 |
| H | -4.182528 | -0.822785 | 0.361428 | C | -1.232560 | -0.484044 | 0.000754 |
| C | -5.332681 | 0.512814 | -0.886951 | H | -1.619056 | -1.360896 | 0.539559 |
| H | -5.418832 | 1.593512 | -1.065391 | H | -1.499770 | -0.652260 | -1.048689 |
| H | -4.991901 | 0.077046 | -1.836590 | C | -1.149479 | 1.933642 | -0.082430 |
| C | -6.709960 | -0.056779 | -0.531853 | C | -0.413610 | 2.808506 | 0.607190 |
| H | -7.096296 | 0.387211 | 0.392908 | H | -0.527784 | 2.875765 | 1.686714 |
| H | -7.441732 | 0.136192 | -1.323649 | C | 0.766798 | 3.537897 | 0.008202 |
| H | -6.662486 | -1.141412 | -0.380121 | H | -1.003595 | 1.883906 | -1.165363 |
| H | 0.758751 | 4.447805 | 0.953904 | H | 0.464559 | 4.356321 | -0.660210 |
| Zr | 0.739267 | -0.770328 | 0.062917 | C | -2.195046 | 0.878286 | 1.969196 |
| C | 0.811870 | -0.542547 | -2.520907 | H | -2.748918 | 1.779752 | 2.256438 |
| H | 0.883068 | 0.458275 | -2.924101 | H | -2.755655 | 0.013092 | 2.336314 |
| C | -0.384231 | -1.249009 | -2.257439 | H | -1.238161 | 0.897562 | 2.495276 |
| H | -1.388096 | -0.882460 | -2.419729 | C | -3.402775 | 0.888593 | -0.252277 |
| C | -0.040411 | -2.519906 | -1.725310 | H | -3.868755 | 1.845408 | 0.026552 |
| H | -0.735504 | -3.288283 | -1.415374 | H | -3.234194 | 0.941249 | -1.337735 |
| C | 1.372461 | -2.601055 | -1.673616 | C | -4.394869 | -0.247988 | 0.028749 |
| H | 1.948222 | -3.448685 | -1.327001 | H | -4.624921 | -0.293596 | 1.101429 |
| C | 1.904068 | -1.372124 | -2.146589 | H | -3.935900 | -1.211747 | -0.227697 |
| H | 2.951039 | -1.114362 | -2.222521 | C | -5.709257 | -0.094691 | -0.749768 |
| C | 2.997780 | -1.213220 | 1.167369 | H | -6.167063 | 0.872950 | -0.502327 |
| H | 3.857047 | -1.222346 | 0.511019 | H | -5.490160 | -0.057986 | -1.825846 |
| C | 2.488741 | -0.080687 | 1.852522 | C | -6.711921 | -1.219164 | -0.471094 |
| H | 2.873882 | 0.926146 | 1.778928 | H | -6.980736 | -1.256337 | 0.590982 |
| C | 1.358063 | -0.491239 | 2.598013 | H | -7.636383 | -1.084611 | -1.042663 |
| H | 0.752755 | 0.142222 | 3.230102 | H | -6.294865 | -2.196989 | -0.738622 |
| C | 1.170763 | -1.883641 | 2.390642 | H | 1.352365 | 3.996861 | 0.813664 |
| H | 0.393627 | -2.494138 | 2.827853 | Zr | 1.166424 | -0.540500 | 0.010164 |
| C | 2.187067 | -2.331366 | 1.512380 | C | 2.088295 | -0.595545 | -2.435687 |
| H | 2.327004 | -3.348916 | 1.172942 | H | 2.557409 | 0.310328 | -2.794358 |
| C | 3.711643 | 3.492108 | -1.129291 | C | 0.720997 | -0.923276 | -2.548113 |
| H | 4.084373 | 3.799008 | -2.114596 | H | -0.040415 | -0.323116 | -3.027883 |
| H | 4.544125 | 3.179372 | -0.496481 | C | 0.515962 | -2.188025 | -1.921049 |
| H | 3.209431 | 4.360696 | -0.690506 | H | -0.426364 | -2.713092 | -1.845279 |
| C | 2.718471 | 2.375600 | -1.290477 | C | 1.757199 | -2.631154 | -1.420169 |
| H | 1.839332 | 2.602390 | -1.922737 | H | 1.937872 | -3.561792 | -0.899785 |
| O | 2.853693 | 1.268322 | -0.799646 | C | 2.731425 | -1.628871 | -1.702974 |
| | | | | H | 3.784691 | -1.674754 | -1.459076 |
| | | | | C | 2.705194 | -0.560266 | 2.096016 |
| | | | | H | 3.568766 | 0.088835 | 2.042906 |
| | | | | C | 1.424465 | -0.200702 | 2.579931 |
| | | | | H | 1.145517 | 0.769501 | 2.967319 |

2rIM17
SCF energy in gas phase: -979.502316
Free energy in Et₂O : -979.037208
Enthalpy in Et₂O : -978.952867

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 0.566574 | -1.323790 | 2.435304 | H | 7.718304 | -0.210151 | 1.420976 |
| H | -0.472550 | -1.371363 | 2.723538 | H | 6.525686 | -1.484086 | 1.129627 |
| C | 1.315972 | -2.375793 | 1.854126 | H | -1.717807 | 3.484079 | -1.339938 |
| H | 0.946031 | -3.364975 | 1.617847 | Zr | -1.292301 | -0.364445 | 0.205541 |
| C | 2.639867 | -1.901238 | 1.638679 | C | -2.078834 | -0.752449 | 2.676083 |
| H | 3.460338 | -2.469802 | 1.221379 | H | -2.505400 | 0.105725 | 3.176445 |
| C | 3.083989 | 3.185929 | -0.994584 | C | -0.718600 | -1.116516 | 2.669009 |
| H | 3.713720 | 2.529109 | -1.602855 | H | 0.074960 | -0.612005 | 3.203808 |
| H | 3.574978 | 3.327915 | -0.026083 | C | -0.569072 | -2.273749 | 1.842351 |
| H | 3.016090 | 4.158583 | -1.494963 | H | 0.352484 | -2.795638 | 1.624451 |
| C | 1.695461 | 2.577698 | -0.795566 | C | -1.841685 | -2.617466 | 1.345080 |
| H | 1.241486 | 2.418563 | -1.788884 | H | -2.061224 | -3.453033 | 0.695832 |
| O | 1.798617 | 1.338750 | -0.134836 | C | -2.778154 | -1.651536 | 1.825603 |

2rTS17

SCF energy in gas phase: -1440.285466

Free energy in Et₂O : -1439.827445

Enthalpy in Et₂O : -1439.739402

| | | | |
|---|-----------|-----------|-----------|
| C | 2.018127 | 0.921928 | -0.491514 |
| C | 1.285826 | -0.272721 | 0.214264 |
| H | 2.025600 | -1.012601 | 0.542886 |
| H | 0.939293 | 0.106926 | 1.189745 |
| C | 1.085733 | 2.083942 | -0.226383 |
| C | 0.256013 | 2.724094 | -1.053086 |
| H | 0.339753 | 2.582037 | -2.128398 |
| C | -0.948294 | 3.494017 | -0.556770 |
| H | 0.972478 | 2.277862 | 0.841457 |
| H | -0.725055 | 4.555778 | -0.377551 |
| C | 2.269279 | 0.674674 | -1.986262 |
| H | 2.863524 | 1.487551 | -2.419667 |
| H | 2.803018 | -0.264741 | -2.146720 |
| H | 1.333390 | 0.612943 | -2.545675 |
| C | 3.366734 | 1.225650 | 0.234539 |
| H | 3.741852 | 2.188410 | -0.141590 |
| H | 3.151413 | 1.382413 | 1.301714 |
| C | 4.484450 | 0.181675 | 0.103677 |
| H | 4.784174 | 0.084105 | -0.947263 |
| H | 4.122081 | -0.809502 | 0.406845 |
| C | 5.720757 | 0.535602 | 0.942789 |
| H | 6.087904 | 1.528223 | 0.647560 |
| H | 5.428924 | 0.623521 | 1.998532 |
| C | 6.852859 | -0.488097 | 0.810182 |
| H | 7.191700 | -0.571694 | -0.228681 |

| | | | |
|----|-----------|-----------|-----------|
| H | 7.718304 | -0.210151 | 1.420976 |
| H | 6.525686 | -1.484086 | 1.129627 |
| H | -1.717807 | 3.484079 | -1.339938 |
| Zr | -1.292301 | -0.364445 | 0.205541 |
| C | -2.078834 | -0.752449 | 2.676083 |
| H | -2.505400 | 0.105725 | 3.176445 |
| C | -0.718600 | -1.116516 | 2.669009 |
| H | 0.074960 | -0.612005 | 3.203808 |
| C | -0.569072 | -2.273749 | 1.842351 |
| H | 0.352484 | -2.795638 | 1.624451 |
| C | -1.841685 | -2.617466 | 1.345080 |
| H | -2.061224 | -3.453033 | 0.695832 |
| C | -2.778154 | -1.651536 | 1.825603 |
| H | -3.845071 | -1.650567 | 1.647092 |
| C | -3.136045 | 0.119490 | -1.551385 |
| H | -3.904173 | 0.829220 | -1.274228 |
| C | -1.913781 | 0.421587 | -2.200111 |
| H | -1.589800 | 1.401325 | -2.515248 |
| C | -1.184864 | -0.785631 | -2.350906 |
| H | -0.214578 | -0.908468 | -2.807309 |
| C | -1.958795 | -1.839128 | -1.801352 |
| H | -1.659507 | -2.876342 | -1.770945 |
| C | -3.166256 | -1.279353 | -1.307628 |
| H | -3.978947 | -1.823998 | -0.847095 |
| C | -2.969063 | 3.460876 | 0.991789 |
| H | -3.369437 | 3.089513 | 1.939378 |
| H | -3.645055 | 3.153000 | 0.186798 |
| H | -2.957067 | 4.555658 | 1.028177 |
| C | -1.561535 | 2.914781 | 0.749285 |
| H | -0.926289 | 3.228305 | 1.592703 |
| O | -1.578129 | 1.501882 | 0.761650 |
| Cl | 1.228718 | -2.870731 | -1.296902 |
| H | 0.982940 | -1.528613 | -0.626742 |

