

Electronic Supplementary Information

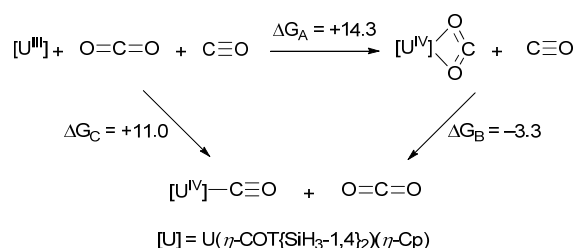
Computational Insight into the Reductive Oligomerisation of CO at Uranium (III) Mixed-Sandwich Complexes

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Supplementary Information

Computational Details:

DFT Calculations were run with the Gaussian 03, Revision E.01,¹ via the B3PW91 method.² 6-31G** basis sets were used for C, H and O and the Stuttgart-Dresden relativistic Effective Core Potential (ECP) and associated basis sets,³ for Si and U (small core). Basis sets augmented with d-polarisation function⁴ in the case of Si. Large core description of U adopted the ECP80MWB quasi-relativistic pseudopotential⁵ with associated ECP80MWB-AVTZ basis sets, augmented with a single f-polarisation function from ECP80MWB2f. Geometry optimisations were performed without constraints. Minima and transition states were subjected to analytical frequency calculations and transition states further characterised through IRC calculations.⁶



ESI Scheme 1 Indirect calculation of ΔG_{C} , the free energies of binding CO to and oxidation of U to give **2**. Energies in kcal.mol⁻¹.

Computed Geometries:

1 / small core

SCF (B3PW91) Energy = -990.305969
 Enthalpy 0K = -990.058645
 Enthalpy 298K = -990.040544
 Free Energy 298K = -990.109759

| | | | |
|----|-----------|-----------|-----------|
| U | -0.251894 | -0.050537 | -1.159708 |
| C | -2.457109 | 1.367284 | -0.729280 |
| C | -2.248340 | 1.400916 | -2.139950 |
| C | -1.989423 | 0.446094 | -3.149002 |
| C | -1.776926 | -0.951590 | -3.179400 |
| C | -1.733977 | -1.982053 | -2.213385 |
| C | -1.931665 | -2.070895 | -0.803485 |
| C | -2.262204 | -1.098746 | 0.187065 |
| C | -2.476703 | 0.299965 | 0.217276 |
| C | 1.732958 | 1.325103 | 0.106362 |
| C | 2.259394 | 0.972385 | -1.163710 |
| C | 1.577834 | 0.135486 | 0.862072 |
| C | 2.011780 | -0.952994 | 0.063896 |
| C | 2.432463 | -0.437788 | -1.189530 |
| H | -2.259957 | -1.508093 | 1.196221 |
| H | -2.591299 | 0.648325 | 1.242714 |
| Si | -2.790758 | 3.063434 | 0.029120 |
| H | -2.333943 | 3.098216 | 1.454096 |
| H | -2.221758 | 2.413471 | -2.541145 |
| H | -1.826506 | 0.909378 | -4.120267 |
| H | -1.490214 | -1.303931 | -4.168374 |

| | | | |
|----|-----------|-----------|-----------|
| H | -1.409635 | -2.922730 | -2.656690 |
| H | -3.027689 | -4.570765 | -0.143887 |
| Si | -1.732089 | -3.818576 | -0.118048 |
| H | -1.261915 | -3.772629 | 1.302114 |
| H | -0.745836 | -4.590356 | -0.938793 |
| H | 2.858299 | -1.013202 | -2.004065 |
| H | 2.046929 | -1.992217 | 0.369893 |
| H | 1.215147 | 0.072237 | 1.881280 |
| H | 2.530763 | 1.662632 | -1.954871 |
| H | 1.519108 | 2.330370 | 0.450873 |
| H | -4.251822 | 3.395145 | 0.012518 |
| H | -2.077728 | 4.129802 | -0.743208 |

2

SCF (B3PW91) Energy = -664.011759
 Enthalpy 0K = -663.757014
 Enthalpy 298K = -663.736141
 Free Energy 298K = -663.809808

| | | | |
|---|-----------|-----------|-----------|
| U | -0.275910 | -0.251774 | -0.349300 |
| C | -2.488214 | 1.285338 | -0.481036 |
| C | -1.901470 | 1.452073 | -1.776374 |
| C | -1.449383 | 0.582888 | -2.788762 |
| C | -1.262849 | -0.810899 | -2.924829 |
| C | -1.469873 | -1.938109 | -2.096573 |
| C | -2.134459 | -2.168234 | -0.850538 |
| C | -2.758034 | -1.281942 | 0.070735 |

| | | | |
|----|-----------|-----------|-----------|
| C | -2.896817 | 0.120304 | 0.230188 |
| C | 1.853752 | 1.474788 | -0.630220 |
| C | 1.957758 | 0.593658 | -1.738537 |
| C | 2.122522 | 0.728322 | 0.546467 |
| C | 2.397163 | -0.618005 | 0.159989 |
| C | 2.295972 | -0.696686 | -1.252636 |
| C | -0.018357 | -0.892567 | 2.006068 |
| O | 0.096543 | -1.187651 | 3.129108 |
| H | -3.115631 | -1.796720 | 0.960738 |
| H | -3.315501 | 0.351293 | 1.207918 |
| Si | -2.957708 | 2.909307 | 0.364081 |
| H | -2.981426 | 2.735388 | 1.848470 |