2rIM18

SCF energy in gas phase: -1440.410245

Free energy in Et₂O : -1439.933519

Enthalpy in Et₂O : -1439.838485

| | | | |
|---|----------|-----------|----------|
| C | 3.894450 | -0.003987 | 0.461323 |
| C | 4.087906 | -0.328184 | 1.962439 |
| H | 4.769697 | -1.172299 | 2.108060 |
| H | 4.496334 | 0.531944 | 2.505956 |
| C | 2.944365 | 1.179191 | 0.366737 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -0.786973 | -1.312325 | 1.731754 | C | -2.814674 | -0.946334 | 0.016831 |
| H | -0.271168 | -0.525939 | 2.267177 | H | -0.476178 | -0.826318 | -1.355174 |
| C | -0.356873 | -1.945233 | 0.535366 | H | -2.694724 | -1.539935 | -0.897189 |
| H | 0.563888 | -1.742316 | 0.005908 | C | 0.757050 | 1.540079 | 0.926381 |
| C | -1.354317 | -2.875400 | 0.145215 | H | 0.622732 | 0.983061 | 1.859785 |
| H | -1.328285 | -3.500670 | -0.735778 | H | 1.675052 | 2.128239 | 1.015968 |
| C | -2.417828 | -2.798097 | 1.079343 | H | -0.076179 | 2.243965 | 0.831816 |
| H | -3.319299 | -3.395972 | 1.065071 | C | 1.952339 | -0.461069 | -0.104396 |
| C | -2.061315 | -1.831423 | 2.067002 | H | 1.704038 | -1.066557 | 0.777866 |
| H | -2.646567 | -1.557032 | 2.933769 | H | 1.916174 | -1.150549 | -0.960099 |
| C | -4.040722 | 1.440054 | 0.294058 | C | 3.390447 | 0.058783 | 0.040231 |
| H | -3.592288 | 2.415183 | 0.420712 | H | 3.462567 | 0.738660 | 0.899155 |
| C | -4.440016 | 0.842175 | -0.923152 | H | 3.671931 | 0.648506 | -0.841942 |
| H | -4.373672 | 1.283995 | -1.907395 | C | 4.409443 | -1.075469 | 0.221411 |
| C | -4.936155 | -0.462776 | -0.632097 | H | 4.135841 | -1.670054 | 1.103695 |
| H | -5.313660 | -1.170536 | -1.357636 | H | 4.345675 | -1.760215 | -0.635435 |
| C | -4.828404 | -0.668968 | 0.762615 | C | 5.850256 | -0.576078 | 0.368891 |
| H | -5.136041 | -1.554871 | 1.300801 | H | 5.955020 | 0.081907 | 1.239221 |
| C | -4.245213 | 0.499981 | 1.337522 | H | 6.551496 | -1.407617 | 0.495344 |
| H | -4.028414 | 0.669518 | 2.383359 | H | 6.165359 | -0.007203 | -0.513488 |
| C | -1.325814 | 2.504704 | -2.125615 | H | -2.995873 | -1.651396 | 0.841524 |
| H | -2.177264 | 3.015603 | -1.667325 | C | -5.313965 | -0.900552 | -0.467912 |
| H | -1.695701 | 1.704076 | -2.772852 | H | -6.201499 | -0.260051 | -0.536030 |
| H | -0.797992 | 3.232382 | -2.750766 | H | -5.500132 | -1.656724 | 0.301740 |
| C | -0.379965 | 1.964485 | -1.057650 | H | -5.195759 | -1.405182 | -1.432918 |
| H | -0.018184 | 2.799045 | -0.444103 | C | -4.073847 | -0.077570 | -0.115396 |
| O | -1.076982 | 1.094335 | -0.121231 | H | -3.895882 | 0.666615 | -0.909767 |
| Cl | -2.246881 | -1.196316 | -2.446264 | O | -4.239735 | 0.583769 | 1.141784 |
| H | 4.410176 | 3.004577 | 0.761533 | H | 0.232296 | 2.126924 | -1.733859 |
| Cl | -0.998116 | 2.282698 | 2.376277 | H | -4.981558 | 1.196427 | 1.060258 |
| H | -1.016586 | 1.635337 | 1.014837 | | | | |

2rTS19

SCF energy in gas phase: -979.42286

Free energy in Et₂O : -978.971897

Enthalpy in Et₂O : -978.884954

(E)2p

SCF energy in gas phase: -546.969547

Free energy in Et₂O : -546.391166

Enthalpy in Et₂O : -546.328088

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.822286 | 0.597433 | -0.287423 | C | -1.744693 | 0.520094 | 0.449446 |
| C | 1.061721 | 1.431426 | -1.568859 | C | -1.420971 | -1.007943 | 0.594458 |
| H | 1.982752 | 2.019276 | -1.501035 | H | -1.700829 | -1.412565 | 1.570297 |
| H | 1.138367 | 0.787372 | -2.452584 | H | -1.952955 | -1.591391 | -0.162240 |
| C | -0.474329 | -0.173652 | -0.477688 | C | -0.515777 | 1.139474 | -0.327440 |
| C | -1.568472 | -0.146794 | 0.287989 | C | -0.085436 | 2.545943 | -0.226418 |
| H | -1.613177 | 0.489486 | 1.168507 | H | 0.222406 | 2.953680 | -1.193617 |
| | | | | C | 0.042771 | 3.409944 | 0.804369 |

| | | | | | | | |
|----|-----------|-----------|-----------|--|-----------|-----------|-----------|
| H | -0.707321 | 0.949128 | -1.390463 | H | 4.335015 | 4.033985 | -1.280957 |
| H | -0.220016 | 3.173637 | 1.828821 | C | 3.021204 | 2.454091 | -0.690198 |
| C | -1.984735 | 1.161466 | 1.828353 | H | 3.041886 | 2.623650 | 0.403411 |
| H | -2.313478 | 2.200269 | 1.730423 | O | 2.759431 | 1.351555 | -1.138880 |
| H | -2.760629 | 0.612402 | 2.371865 | | | | |
| H | -1.088114 | 1.157609 | 2.450721 | | | | |
| C | -3.014196 | 0.737078 | -0.428852 | 2rIM19 | | | |
| H | -3.115083 | 1.814928 | -0.623042 | SCF energy in gas phase: -979.506679 | | | |
| H | -2.829150 | 0.269091 | -1.406769 | Free energy in Et ₂ O : -979.039283 | | | |
| C | -4.341404 | 0.196686 | 0.122418 | Enthalpy in Et ₂ O : -978.956379 | | | |
| H | -4.613427 | 0.731230 | 1.041673 | C | -1.909061 | 0.886471 | -0.009702 |
| H | -4.221784 | -0.858124 | 0.404434 | C | -1.089830 | -0.336157 | -0.531508 |
| C | -5.497092 | 0.323088 | -0.880382 | H | -1.593340 | -1.262070 | -0.223130 |
| H | -5.603894 | 1.374995 | -1.179489 | H | -1.167920 | -0.319308 | -1.624868 |
| H | -5.242774 | -0.226305 | -1.797501 | C | -1.351133 | 2.143565 | -0.677436 |
| C | -6.833542 | -0.189093 | -0.333294 | C | -0.532567 | 3.130527 | -0.283139 |
| H | -7.132799 | 0.365933 | 0.563348 | H | -0.326630 | 3.896027 | -1.032158 |
| H | -7.636771 | -0.086290 | -1.070885 | C | 0.222437 | 3.307395 | 1.009876 |
| H | -6.768935 | -1.248083 | -0.057515 | H | -1.705088 | 2.234472 | -1.707338 |
| H | 0.388375 | 4.424619 | 0.624860 | H | -0.329334 | 2.900364 | 1.856978 |
| Zr | 0.799958 | -0.760353 | 0.088973 | C | -1.936443 | 0.947075 | 1.528525 |
| C | 2.263581 | -1.729098 | -1.761716 | H | -2.489228 | 1.825612 | 1.881480 |
| H | 3.313496 | -1.472901 | -1.722294 | H | -2.434758 | 0.061378 | 1.934138 |
| C | 1.255318 | -1.001604 | -2.451818 | H | -0.934539 | 0.975434 | 1.956175 |
| H | 1.408398 | -0.080801 | -2.996835 | C | -3.391655 | 0.800852 | -0.523878 |
| C | 0.023470 | -1.664774 | -2.250320 | H | -3.893436 | 1.748678 | -0.277225 |
| H | -0.940192 | -1.343912 | -2.622231 | H | -3.360226 | 0.753850 | -1.621395 |
| C | 0.261503 | -2.810420 | -1.444908 | C | -4.263972 | -0.355848 | -0.018631 |
| H | -0.483706 | -3.519392 | -1.110813 | H | -4.405459 | -0.282222 | 1.067331 |
| C | 1.647590 | -2.858608 | -1.157060 | H | -3.761624 | -1.315080 | -0.199930 |
| H | 2.146454 | -3.618413 | -0.570215 | C | -5.645636 | -0.387123 | -0.688759 |
| C | 2.775249 | -0.163190 | 1.632604 | H | -6.150977 | 0.574480 | -0.524202 |
| H | 3.572437 | 0.420370 | 1.196006 | H | -5.518824 | -0.479177 | -1.776107 |
| C | 1.604519 | 0.346653 | 2.262667 | C | -6.536891 | -1.524839 | -0.180244 |
| H | 1.363740 | 1.392179 | 2.399435 | H | -6.711940 | -1.439451 | 0.898506 |
| C | 0.829907 | -0.763405 | 2.689130 | H | -7.513499 | -1.522485 | -0.675866 |
| H | -0.113666 | -0.720146 | 3.211122 | H | -6.074678 | -2.502149 | -0.361728 |
| C | 1.501358 | -1.949156 | 2.299988 | H | 0.366006 | 4.376813 | 1.212441 |
| H | 1.154096 | -2.960424 | 2.469152 | Zr | 1.208379 | -0.535036 | -0.003906 |
| C | 2.713243 | -1.575968 | 1.662272 | C | 3.208129 | -1.067045 | -1.535842 |
| H | 3.454944 | -2.250590 | 1.256096 | H | 4.157753 | -1.287740 | -1.065611 |
| C | 3.339361 | 3.652262 | -1.538697 | C | 2.762971 | 0.214239 | -1.957936 |
| H | 2.625763 | 4.453233 | -1.312940 | H | 3.291842 | 1.145402 | -1.813930 |
| H | 3.297373 | 3.398952 | -2.599358 | C | 1.483298 | 0.066558 | -2.536399 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 0.860019 | 0.864192 | -2.916658 | H | -3.348405 | 1.297408 | -1.544174 |
| C | 1.148247 | -1.318353 | -2.513828 | C | -4.235279 | 0.135814 | 0.038380 |
| H | 0.234784 | -1.756490 | -2.892166 | H | -4.371408 | 0.193483 | 1.125727 |
| C | 2.215865 | -2.017683 | -1.913508 | H | -3.746024 | -0.825963 | -0.152706 |
| H | 2.265116 | -3.086363 | -1.754966 | C | -5.619206 | 0.136761 | -0.627967 |
| C | 2.335403 | -1.545098 | 2.102168 | H | -6.108581 | 1.105738 | -0.455426 |
| H | 3.283609 | -1.118067 | 2.402274 | H | -5.496984 | 0.050277 | -1.716598 |
| C | 1.053287 | -1.127834 | 2.544430 | C | -6.526737 | -0.990707 | -0.125633 |
| H | 0.853533 | -0.305464 | 3.217338 | H | -6.699861 | -0.907789 | 0.953499 |
| C | 0.085071 | -1.939443 | 1.909793 | H | -7.503205 | -0.970971 | -0.621417 |
| H | -0.984730 | -1.868625 | 2.036718 | H | -6.076633 | -1.972282 | -0.310831 |
| C | 0.765593 | -2.875920 | 1.082948 | H | 1.060162 | 4.312643 | 1.174640 |
| H | 0.301329 | -3.639940 | 0.472769 | Zr | 1.307908 | -0.485160 | -0.074799 |
| C | 2.155758 | -2.641182 | 1.216182 | C | 2.964778 | -1.804004 | -1.504009 |
| H | 2.946567 | -3.193696 | 0.727457 | H | 3.948473 | -1.999598 | -1.098853 |
| C | 2.596133 | 3.328081 | 0.024151 | C | 2.612218 | -0.701704 | -2.329733 |
| H | 2.741670 | 4.376425 | 0.307048 | H | 3.254967 | 0.127970 | -2.589671 |
| H | 2.215980 | 3.296550 | -1.001162 | C | 1.253928 | -0.838538 | -2.680591 |
| H | 3.571268 | 2.831804 | 0.048737 | H | 0.683329 | -0.147369 | -3.286007 |
| C | 1.624622 | 2.640950 | 0.987294 | C | 0.761393 | -2.045311 | -2.097437 |
| H | 2.039146 | 2.717222 | 2.005992 | H | -0.246147 | -2.430776 | -2.171892 |
| O | 1.486835 | 1.278242 | 0.673994 | C | 1.822102 | -2.651855 | -1.391435 |

2rTS20

SCF energy in gas phase: -1440.287001

Free energy in Et₂O : -1439.824513

Enthalpy in Et₂O : -1439.738084

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | -1.868772 | 1.352107 | 0.037113 | H | -0.398443 | -1.001574 | 2.627470 |
| C | -1.052334 | 0.171299 | -0.621693 | C | 1.349282 | -2.153831 | 1.874500 |
| H | -1.719866 | -0.391568 | -1.285238 | H | 0.913359 | -3.126248 | 1.698584 |
| H | -0.380614 | 0.635214 | -1.359253 | C | 2.701468 | -1.775522 | 1.672194 |
| C | -1.333027 | 2.671893 | -0.540294 | H | 3.495762 | -2.419718 | 1.321457 |
| C | -0.287040 | 3.462453 | -0.256471 | C | 2.797115 | 3.518155 | -0.839760 |
| H | -0.176013 | 4.334900 | -0.901086 | H | 3.058454 | 4.509501 | -0.453776 |
| C | 0.800639 | 3.321628 | 0.777748 | H | 2.148345 | 3.641692 | -1.711491 |
| H | -1.926277 | 3.010078 | -1.391798 | H | 3.717200 | 3.023746 | -1.165465 |
| H | 0.462319 | 2.726733 | 1.626510 | C | 2.102072 | 2.680633 | 0.235190 |
| C | -1.860377 | 1.320036 | 1.577422 | H | 2.790724 | 2.566377 | 1.089085 |
| H | -2.434823 | 2.158932 | 1.986091 | O | 1.819298 | 1.397545 | -0.285803 |
| H | -2.308309 | 0.391628 | 1.941565 | Cl | -1.699454 | -2.592488 | 0.495609 |
| H | -0.852926 | 1.373627 | 1.986999 | H | -1.190298 | -1.252107 | 0.086779 |
| C | -3.358200 | 1.296575 | -0.444561 | | | | |
| H | -3.837989 | 2.241438 | -0.149843 | | | | |

2rIM20

SCF energy in gas phase: -1440.401865

Free energy in Et₂O : -1439.926768

Enthalpy in Et₂O : -1439.831461

| | | | |
|----|-----------|-----------|-----------|
| C | 4.491679 | -0.170350 | 0.027116 |
| C | 4.216612 | 0.803049 | -1.143131 |
| H | 4.794067 | 1.726898 | -1.033678 |
| H | 4.484757 | 0.347030 | -2.102308 |
| C | 3.674836 | -1.456296 | -0.144323 |
| C | 2.350327 | -1.661802 | -0.137796 |
| H | 2.028405 | -2.698428 | -0.261926 |
| C | 1.209383 | -0.693446 | 0.036064 |
| H | 4.282606 | -2.351734 | -0.280144 |
| H | 1.531423 | 0.349245 | -0.016204 |
| C | 4.153584 | 0.510828 | 1.373642 |
| H | 4.374760 | -0.156037 | 2.213836 |
| H | 4.734358 | 1.429293 | 1.507232 |
| H | 3.096801 | 0.780584 | 1.436345 |
| C | 5.989460 | -0.599191 | 0.013837 |
| H | 6.132480 | -1.346486 | 0.807596 |
| H | 6.180032 | -1.126822 | -0.931976 |
| C | 7.049098 | 0.497590 | 0.181807 |
| H | 6.904849 | 1.022272 | 1.134904 |
| H | 6.941307 | 1.255674 | -0.604784 |
| C | 8.480427 | -0.057495 | 0.137007 |
| H | 8.599198 | -0.816605 | 0.922192 |
| H | 8.635950 | -0.581713 | -0.815881 |
| C | 9.552053 | 1.024128 | 0.306168 |
| H | 9.443354 | 1.542837 | 1.265567 |
| H | 10.560404 | 0.598607 | 0.271075 |
| H | 9.482098 | 1.778802 | -0.485693 |
| H | 0.758089 | -0.830584 | 1.028772 |
| Zr | -2.811443 | 0.130888 | 0.120089 |
| C | -3.890168 | 1.517177 | -1.747625 |
| H | -4.110137 | 1.032067 | -2.689807 |
| C | -2.698341 | 2.219711 | -1.429513 |
| H | -1.817836 | 2.284629 | -2.052894 |
| C | -2.819392 | 2.716164 | -0.114440 |
| H | -2.062364 | 3.253456 | 0.439813 |
| C | -4.117543 | 2.370758 | 0.371391 |
| H | -4.505128 | 2.604543 | 1.353535 |
| C | -4.782841 | 1.647822 | -0.639670 |
| H | -5.786557 | 1.248914 | -0.583517 |
| C | -3.186405 | -2.253931 | -0.801759 |

| | | | |
|----|-----------|-----------|-----------|
| H | -2.631944 | -2.535850 | -1.687140 |
| C | -2.763254 | -2.432175 | 0.542394 |
| H | -1.829135 | -2.872254 | 0.864467 |
| C | -3.777624 | -1.924653 | 1.392157 |
| H | -3.740671 | -1.892707 | 2.471305 |
| C | -4.816547 | -1.407099 | 0.579966 |
| H | -5.736039 | -0.959900 | 0.933396 |
| C | -4.452245 | -1.618121 | -0.782197 |
| H | -5.047272 | -1.360665 | -1.647793 |
| C | 0.523459 | -0.584296 | -2.428802 |
| H | 1.383811 | -1.195538 | -2.718135 |
| H | 0.808906 | 0.470183 | -2.506027 |
| H | -0.292460 | -0.771468 | -3.134036 |
| C | 0.086157 | -0.908961 | -1.000212 |
| H | -0.217639 | -1.969476 | -0.956536 |
| O | -1.016729 | -0.103309 | -0.646148 |
| Cl | -2.163918 | 0.647853 | 2.462637 |
| H | 3.161363 | 1.082192 | -1.193261 |

2rTS21

SCF energy in gas phase: -1901.206286

Free energy in Et₂O : -1900.737367

Enthalpy in Et₂O : -1900.639733

| | | | |
|---|-----------|-----------|-----------|
| C | -4.184187 | 0.430968 | 0.068448 |
| C | -3.721847 | -0.373650 | -1.169031 |
| H | -4.170762 | -1.372069 | -1.180807 |
| H | -4.006830 | 0.137050 | -2.095183 |
| C | -3.561866 | 1.831957 | 0.054479 |
| C | -2.286086 | 2.228029 | 0.162341 |
| H | -2.113312 | 3.305994 | 0.145256 |
| C | -1.026380 | 1.416250 | 0.334774 |
| H | -4.288576 | 2.638504 | -0.049300 |
| H | -1.192732 | 0.351767 | 0.157179 |
| C | -3.800058 | -0.321826 | 1.363314 |
| H | -4.145513 | 0.222259 | 2.248973 |
| H | -4.244150 | -1.322067 | 1.383558 |
| H | -2.718181 | -0.446654 | 1.450741 |
| C | -5.728008 | 0.637498 | 0.019231 |
| H | -6.009605 | 1.278317 | 0.867169 |
| H | -5.961422 | 1.217494 | -0.885286 |
| C | -6.616032 | -0.613575 | 0.038561 |
| H | -6.429904 | -1.197284 | 0.949164 |
| H | -6.365561 | -1.271072 | -0.803794 |

| | | | | | | | |
|----|------------|-----------|-----------|---|-----------|-----------|-----------|
| C | -8.112227 | -0.273334 | -0.030278 | Enthalpy in Et ₂ O : -546.322407 | | | |
| H | -8.373102 | 0.386006 | 0.808808 | | | | |
| H | -8.310511 | 0.305627 | -0.942599 | C | -0.605549 | -0.201202 | 0.006461 |
| C | -9.012702 | -1.512557 | -0.005358 | C | -0.297130 | 1.063424 | -0.829238 |
| H | -8.862571 | -2.092653 | 0.912393 | H | -0.999816 | 1.169148 | -1.662399 |
| H | -10.071914 | -1.239694 | -0.056286 | H | -0.364920 | 1.965569 | -0.211865 |
| H | -8.798764 | -2.174790 | -0.852096 | C | 0.393335 | -0.330484 | 1.162112 |
| H | -0.673481 | 1.523018 | 1.370528 | C | 1.716521 | -0.542856 | 1.157269 |
| Zr | 2.300013 | -0.602709 | -0.016123 | H | 2.193203 | -0.611995 | 2.137521 |
| C | 4.695446 | -0.372345 | -0.827295 | C | 2.676450 | -0.717681 | 0.009355 |
| H | 5.449322 | -0.083737 | -0.107909 | H | -0.059125 | -0.242550 | 2.150581 |
| C | 3.945244 | 0.513770 | -1.638504 | H | 2.235985 | -0.450000 | -0.954294 |
| H | 3.985367 | 1.594147 | -1.587191 | C | -0.560750 | -1.456314 | -0.895517 |
| C | 3.077881 | -0.264219 | -2.450080 | H | -0.807293 | -2.356949 | -0.322933 |
| H | 2.357549 | 0.118187 | -3.159906 | H | -1.274817 | -1.373018 | -1.721132 |
| C | 3.313072 | -1.634043 | -2.162177 | H | 0.428963 | -1.603554 | -1.333888 |
| H | 2.797275 | -2.472868 | -2.607614 | C | -2.014761 | -0.072177 | 0.658204 |
| C | 4.300781 | -1.706779 | -1.148976 | H | -2.169697 | -0.950225 | 1.301629 |
| H | 4.709365 | -2.614702 | -0.725832 | H | -1.994936 | 0.794627 | 1.334316 |
| C | 3.430737 | -0.197331 | 2.214570 | C | -3.224521 | 0.066914 | -0.275259 |
| H | 4.234704 | 0.525525 | 2.241062 | H | -3.288648 | -0.799040 | -0.946536 |
| C | 2.062570 | 0.091275 | 2.457538 | H | -3.108419 | 0.947315 | -0.920549 |
| H | 1.663463 | 1.077901 | 2.645539 | C | -4.547733 | 0.191627 | 0.494289 |
| C | 1.326357 | -1.107224 | 2.317923 | H | -4.672332 | -0.685141 | 1.144470 |
| H | 0.253927 | -1.215214 | 2.401789 | H | -4.496320 | 1.060204 | 1.164933 |
| C | 2.244867 | -2.158138 | 2.024934 | C | -5.768340 | 0.324926 | -0.421804 |
| H | 1.986225 | -3.195169 | 1.858285 | H | -5.867639 | -0.546479 | -1.079206 |
| C | 3.543863 | -1.599487 | 1.975413 | H | -6.694802 | 0.412591 | 0.155281 |
| H | 4.462330 | -2.140313 | 1.794097 | H | -5.690032 | 1.211995 | -1.060896 |
| C | -0.163263 | 1.674824 | -2.064184 | H | 2.952730 | -1.783258 | -0.058922 |
| H | -1.090174 | 2.179057 | -2.353518 | C | 3.763659 | 1.592954 | 0.132748 |
| H | -0.276435 | 0.607558 | -2.279115 | H | 3.069740 | 1.912657 | 0.914934 |
| H | 0.651779 | 2.078757 | -2.671596 | H | 3.348402 | 1.878101 | -0.839675 |
| C | 0.106941 | 1.905354 | -0.582463 | H | 4.713849 | 2.117782 | 0.264313 |
| H | 0.263499 | 2.977538 | -0.406059 | C | 3.981866 | 0.086323 | 0.185178 |
| O | 1.363992 | 1.286058 | -0.193251 | H | 4.416561 | -0.174403 | 1.166686 |
| Cl | 0.427822 | -2.003786 | -0.767527 | O | 4.908109 | -0.222651 | -0.855203 |
| H | -2.637503 | -0.507513 | -1.182089 | H | 0.709523 | 1.028758 | -1.253060 |
| Cl | 3.095525 | 3.233895 | 0.707902 | H | 5.076687 | -1.173652 | -0.830472 |
| H | 2.106233 | 2.156665 | 0.197119 | | | | |

3r

(Z)3p

SCF energy in gas phase: -546.9609

Free energy in Et₂O : -546.386086

SCF energy in gas phase: -195.297523

Free energy in Et₂O : -195.100335

Enthalpy in Et₂O : -195.065734

| | | | |
|---|-----------|-----------|-----------|
| C | 1.129210 | 0.863689 | 0.190980 |
| C | 1.430337 | -0.401765 | -0.572003 |
| H | 1.095329 | -0.457230 | -1.603397 |
| H | 2.359122 | -0.927146 | -0.369524 |
| C | 0.358106 | -0.392215 | 0.506171 |
| C | -1.074228 | -0.568263 | 0.141733 |
| H | -1.424723 | -1.601614 | 0.143774 |
| C | -1.933489 | 0.398097 | -0.187407 |
| H | -1.648030 | 1.446419 | -0.190103 |
| H | -2.959071 | 0.172488 | -0.463734 |
| H | 0.620981 | 1.661668 | -0.340913 |
| H | 1.852847 | 1.211555 | 0.921918 |
| H | 0.643934 | -0.903397 | 1.425139 |

3rIM1

SCF energy in gas phase: -629.008385

Free energy in Et₂O : -628.917102

Enthalpy in Et₂O : -628.855778

| | | | |
|----|-----------|-----------|-----------|
| C | -4.190169 | -0.930399 | 0.047803 |
| C | -3.580344 | -0.437336 | -1.244620 |
| H | -3.128367 | -1.175051 | -1.903408 |
| H | -4.072175 | 0.378429 | -1.768457 |
| C | -2.882646 | -0.158641 | 0.066318 |
| C | -1.593633 | -0.846684 | 0.419741 |
| H | -1.603026 | -1.884723 | 0.079281 |
| C | -0.977653 | -0.638683 | 1.744328 |
| H | -2.970982 | 0.863242 | 0.430335 |
| H | -1.431988 | 0.124813 | 2.376098 |
| H | -0.695897 | -1.519973 | 2.320521 |
| Zr | 0.530613 | 0.052295 | 0.169440 |
| C | 0.831416 | 2.514518 | 0.977817 |
| H | 1.218229 | 2.707467 | 1.971064 |
| C | -0.534498 | 2.374692 | 0.632045 |
| H | -1.367826 | 2.448097 | 1.316324 |
| C | -0.619249 | 2.121971 | -0.764672 |
| H | -1.529149 | 1.981886 | -1.330982 |
| C | 0.709011 | 2.099476 | -1.280148 |
| H | 0.988435 | 1.960725 | -2.316803 |
| C | 1.605110 | 2.344486 | -0.200253 |
| H | 2.683159 | 2.408200 | -0.269038 |
| C | 2.246966 | -1.777250 | 0.852664 |
| H | 2.530859 | -1.868687 | 1.893568 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.198761 | -2.482197 | 0.214837 |
| H | 0.534209 | -3.191020 | 0.689826 |
| C | 1.147213 | -2.078262 | -1.143635 |
| H | 0.459827 | -2.450732 | -1.891490 |
| C | 2.169407 | -1.107879 | -1.348215 |
| H | 2.415726 | -0.627965 | -2.286395 |
| C | 2.850528 | -0.920052 | -0.109213 |
| H | 3.701541 | -0.272791 | 0.057721 |
| H | -4.146029 | -1.996194 | 0.255443 |
| H | -5.092397 | -0.444085 | 0.409996 |

3rTS1

SCF energy in gas phase: -628.998029

Free energy in Et₂O : -628.905894

Enthalpy in Et₂O : -628.846298

| | | | |
|----|-----------|-----------|-----------|
| C | -3.720499 | -0.841015 | -0.534082 |
| C | -2.610979 | -0.184102 | -1.318940 |
| H | -1.888593 | -0.852149 | -1.787581 |
| H | -2.848205 | 0.698404 | -1.904592 |
| C | -2.665975 | -0.106215 | 0.241366 |
| C | -1.645744 | -0.842749 | 1.045283 |
| H | -1.744142 | -1.925554 | 1.005482 |
| C | -0.847962 | -0.290215 | 2.108901 |
| H | -2.958068 | 0.873001 | 0.615702 |
| H | -1.113710 | 0.682251 | 2.520430 |
| H | -0.475625 | -0.976946 | 2.864414 |
| Zr | 0.267418 | -0.005395 | 0.053031 |
| C | 0.796752 | 2.293444 | 1.094228 |
| H | 0.976166 | 2.350564 | 2.158491 |
| C | -0.457832 | 2.477375 | 0.440312 |
| H | -1.400084 | 2.687060 | 0.927236 |
| C | -0.247376 | 2.372761 | -0.955135 |
| H | -1.005691 | 2.467289 | -1.721895 |
| C | 1.126365 | 2.110190 | -1.181714 |
| H | 1.603920 | 1.997848 | -2.146150 |
| C | 1.771721 | 2.074098 | 0.090490 |
| H | 2.829168 | 1.916723 | 0.258811 |
| C | 2.382637 | -1.389804 | 0.573029 |
| H | 3.056954 | -1.045283 | 1.346566 |
| C | 1.301550 | -2.282727 | 0.756101 |
| H | 1.004942 | -2.733282 | 1.692835 |
| C | 0.655131 | -2.459102 | -0.496771 |
| H | -0.189662 | -3.106914 | -0.687716 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| C | 1.346221 | -1.670897 | -1.466452 | H | -2.566239 | 2.128167 | -0.900834 |
| H | 1.138493 | -1.632892 | -2.528066 | H | -1.536489 | 3.451034 | -1.460399 |
| C | 2.417748 | -1.012640 | -0.797225 | | | | |
| H | 3.140327 | -0.351960 | -1.256157 | | | | |
| H | -3.724432 | -1.926077 | -0.471800 | | | | |
| H | -4.709035 | -0.396685 | -0.603615 | | | | |

3rIM2

SCF energy in gas phase: -629.030218

Free energy in Et₂O : -628.925264

Enthalpy in Et₂O : -628.86639

| | | | |
|----|-----------|-----------|-----------|
| C | -1.522011 | 2.443544 | -1.021148 |
| C | -0.701497 | 1.395601 | -1.792050 |
| H | -1.281722 | 0.859106 | -2.549136 |
| H | 0.140966 | 1.876285 | -2.295267 |
| C | -0.811361 | 2.371185 | 0.313086 |
| C | -1.236681 | 1.620945 | 1.389318 |
| H | -2.278772 | 1.299687 | 1.371885 |
| C | -0.350802 | 0.917602 | 2.270533 |
| H | 0.187402 | 2.807527 | 0.341002 |
| H | 0.584194 | 1.408046 | 2.533868 |
| H | -0.791345 | 0.362221 | 3.093765 |
| Zr | 0.059498 | -0.043353 | 0.045962 |
| C | 2.440088 | -0.059160 | 1.075099 |
| H | 2.531106 | -0.055468 | 2.152003 |
| C | 2.404712 | 1.084253 | 0.229195 |
| H | 2.484554 | 2.114004 | 0.551278 |
| C | 2.305197 | 0.636506 | -1.113367 |
| H | 2.274653 | 1.263121 | -1.992281 |
| C | 2.244220 | -0.775968 | -1.100159 |
| H | 2.165093 | -1.415558 | -1.969450 |
| C | 2.334553 | -1.206823 | 0.256736 |
| H | 2.338335 | -2.232088 | 0.601422 |
| C | -0.856665 | -2.321891 | 0.812211 |
| H | -0.372946 | -2.806887 | 1.649561 |
| C | -1.974882 | -1.455326 | 0.883937 |
| H | -2.477417 | -1.151368 | 1.791720 |
| C | -2.298087 | -1.037179 | -0.430553 |
| H | -3.095359 | -0.361543 | -0.708646 |
| C | -1.393960 | -1.669927 | -1.326879 |
| H | -1.382457 | -1.559314 | -2.402058 |
| C | -0.513546 | -2.470352 | -0.561599 |
| H | 0.280853 | -3.090891 | -0.953093 |

3rIM3

SCF energy in gas phase: -629.002935

Free energy in Et₂O : -628.913061

Enthalpy in Et₂O : -628.851203

| | | | |
|----|-----------|-----------|-----------|
| C | -2.862052 | -0.717183 | -1.220229 |
| C | -2.170091 | -2.063963 | -1.145464 |
| H | -2.682708 | -2.857722 | -0.601558 |
| H | -1.636420 | -2.416426 | -2.027315 |
| C | -1.639861 | -0.892937 | -0.364333 |
| C | -1.541799 | -0.739372 | 1.103332 |
| H | -1.295887 | -1.668847 | 1.626462 |
| C | -2.603412 | 0.046403 | 1.861968 |
| H | -3.536626 | -0.530211 | 1.963912 |
| H | -2.868819 | 0.981217 | 1.358799 |
| H | -2.276895 | 0.299970 | 2.878071 |
| Zr | 0.327993 | 0.100129 | 0.045439 |
| C | 1.118100 | -2.383180 | 0.203628 |
| H | 0.360561 | -3.150086 | 0.282065 |
| C | 1.712542 | -1.685186 | 1.284828 |
| H | 1.516980 | -1.856505 | 2.335274 |
| C | 2.616952 | -0.727225 | 0.743080 |
| H | 3.250861 | -0.055503 | 1.307584 |
| C | 2.577020 | -0.843162 | -0.676309 |
| H | 3.171468 | -0.272762 | -1.377933 |
| C | 1.648183 | -1.869394 | -1.004373 |
| H | 1.385043 | -2.198232 | -2.001791 |
| C | -0.037519 | 2.192358 | -1.452994 |
| H | -0.200616 | 2.060242 | -2.515694 |
| C | -1.045104 | 2.240084 | -0.458929 |
| H | -2.105938 | 2.133806 | -0.633190 |
| C | -0.416936 | 2.418783 | 0.802535 |
| H | -0.920765 | 2.510318 | 1.754869 |
| C | 0.990270 | 2.480149 | 0.583288 |
| H | 1.748449 | 2.639880 | 1.339621 |
| C | 1.222087 | 2.342744 | -0.813706 |
| H | 2.186559 | 2.364203 | -1.303743 |
| H | -3.830746 | -0.625595 | -0.729220 |
| H | -2.794499 | -0.156402 | -2.151693 |

3rTS2

SCF energy in gas phase: -628.963127

Free energy in Et₂O : -628.871287

Enthalpy in Et₂O : -628.810078

| | | | |
|----|-----------|-----------|-----------|
| C | 1.441674 | -0.800710 | 1.677791 |
| C | 2.158481 | -2.053823 | 1.115039 |
| H | 3.255005 | -2.050214 | 1.141065 |
| H | 1.763606 | -2.987099 | 1.522803 |
| C | 1.476659 | -1.507205 | -0.048907 |
| C | 1.827661 | -0.668178 | -1.117314 |
| H | 1.241529 | -0.915859 | -2.019833 |
| C | 3.185304 | -0.049199 | -1.406763 |
| H | 3.927742 | -0.803863 | -1.703498 |
| H | 3.586698 | 0.465438 | -0.525236 |
| H | 3.134462 | 0.685322 | -2.218816 |
| Zr | -0.141716 | 0.001264 | 0.029726 |
| C | -1.402115 | -2.268880 | -0.365981 |
| H | -0.804362 | -3.165512 | -0.429966 |
| C | -1.744039 | -1.417772 | -1.447398 |
| H | -1.494027 | -1.578892 | -2.488480 |
| C | -2.560981 | -0.362883 | -0.932223 |
| H | -2.998902 | 0.438106 | -1.512904 |
| C | -2.684414 | -0.545347 | 0.458565 |
| H | -3.231139 | 0.093093 | 1.140349 |
| C | -1.945457 | -1.713197 | 0.820940 |
| H | -1.872681 | -2.138584 | 1.813871 |
| C | -0.445946 | 2.250746 | 1.346404 |
| H | -0.782492 | 2.230148 | 2.375652 |
| C | 0.912854 | 2.216287 | 0.907225 |
| H | 1.782145 | 2.151735 | 1.545398 |
| C | 0.921362 | 2.307472 | -0.499734 |
| H | 1.797349 | 2.322526 | -1.131230 |
| C | -0.434086 | 2.404900 | -0.941918 |
| H | -0.760058 | 2.519758 | -1.968141 |
| C | -1.265098 | 2.419113 | 0.204948 |
| H | -2.344470 | 2.485952 | 0.204768 |
| H | 2.125421 | -0.021564 | 2.003675 |
| H | 0.691645 | -1.048986 | 2.437468 |

3rIM4

SCF energy in gas phase: -629.025228

Free energy in Et₂O : -628.921628

Enthalpy in Et₂O : -628.857257

| | | | |
|----|-----------|-----------|-----------|
| C | 0.595281 | -0.000970 | 2.164591 |
| C | 1.964579 | -0.002363 | 1.369151 |
| H | 2.542875 | 0.882072 | 1.659683 |
| H | 2.540685 | -0.888502 | 1.658849 |
| C | 1.820923 | -0.001462 | -0.192335 |
| C | 2.868327 | -0.001341 | -1.026472 |
| H | 2.673691 | -0.000806 | -2.101953 |
| C | 4.333437 | -0.002152 | -0.660539 |
| H | 4.844066 | -0.882405 | -1.074270 |
| H | 4.493601 | -0.000013 | 0.420674 |
| H | 4.846006 | 0.875090 | -1.078169 |
| Zr | -0.354517 | 0.000069 | 0.128852 |
| C | -0.181909 | -2.576851 | 0.303381 |
| H | 0.666145 | -2.985481 | 0.836570 |
| C | -0.225743 | -2.281110 | -1.084234 |
| H | 0.581326 | -2.424444 | -1.788581 |
| C | -1.502951 | -1.737589 | -1.371619 |
| H | -1.854994 | -1.418832 | -2.344081 |
| C | -2.253596 | -1.711725 | -0.160850 |
| H | -3.275414 | -1.372349 | -0.053695 |
| C | -1.436077 | -2.235609 | 0.872164 |
| H | -1.715586 | -2.346414 | 1.910980 |
| C | -1.420153 | 2.242672 | 0.875334 |
| H | -1.689092 | 2.358336 | 1.916374 |
| C | -0.170430 | 2.577116 | 0.293052 |
| H | 0.684477 | 2.984302 | 0.816302 |
| C | -0.229096 | 2.276765 | -1.093052 |
| H | 0.571575 | 2.414740 | -1.805780 |
| C | -1.511111 | 1.737299 | -1.365989 |
| H | -1.874028 | 1.416552 | -2.333780 |
| C | -2.249713 | 1.718035 | -0.147673 |
| H | -3.271744 | 1.383122 | -0.029112 |
| H | 0.504314 | 0.885464 | 2.793420 |
| H | 0.502175 | -0.887472 | 2.793035 |

4r

SCF energy in gas phase: -234.614813

Free energy in Et₂O : -234.362274

Enthalpy in Et₂O : -234.324916

| | | | |
|---|----------|-----------|-----------|
| C | 0.702955 | 0.986957 | 0.554936 |
| C | 1.145017 | -0.991586 | -0.227396 |
| H | 0.836659 | -1.689106 | -1.012222 |
| H | 1.935975 | -1.460360 | 0.366203 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 0.009884 | -0.401062 | 0.680352 | C | -0.982143 | 2.246179 | -1.044238 |
| C | -1.362693 | -0.552560 | 0.086091 | H | -0.201463 | 2.557702 | -1.725187 |
| H | -1.701867 | -1.588056 | 0.011709 | C | -2.116492 | 1.449082 | -1.371869 |
| C | -2.175480 | 0.410702 | -0.350116 | H | -2.367510 | 1.068236 | -2.353411 |
| H | -0.005194 | -0.818836 | 1.695727 | C | -2.897917 | 1.293159 | -0.189193 |
| H | -1.910010 | 1.463082 | -0.305842 | H | -3.840652 | 0.767400 | -0.113777 |
| H | -3.150934 | 0.177505 | -0.766674 | H | 3.974770 | 1.014225 | 1.508671 |
| H | 0.070689 | 1.864881 | 0.398642 | H | 4.730447 | -0.519420 | 1.026489 |
| H | 1.346122 | 1.182434 | 1.418387 | C | 4.363850 | 0.787616 | -0.719272 |
| C | 1.508632 | 0.453453 | -0.658424 | H | 4.139298 | 1.852240 | -0.838094 |
| H | 1.038063 | 0.723073 | -1.608142 | H | 5.374846 | 0.610198 | -1.098765 |
| H | 2.570607 | 0.709960 | -0.710448 | | | | |

4rTS1

SCF energy in gas phase: -668.296808

Free energy in Et₂O : -668.146596

Enthalpy in Et₂O : -668.084635

4rIM1

SCF energy in gas phase: -668.326003

Free energy in Et₂O : -668.179999

Enthalpy in Et₂O : -668.115422

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 4.042460 | 0.271583 | 0.707855 | C | -3.673472 | 0.395004 | 0.189819 |
| C | 3.230614 | -0.117223 | -1.274286 | C | -1.995664 | 0.491552 | -1.307069 |
| H | 2.541611 | 0.336032 | -1.995435 | H | -1.261683 | -0.038300 | -1.923550 |
| H | 3.616381 | -1.048839 | -1.702975 | H | -2.079739 | 1.508522 | -1.692198 |
| C | 2.679654 | -0.302091 | 0.176513 | C | -2.199486 | 0.706632 | 0.541213 |
| C | 1.465790 | 0.543672 | 0.510946 | C | -1.523089 | -0.182600 | 1.477339 |
| H | 1.625351 | 1.586053 | 0.221272 | H | -1.945402 | -1.181929 | 1.555891 |
| C | 0.777574 | 0.379762 | 1.805250 | C | -0.376695 | 0.149411 | 2.299793 |
| H | 2.506857 | -1.343387 | 0.468657 | H | -1.989348 | 1.762776 | 0.720722 |
| H | 1.076485 | -0.475257 | 2.412308 | H | -0.277370 | 1.177460 | 2.649511 |
| H | 0.609853 | 1.266178 | 2.416896 | H | -0.119804 | -0.573180 | 3.070088 |
| Zr | -0.753064 | -0.019703 | 0.150042 | Zr | 0.360921 | -0.029217 | 0.107880 |
| C | -1.461455 | -2.404736 | 0.930678 | C | 1.773669 | 1.977280 | 0.912932 |
| H | -1.890680 | -2.535543 | 1.916538 | H | 1.999409 | 2.050826 | 1.966971 |
| C | -0.086475 | -2.494215 | 0.606963 | C | 0.645084 | 2.539706 | 0.251884 |
| H | 0.712126 | -2.708200 | 1.302832 | H | -0.129816 | 3.133698 | 0.716899 |
| C | 0.062950 | -2.248330 | -0.784840 | C | 0.755378 | 2.244613 | -1.135036 |
| H | 0.990747 | -2.274569 | -1.339106 | H | 0.063068 | 2.550432 | -1.908298 |
| C | -1.234345 | -2.000339 | -1.321798 | C | 1.932804 | 1.490922 | -1.333156 |
| H | -1.469511 | -1.814167 | -2.361981 | H | 2.295827 | 1.113071 | -2.280234 |
| C | -2.176206 | -2.099537 | -0.257954 | C | 2.561414 | 1.324234 | -0.063581 |
| H | -3.248491 | -1.983206 | -0.344247 | H | 3.491930 | 0.803970 | 0.121591 |
| C | -2.242927 | 1.992991 | 0.861340 | C | 1.744861 | -2.116449 | 0.666387 |
| H | -2.579383 | 2.062464 | 1.888203 | H | 2.438744 | -2.066926 | 1.494716 |
| C | -1.064845 | 2.572708 | 0.333550 | C | 0.408547 | -2.580079 | 0.727915 |
| H | -0.339061 | 3.148275 | 0.891543 | H | -0.102762 | -2.914198 | 1.619967 |
| | | | | C | -0.154634 | -2.490862 | -0.568347 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -1.166201 | -2.764218 | -0.838965 | C | -1.121216 | 2.080323 | -1.140174 |
| C | 0.835656 | -1.975490 | -1.448086 | H | -1.689983 | 1.918473 | -2.045948 |
| H | 0.726997 | -1.822700 | -2.514235 | C | -1.647585 | 2.153270 | 0.184747 |
| C | 2.015878 | -1.751363 | -0.683867 | H | -2.686246 | 2.041467 | 0.465546 |
| H | 2.962369 | -1.401170 | -1.070016 | H | 4.103559 | -0.552794 | 0.341391 |
| H | -4.168923 | -0.261781 | 0.912252 | H | 3.517954 | -1.958334 | -0.538275 |
| H | -4.259130 | 1.317379 | 0.112200 | C | 2.766258 | -0.078853 | -1.331951 |
| C | -3.354413 | -0.208289 | -1.182869 | H | 2.844394 | 0.969056 | -1.010084 |
| H | -3.223375 | -1.293101 | -1.105850 | H | 3.460909 | -0.181974 | -2.181975 |
| H | -4.066650 | -0.017299 | -1.994268 | | | | |

4rIM2

SCF energy in gas phase: -668.357037

Free energy in Et₂O : -668.201546

Enthalpy in Et₂O : -668.14031

| | | | |
|----|-----------|-----------|-----------|
| C | 3.220646 | -0.975039 | -0.156007 |
| C | 1.315098 | -0.425743 | -1.694133 |
| H | 1.002939 | 0.095202 | -2.609183 |
| H | 1.269440 | -1.496090 | -1.933323 |
| C | 2.074555 | -1.148789 | 0.813347 |
| C | 1.687249 | -0.220116 | 1.753826 |
| H | 2.267209 | 0.702794 | 1.800351 |
| C | 0.424600 | -0.242946 | 2.424866 |
| H | 1.576748 | -2.118178 | 0.825631 |
| H | 0.038790 | -1.213784 | 2.723447 |
| H | 0.233917 | 0.533164 | 3.159285 |
| Zr | -0.229617 | 0.019401 | 0.073117 |
| C | -1.480229 | -2.204902 | 0.733594 |
| H | -1.204158 | -2.725736 | 1.639796 |
| C | -0.932544 | -2.427717 | -0.550681 |
| H | -0.158374 | -3.140550 | -0.798831 |
| C | -1.577845 | -1.550556 | -1.464084 |
| H | -1.381634 | -1.482391 | -2.525199 |
| C | -2.532286 | -0.796301 | -0.736967 |
| H | -3.201546 | -0.054606 | -1.150730 |
| C | -2.455964 | -1.179500 | 0.628660 |
| H | -3.055473 | -0.786176 | 1.438932 |
| C | -0.575723 | 2.406050 | 1.067789 |
| H | -0.651152 | 2.521548 | 2.139218 |
| C | 0.617290 | 2.488245 | 0.294700 |
| H | 1.608004 | 2.696737 | 0.674384 |
| C | 0.273050 | 2.309960 | -1.067054 |
| H | 0.957269 | 2.331833 | -1.901988 |

4rIM3

SCF energy in gas phase: -668.31043

Free energy in Et₂O : -668.159462

Enthalpy in Et₂O : -668.09687

| | | | |
|----|-----------|-----------|-----------|
| C | -3.935260 | -0.221675 | -0.729079 |
| C | -2.917358 | 0.847746 | -0.245529 |
| H | -2.654206 | 1.549579 | -1.042359 |
| H | -3.195397 | 1.424331 | 0.644513 |
| C | -1.889151 | -0.300543 | -0.035741 |
| C | -1.469794 | -0.741710 | 1.264783 |
| H | -1.449076 | -1.815794 | 1.430277 |
| C | -0.898742 | 0.061592 | 2.359093 |
| H | -0.921960 | -0.442923 | 3.327021 |
| H | -1.287855 | 1.078731 | 2.456085 |
| H | 0.302818 | 0.249238 | 2.274635 |
| Zr | 0.491870 | 0.016893 | 0.209689 |
| C | 1.404723 | -1.676698 | -1.497982 |
| H | 1.234709 | -1.490511 | -2.550585 |
| C | 0.573286 | -2.439842 | -0.648716 |
| H | -0.348211 | -2.926660 | -0.935891 |
| C | 1.141709 | -2.423024 | 0.654918 |
| H | 0.747676 | -2.929508 | 1.525976 |
| C | 2.339138 | -1.655079 | 0.611140 |
| H | 3.027798 | -1.495557 | 1.429640 |
| C | 2.497609 | -1.190583 | -0.725285 |
| H | 3.320347 | -0.594782 | -1.095409 |
| C | 0.060598 | 2.085406 | -1.228050 |
| H | -0.681822 | 2.026005 | -2.010509 |
| C | -0.159005 | 2.503546 | 0.118402 |
| H | -1.105395 | 2.816032 | 0.536557 |
| C | 1.088564 | 2.491468 | 0.794890 |
| H | 1.257402 | 2.765080 | 1.828440 |
| C | 2.077982 | 2.049105 | -0.112564 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 3.131321 | 1.928657 | 0.103766 | C | 1.012516 | 2.421380 | -0.735166 |
| C | 1.441415 | 1.806622 | -1.366014 | H | 1.731682 | 2.473816 | -1.541120 |
| H | 1.932955 | 1.473951 | -2.270913 | H | -3.050250 | 0.914604 | -1.519596 |
| H | -4.519726 | 0.017852 | -1.623718 | H | -3.743950 | -0.571955 | -2.191704 |
| H | -4.620650 | -0.518919 | 0.069990 | C | -1.635419 | -0.738506 | -1.486564 |
| C | -2.768717 | -1.234507 | -0.889989 | H | -0.966678 | -0.222727 | -2.191503 |
| H | -2.432712 | -1.314667 | -1.929598 | H | -1.611342 | -1.803829 | -1.731256 |
| H | -2.934790 | -2.246792 | -0.501152 | | | | |

4rTS2

SCF energy in gas phase: -668.265561

Free energy in Et₂O : -668.119902

Enthalpy in Et₂O : -668.058365

| | | | |
|----|-----------|-----------|-----------|
| C | -3.062160 | -0.175873 | -1.431082 |
| C | -3.324211 | -0.611173 | 0.017350 |
| H | -3.927853 | 0.062511 | 0.641045 |
| H | -3.798226 | -1.604056 | 0.056058 |
| C | -1.856498 | -0.674980 | 0.389812 |
| C | -1.117510 | -1.631410 | 1.155698 |
| H | -1.199402 | -2.716685 | 1.041269 |
| C | -0.480280 | -1.149001 | 2.434387 |
| H | 0.028542 | -1.963939 | 2.956040 |
| H | -1.148963 | -0.631795 | 3.130892 |
| H | 0.357555 | -0.379943 | 2.297627 |
| Zr | 0.178265 | -0.019225 | 0.143859 |
| C | 2.139007 | -0.585804 | -1.608433 |
| H | 2.182341 | -0.049442 | -2.548020 |
| C | 1.371873 | -1.767982 | -1.358853 |
| H | 0.750453 | -2.285301 | -2.077244 |
| C | 1.621115 | -2.176536 | -0.030837 |
| H | 1.217963 | -3.054675 | 0.451794 |
| C | 2.513868 | -1.228939 | 0.554792 |
| H | 2.922473 | -1.280385 | 1.556631 |
| C | 2.870676 | -0.285877 | -0.443357 |
| H | 3.534081 | 0.557226 | -0.308144 |
| C | -0.400266 | 2.351121 | -0.884298 |
| H | -0.944068 | 2.405522 | -1.819081 |
| C | -0.981014 | 2.307059 | 0.413840 |
| H | -2.036936 | 2.278124 | 0.638939 |
| C | 0.071483 | 2.272224 | 1.354051 |
| H | -0.038390 | 2.249686 | 2.431387 |
| C | 1.309477 | 2.344462 | 0.639501 |
| H | 2.294438 | 2.371256 | 1.086564 |

4rIM4

SCF energy in gas phase: -668.346184

Free energy in Et₂O : -668.193586

Enthalpy in Et₂O : -668.12968

| | | | |
|----|-----------|-----------|-----------|
| C | -1.767399 | 0.283384 | -2.339878 |
| C | -2.437981 | -0.659850 | -1.317690 |
| H | -3.531846 | -0.534468 | -1.327946 |
| H | -2.247310 | -1.692753 | -1.651704 |
| C | -1.883418 | -0.491447 | 0.102392 |
| C | -2.712893 | -0.632664 | 1.148539 |
| H | -3.776430 | -0.834631 | 0.962947 |
| C | -2.351924 | -0.566516 | 2.609123 |
| H | -2.639134 | -1.489496 | 3.131756 |
| H | -2.878162 | 0.251027 | 3.121972 |
| H | -1.277129 | -0.422686 | 2.759578 |
| Zr | 0.327131 | 0.047007 | -0.141991 |
| C | 2.011867 | -1.770544 | -0.910744 |
| H | 2.420861 | -1.693147 | -1.909322 |
| C | 0.837784 | -2.477209 | -0.542988 |
| H | 0.189593 | -3.023258 | -1.214797 |
| C | 0.646409 | -2.325929 | 0.852796 |
| H | -0.167376 | -2.742377 | 1.429076 |
| C | 1.694320 | -1.506999 | 1.350586 |
| H | 1.840856 | -1.216467 | 2.382913 |
| C | 2.544918 | -1.171569 | 0.257961 |
| H | 3.445929 | -0.574865 | 0.313918 |
| C | 0.372847 | 2.574359 | -0.679029 |
| H | 0.160552 | 2.883599 | -1.692285 |
| C | -0.575902 | 2.425053 | 0.364245 |
| H | -1.641423 | 2.586518 | 0.287120 |
| C | 0.118256 | 2.015167 | 1.533449 |
| H | -0.328436 | 1.819596 | 2.499058 |
| C | 1.495957 | 1.916353 | 1.214474 |
| H | 2.287723 | 1.633835 | 1.895712 |
| C | 1.653844 | 2.249890 | -0.157022 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 2.587656 | 2.268822 | -0.704683 | H | 3.646314 | 1.224611 | 2.030354 |
| H | -1.998581 | 1.322473 | -2.068323 | H | 3.862329 | -0.519400 | 1.943560 |
| H | -2.215891 | 0.125338 | -3.332921 | C | 3.374933 | 0.378011 | 0.024538 |
| C | -0.237344 | 0.064229 | -2.379441 | H | 3.132303 | 1.397699 | -0.299760 |
| H | 0.257186 | 0.811767 | -3.010771 | H | 4.419390 | 0.208298 | -0.279799 |
| H | -0.029926 | -0.913373 | -2.832282 | Cl | -3.348692 | 0.816231 | 1.145216 |
| | | | | H | -1.772112 | 0.724898 | 1.377642 |

4rTS3

SCF energy in gas phase: -1129.149171

Free energy in Et₂O : -1128.996587

Enthalpy in Et₂O : -1128.931337

| | | | |
|----|-----------|-----------|-----------|
| C | 3.256956 | 0.311002 | 1.564427 |
| C | 2.410483 | -0.643346 | -0.593429 |
| H | 2.586696 | -0.756552 | -1.670832 |
| H | 2.630659 | -1.621697 | -0.150397 |
| C | 1.815636 | 0.081595 | 1.956554 |
| C | 0.847710 | 1.041875 | 1.966709 |
| H | 1.144728 | 2.059913 | 1.718332 |
| C | -0.580901 | 0.805681 | 2.192190 |
| H | 1.545523 | -0.913964 | 2.305753 |
| H | -0.774526 | -0.044091 | 2.848931 |
| H | -1.061893 | 1.701732 | 2.587668 |
| Zr | 0.109162 | -0.149616 | -0.209199 |
| C | -1.317482 | -2.056608 | 0.795808 |
| H | -1.835208 | -1.873672 | 1.726307 |
| C | -0.015160 | -2.598455 | 0.634407 |
| H | 0.640160 | -2.937695 | 1.425540 |
| C | 0.258460 | -2.675001 | -0.758303 |
| H | 1.161333 | -3.058965 | -1.210389 |
| C | -0.865757 | -2.164026 | -1.450692 |
| H | -0.975433 | -2.109431 | -2.524958 |
| C | -1.839227 | -1.770118 | -0.488597 |
| H | -2.809043 | -1.334057 | -0.678131 |
| C | -0.833682 | 2.186133 | -0.799151 |
| H | -1.411149 | 2.702550 | -0.045676 |
| C | 0.567954 | 2.283791 | -1.020713 |
| H | 1.253416 | 2.930725 | -0.490994 |
| C | 0.903985 | 1.432801 | -2.103020 |
| H | 1.889106 | 1.300594 | -2.524994 |
| C | -0.282371 | 0.787004 | -2.533334 |
| H | -0.360073 | 0.096859 | -3.362046 |
| C | -1.360221 | 1.259652 | -1.726578 |
| H | -2.399126 | 0.970428 | -1.791690 |

4rTS4

SCF energy in gas phase: -1129.13658

Free energy in Et₂O : -1128.98569

Enthalpy in Et₂O : -1128.920218

| | | | |
|----|-----------|-----------|-----------|
| C | 2.507610 | 2.147108 | -0.998792 |
| C | -0.034710 | 1.927440 | -1.157069 |
| H | -0.795104 | 2.627358 | -1.520763 |
| H | 0.252231 | 1.422482 | -2.085746 |
| C | 2.419941 | 0.645173 | -1.023783 |
| C | 2.755848 | -0.203049 | 0.003216 |
| H | 3.148358 | 0.239283 | 0.917745 |
| C | 2.340086 | -1.569359 | 0.023843 |
| H | 2.146508 | 0.185948 | -1.973723 |
| H | 2.358091 | -2.082996 | -0.933340 |
| H | 2.661866 | -2.195114 | 0.850120 |
| Zr | 0.164503 | -0.425239 | 0.044736 |
| C | -0.183689 | -2.605089 | -1.305548 |
| H | 0.554288 | -3.391956 | -1.252183 |
| C | -0.216306 | -1.540141 | -2.250178 |
| H | 0.489017 | -1.383363 | -3.055964 |
| C | -1.385708 | -0.772788 | -2.000276 |
| H | -1.713908 | 0.099943 | -2.545647 |
| C | -2.049244 | -1.328910 | -0.883127 |
| H | -2.959145 | -0.943168 | -0.447954 |
| C | -1.304558 | -2.465313 | -0.454029 |
| H | -1.569736 | -3.131102 | 0.355588 |
| C | 0.840942 | -0.716973 | 2.541269 |
| H | 1.713663 | -1.299666 | 2.798190 |
| C | 0.805489 | 0.686316 | 2.313388 |
| H | 1.645158 | 1.363823 | 2.382784 |
| C | -0.536024 | 1.055031 | 2.042685 |
| H | -0.905067 | 2.047031 | 1.830103 |
| C | -1.327554 | -0.117497 | 2.071516 |
| H | -2.393910 | -0.148587 | 1.903926 |
| C | -0.472888 | -1.216415 | 2.383021 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -0.776813 | -2.246026 | 2.513063 | C | -3.130026 | 1.372234 | 0.032395 |
| H | 3.288766 | 2.477024 | -0.303052 | H | -4.091621 | 0.892466 | 0.154848 |
| H | 2.798201 | 2.507484 | -1.992521 | H | 3.895792 | 2.236140 | -0.625623 |
| C | 1.139106 | 2.765854 | -0.608202 | H | 3.286327 | 1.434335 | -2.072542 |
| H | 1.090743 | 2.833044 | 0.484300 | C | 1.937564 | 1.331531 | -0.381238 |
| H | 1.090728 | 3.802513 | -0.968636 | H | 2.022326 | 1.240404 | 0.708694 |
| Cl | -2.888288 | 1.905964 | -0.144679 | H | 1.503965 | 2.321049 | -0.574125 |
| H | -1.393221 | 1.675914 | -0.473791 | Cl | -0.174958 | -0.279554 | 2.385190 |
| | | | | H | 6.171455 | -1.219197 | 1.547158 |

4rIM5

SCF energy in gas phase: -1129.236328

Free energy in Et₂O : -1129.071946

Enthalpy in Et₂O : -1128.998937

| | | | |
|----|-----------|-----------|-----------|
| C | 3.371003 | 1.338810 | -0.979131 |
| C | 1.021513 | 0.228412 | -0.932548 |
| H | 0.911280 | 0.340006 | -2.021930 |
| H | 1.506097 | -0.745318 | -0.780405 |
| C | 4.194550 | 0.125561 | -0.643163 |
| C | 5.299265 | 0.132997 | 0.108602 |
| H | 5.653097 | 1.085123 | 0.509000 |
| C | 6.118402 | -1.076124 | 0.460163 |
| H | 3.847810 | -0.827508 | -1.045505 |
| H | 5.699195 | -1.986759 | 0.020709 |
| H | 7.153402 | -0.975440 | 0.108011 |
| Zr | -1.021408 | -0.075797 | 0.093433 |
| C | -1.769911 | -2.520502 | 0.508630 |
| H | -1.880931 | -2.827326 | 1.539448 |
| C | -0.582032 | -2.607489 | -0.258623 |
| H | 0.365203 | -2.999565 | 0.086420 |
| C | -0.847228 | -2.070212 | -1.545970 |
| H | -0.142965 | -2.000236 | -2.362985 |
| C | -2.194838 | -1.633290 | -1.568148 |
| H | -2.708075 | -1.197804 | -2.414478 |
| C | -2.766373 | -1.906198 | -0.291357 |
| H | -3.788170 | -1.711919 | 0.005326 |
| C | -2.334307 | 1.919502 | 1.069039 |
| H | -2.555338 | 1.885796 | 2.127087 |
| C | -1.166784 | 2.471755 | 0.483065 |
| H | -0.350117 | 2.935214 | 1.018913 |
| C | -1.248463 | 2.286497 | -0.922062 |
| H | -0.519217 | 2.609899 | -1.650767 |
| C | -2.457099 | 1.600606 | -1.202661 |
| H | -2.820313 | 1.330387 | -2.184767 |

4rIM6

SCF energy in gas phase: -1129.243445

Free energy in Et₂O : -1129.080629

Enthalpy in Et₂O : -1129.008629

| | | | |
|----|-----------|-----------|-----------|
| C | 4.243719 | -0.082330 | -1.139875 |
| C | 4.925542 | 1.002982 | 1.105728 |
| H | 5.381582 | 0.804440 | 2.081340 |
| H | 5.560231 | 1.730402 | 0.585186 |
| C | 2.862239 | 0.509530 | -1.212663 |
| C | 1.783541 | -0.115485 | -1.715253 |
| H | 1.923845 | -1.130409 | -2.095362 |
| C | 0.408279 | 0.436980 | -1.805820 |
| H | 2.741495 | 1.521664 | -0.825105 |
| H | 0.435757 | 1.534576 | -1.806344 |
| H | -0.094898 | 0.117644 | -2.726095 |
| Zr | -0.920507 | 0.006791 | 0.051195 |
| C | -2.335840 | 1.554446 | -1.469706 |
| H | -1.977134 | 1.767159 | -2.466586 |
| C | -2.049492 | 2.306423 | -0.301428 |
| H | -1.415227 | 3.180530 | -0.243162 |
| C | -2.724428 | 1.699258 | 0.789405 |
| H | -2.686089 | 2.028156 | 1.818833 |
| C | -3.409724 | 0.559712 | 0.302013 |
| H | -4.029540 | -0.107046 | 0.885729 |
| C | -3.165019 | 0.466536 | -1.098959 |
| H | -3.569884 | -0.279951 | -1.768782 |
| C | -0.407039 | -2.384402 | -0.777823 |
| H | -0.071635 | -2.527028 | -1.795266 |
| C | 0.424274 | -2.188153 | 0.358392 |
| H | 1.502083 | -2.112091 | 0.350688 |
| C | -0.406974 | -2.070595 | 1.498046 |
| H | -0.071860 | -1.887703 | 2.509444 |
| C | -1.756115 | -2.171004 | 1.071598 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -2.627762 | -2.137057 | 1.711201 | H | 2.391500 | -0.395104 | -1.943874 |
| C | -1.754633 | -2.375715 | -0.338542 | C | 2.446299 | 0.148607 | 0.200874 |
| H | -2.627467 | -2.524190 | -0.959323 | C | 1.113411 | 0.818576 | 0.497241 |
| H | 4.253575 | -1.045622 | -1.666426 | H | 1.146267 | 1.867064 | 0.186295 |
| H | 4.950048 | 0.569970 | -1.677056 | C | 0.429120 | 0.602233 | 1.788059 |
| C | 4.783517 | -0.288649 | 0.293438 | H | 2.392427 | -0.920259 | 0.456423 |
| H | 4.121061 | -0.982151 | 0.827717 | H | 0.824891 | -0.189404 | 2.424839 |
| H | 5.761236 | -0.784015 | 0.225038 | H | 0.140873 | 1.477484 | 2.370158 |
| Cl | 0.404484 | 1.138956 | 1.785168 | Zr | -1.007789 | -0.037069 | 0.131371 |
| H | 3.953581 | 1.471629 | 1.287361 | C | -1.410667 | -2.439933 | 1.061175 |

5r

SCF energy in gas phase: -273.960473

Free energy in Et₂O : -273.655431

Enthalpy in Et₂O : -273.614962

| | | | |
|---|-----------|-----------|-----------|
| C | 0.208113 | 1.133800 | 0.002746 |
| C | 0.606679 | -1.221846 | -0.242777 |
| H | 0.295706 | -1.313929 | -1.290887 |
| H | 0.574352 | -2.225790 | 0.193312 |
| C | -0.341148 | -0.224851 | 0.468574 |
| C | -1.801311 | -0.499894 | 0.233078 |
| H | -2.131598 | -1.499365 | 0.521869 |
| C | -2.699387 | 0.341282 | -0.282225 |
| H | -0.154465 | -0.316217 | 1.552066 |
| H | -2.441488 | 1.352960 | -0.582139 |
| H | -3.735616 | 0.046125 | -0.419618 |
| H | -0.122494 | 1.317723 | -1.027392 |
| H | -0.144236 | 1.972545 | 0.611633 |
| C | 2.003681 | -0.565101 | -0.147186 |
| H | 2.606263 | -0.772074 | -1.036845 |
| H | 2.559137 | -0.967681 | 0.706575 |
| C | 1.743138 | 0.960946 | 0.046295 |
| H | 2.242266 | 1.568538 | -0.714665 |
| H | 2.133579 | 1.291146 | 1.015059 |

5rIM1

SCF energy in gas phase: -707.671142

Free energy in Et₂O : -707.472164

Enthalpy in Et₂O : -707.405227

| | | | |
|---|----------|----------|-----------|
| C | 3.651345 | 0.736198 | 0.975264 |
| C | 2.925277 | 0.276347 | -1.262365 |
| H | 2.718244 | 1.298697 | -1.605941 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.792834 | -2.480119 | 1.377699 |
| C | 0.041712 | -2.216065 | -0.707253 |
| H | 0.952976 | -2.169736 | -1.286945 |
| C | -1.287963 | -2.140868 | -1.216948 |
| H | -1.568773 | -2.044903 | -2.257994 |
| C | -2.185020 | -2.283856 | -0.119645 |
| H | -3.265411 | -2.293141 | -0.178548 |
| C | -2.729541 | 1.803361 | 0.775466 |
| H | -3.061401 | 1.877486 | 1.803417 |
| C | -1.640894 | 2.503538 | 0.203091 |
| H | -0.986561 | 3.188655 | 0.724553 |
| C | -1.531699 | 2.127096 | -1.159650 |
| H | -0.802207 | 2.501854 | -1.865368 |
| C | -2.559123 | 1.179313 | -1.434207 |
| H | -2.769949 | 0.725760 | -2.393981 |
| C | -3.301017 | 0.978727 | -0.233028 |
| H | -4.167637 | 0.340927 | -0.119194 |
| H | 3.633897 | 1.830986 | 0.881400 |
| H | 3.622384 | 0.503478 | 2.044605 |
| C | 4.455507 | 0.021157 | -1.237436 |
| H | 4.985752 | 0.737853 | -1.873096 |
| H | 4.700537 | -0.974038 | -1.623582 |
| C | 4.881790 | 0.154168 | 0.255921 |
| H | 5.778492 | 0.769195 | 0.383960 |
| H | 5.117463 | -0.834419 | 0.667655 |

5rTS1

SCF energy in gas phase: -707.623593

Free energy in Et₂O : -707.419214

Enthalpy in Et₂O : -707.355786

| | | | |
|---|-----------|----------|----------|
| C | -3.477231 | 0.040172 | 0.852018 |
|---|-----------|----------|----------|

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | -1.802961 | 0.472157 | -1.184629 | | | | |
| H | -1.038934 | 0.051605 | -1.846039 | C | 3.307558 | -0.502736 | 0.780501 |
| H | -1.828342 | 1.548013 | -1.364413 | C | 1.180170 | -0.598391 | -1.595656 |
| C | -2.003474 | 0.459678 | 0.844121 | H | 0.648091 | -0.339255 | -2.523276 |
| C | -1.145543 | -0.335931 | 1.694224 | H | 1.255666 | -1.693044 | -1.609307 |
| H | -1.471264 | -1.364055 | 1.825124 | C | 1.913644 | -0.832975 | 1.243792 |
| C | 0.065495 | 0.084064 | 2.380319 | C | 1.196772 | -0.017779 | 2.091529 |
| H | -1.878578 | 1.538131 | 0.962030 | H | 1.629369 | 0.963330 | 2.290637 |
| H | 0.116274 | 1.112582 | 2.739882 | C | -0.161296 | -0.229674 | 2.477823 |
| H | 0.453424 | -0.621903 | 3.110921 | H | 1.579415 | -1.862281 | 1.097978 |
| Zr | 0.559670 | -0.026033 | 0.134088 | H | -0.461097 | -1.256726 | 2.672524 |
| C | 1.847072 | 2.109097 | 0.874399 | H | -0.605756 | 0.482132 | 3.167422 |
| H | 2.034936 | 2.246013 | 1.929398 | Zr | -0.410582 | 0.010291 | 0.077608 |
| C | 0.701294 | 2.549805 | 0.160039 | C | -2.424969 | -1.470712 | 0.797898 |
| H | -0.127561 | 3.110668 | 0.571143 | H | -2.792141 | -1.360396 | 1.808441 |
| C | 0.878538 | 2.197020 | -1.211267 | C | -1.426669 | -2.389261 | 0.359980 |
| H | 0.196751 | 2.419027 | -2.020918 | H | -0.909177 | -3.110077 | 0.979733 |
| C | 2.111504 | 1.526100 | -1.334503 | C | -1.264933 | -2.226197 | -1.035140 |
| H | 2.528309 | 1.125052 | -2.249363 | H | -0.591510 | -2.785809 | -1.666718 |
| C | 2.705254 | 1.455960 | -0.040247 | C | -2.122871 | -1.183817 | -1.461579 |
| H | 3.661420 | 1.009767 | 0.199857 | H | -2.228463 | -0.824147 | -2.476401 |
| C | 1.941637 | -2.120573 | 0.610513 | C | -2.856786 | -0.733824 | -0.326623 |
| H | 2.586393 | -2.131342 | 1.478311 | H | -3.616460 | 0.035874 | -0.325566 |
| C | 0.613381 | -2.614976 | 0.551168 | C | -0.478816 | 2.477131 | 0.938321 |
| H | 0.061109 | -3.036665 | 1.378690 | H | -0.393030 | 2.663649 | 1.999464 |
| C | 0.132222 | -2.446567 | -0.769969 | C | 0.592950 | 2.423983 | 0.007305 |
| H | -0.855216 | -2.712582 | -1.124522 | H | 1.640429 | 2.571560 | 0.231700 |
| C | 1.164837 | -1.854743 | -1.543283 | C | 0.047803 | 2.175271 | -1.277449 |
| H | 1.114010 | -1.615199 | -2.597866 | H | 0.605624 | 2.090083 | -2.198092 |
| C | 2.288424 | -1.661712 | -0.693646 | C | -1.355009 | 2.046514 | -1.138471 |
| H | 3.248410 | -1.266312 | -0.993034 | H | -2.058451 | 1.865574 | -1.939843 |
| H | -3.526972 | -1.035690 | 1.062823 | C | -1.681162 | 2.233491 | 0.237015 |
| H | -3.971335 | 0.547068 | 1.689521 | H | -2.672825 | 2.211376 | 0.668274 |
| C | -3.146261 | -0.162482 | -1.522701 | H | 3.508341 | 0.555434 | 0.997769 |
| H | -3.069404 | -1.258009 | -1.481109 | H | 4.033170 | -1.076242 | 1.377815 |
| H | -3.454306 | 0.092099 | -2.546024 | C | 2.620673 | -0.065963 | -1.669129 |
| C | -4.157477 | 0.316547 | -0.485045 | H | 2.671293 | 1.018250 | -1.488412 |
| H | -5.125270 | -0.190457 | -0.562976 | H | 3.017255 | -0.207833 | -2.687165 |
| H | -4.340903 | 1.391837 | -0.614019 | C | 3.582271 | -0.774794 | -0.707368 |
| | | | | H | 4.616241 | -0.477166 | -0.924553 |
| | | | | H | 3.531313 | -1.857552 | -0.893249 |

5rIM2

SCF energy in gas phase: -707.672493

Free energy in Et₂O : -707.466986

Enthalpy in Et₂O : -707.403528

5rIM3

SCF energy in gas phase: -707.659814

Free energy in Et₂O : -707.4543

Enthalpy in Et₂O : -707.390712

| | | | |
|----|-----------|-----------|-----------|
| C | -3.458471 | 0.095481 | -1.083254 |
| C | -3.051878 | 0.062130 | 0.402139 |
| H | -3.022859 | 1.057159 | 0.858076 |
| H | -3.795689 | -0.508706 | 0.980489 |
| C | -1.729795 | -0.704807 | 0.439521 |
| C | -0.929099 | -0.888661 | 1.610306 |
| H | -0.425426 | -1.853306 | 1.691438 |
| C | -1.391947 | -0.360042 | 2.952359 |
| H | -0.573958 | -0.375235 | 3.679936 |
| H | -2.213376 | -0.959982 | 3.374727 |
| H | -1.752544 | 0.671598 | 2.891115 |
| Zr | 0.498113 | 0.041136 | -0.091875 |
| C | 1.945142 | -1.806650 | -1.235459 |
| H | 1.646515 | -2.190496 | -2.202162 |
| C | 1.551576 | -2.319352 | 0.030012 |
| H | 0.920340 | -3.182035 | 0.195629 |
| C | 2.187625 | -1.544171 | 1.043459 |
| H | 2.116844 | -1.703301 | 2.110302 |
| C | 2.963059 | -0.552621 | 0.396406 |
| H | 3.577872 | 0.190844 | 0.886181 |
| C | 2.811410 | -0.711784 | -1.012009 |
| H | 3.285154 | -0.112113 | -1.777586 |
| C | 0.183488 | 2.226406 | -1.334849 |
| H | -0.073748 | 2.222498 | -2.385277 |
| C | -0.730400 | 2.239359 | -0.239364 |
| H | -1.805293 | 2.273303 | -0.317512 |
| C | 0.021754 | 2.315124 | 0.970739 |
| H | -0.378622 | 2.364920 | 1.973135 |
| C | 1.392798 | 2.348695 | 0.618862 |
| H | 2.221910 | 2.398404 | 1.312670 |
| C | 1.494787 | 2.293881 | -0.795308 |
| H | 2.414175 | 2.301124 | -1.364902 |
| H | -3.032795 | 0.975722 | -1.578621 |
| H | -4.542413 | 0.135724 | -1.228155 |
| C | -2.828545 | -1.178275 | -1.673086 |
| H | -2.678589 | -1.126389 | -2.756670 |
| H | -3.466613 | -2.046467 | -1.468047 |
| C | -1.519190 | -1.348374 | -0.883008 |
| H | -0.677289 | -0.801602 | -1.578013 |
| H | -1.141979 | -2.375157 | -0.866558 |

5rTS2

SCF energy in gas phase: -707.599101

Free energy in Et₂O : -707.396602

Enthalpy in Et₂O : -707.330858

| | | | |
|----|-----------|-----------|-----------|
| C | -3.345798 | 0.684525 | -0.969162 |
| C | -2.989080 | 0.107940 | 0.402636 |
| H | -3.071368 | 0.860169 | 1.196864 |
| H | -3.712520 | -0.681793 | 0.653247 |
| C | -1.588645 | -0.457636 | 0.360422 |
| C | -1.160377 | -1.411702 | 1.282538 |
| H | -0.272798 | -2.010394 | 1.088901 |
| C | -1.992823 | -1.959847 | 2.421708 |
| H | -1.348770 | -2.347241 | 3.217430 |
| H | -2.641436 | -2.788074 | 2.097550 |
| H | -2.640247 | -1.196269 | 2.863697 |
| Zr | 0.475237 | 0.041156 | 0.088864 |
| C | 1.875208 | -1.298366 | -1.657609 |
| H | 1.554465 | -1.248350 | -2.690390 |
| C | 1.439743 | -2.250708 | -0.692397 |
| H | 0.725312 | -3.045324 | -0.862429 |
| C | 2.135443 | -1.994249 | 0.518224 |
| H | 2.046648 | -2.555117 | 1.439926 |
| C | 3.002375 | -0.893872 | 0.301892 |
| H | 3.675647 | -0.466389 | 1.033352 |
| C | 2.854341 | -0.478124 | -1.046397 |
| H | 3.388012 | 0.333299 | -1.522711 |
| C | 0.019256 | 2.489501 | -0.551567 |
| H | -0.532459 | 2.715811 | -1.454083 |
| C | -0.531689 | 2.294816 | 0.744720 |
| H | -1.576100 | 2.364651 | 1.006252 |
| C | 0.539859 | 2.043168 | 1.648576 |
| H | 0.453032 | 1.882071 | 2.714266 |
| C | 1.752007 | 2.111158 | 0.906566 |
| H | 2.746665 | 1.969416 | 1.306446 |
| C | 1.430254 | 2.383415 | -0.444742 |
| H | 2.134775 | 2.490732 | -1.258264 |
| H | -2.841783 | 1.646502 | -1.124107 |
| H | -4.422765 | 0.863001 | -1.066006 |
| C | -2.832904 | -0.340537 | -1.986152 |
| H | -3.008269 | 0.003948 | -3.014268 |
| H | -3.409142 | -1.267117 | -1.862957 |
| C | -1.349246 | -0.621364 | -1.741499 |
| H | -0.739916 | 0.035529 | -2.367912 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -1.064022 | -1.654016 | -1.935920 | C | -0.132450 | -1.069339 | -2.025451 |
| | | | | H | -0.235387 | -0.300276 | -2.801172 |
| | | | | H | 0.666832 | -1.737676 | -2.379507 |

5rIM4

SCF energy in gas phase: -707.660793

Free energy in Et₂O : -707.456293

Enthalpy in Et₂O : -707.388354

| | | | |
|----|-----------|-----------|-----------|
| C | -2.678379 | -0.997327 | -1.523661 |
| C | -2.722402 | -0.570618 | -0.038525 |
| H | -3.740032 | -0.213716 | 0.165599 |
| H | -2.604072 | -1.475487 | 0.576469 |
| C | -1.692909 | 0.473931 | 0.385728 |
| C | -2.065934 | 1.586160 | 1.059139 |
| H | -1.294705 | 2.308971 | 1.334799 |
| C | -3.432464 | 2.015814 | 1.542731 |
| H | -3.694347 | 3.002018 | 1.136392 |
| H | -3.436068 | 2.124631 | 2.635837 |
| H | -4.232877 | 1.322508 | 1.277648 |
| Zr | 0.487745 | -0.033445 | -0.069987 |
| C | 1.307755 | -2.464609 | 0.457119 |
| H | 1.520934 | -3.130694 | -0.367637 |
| C | 0.067434 | -2.348416 | 1.134814 |
| H | -0.826674 | -2.914605 | 0.918371 |
| C | 0.204567 | -1.371492 | 2.151853 |
| H | -0.569982 | -1.051839 | 2.834763 |
| C | 1.531597 | -0.872968 | 2.100517 |
| H | 1.956121 | -0.126687 | 2.759118 |
| C | 2.216511 | -1.555331 | 1.053457 |
| H | 3.251917 | -1.414188 | 0.772490 |
| C | 1.266571 | 1.730177 | -1.831663 |
| H | 0.965803 | 1.604137 | -2.861505 |
| C | 0.553050 | 2.444188 | -0.837425 |
| H | -0.392802 | 2.947829 | -0.970494 |
| C | 1.300674 | 2.375046 | 0.369924 |
| H | 1.030066 | 2.827004 | 1.315649 |
| C | 2.475133 | 1.621499 | 0.116538 |
| H | 3.253740 | 1.397705 | 0.833242 |
| C | 2.447137 | 1.209802 | -1.241502 |
| H | 3.200087 | 0.614478 | -1.742464 |
| H | -2.738480 | -0.099582 | -2.155283 |
| H | -3.589973 | -1.574900 | -1.728120 |
| C | -1.466242 | -1.840574 | -1.958238 |
| H | -1.693580 | -2.255855 | -2.952765 |
| H | -1.384218 | -2.711647 | -1.294091 |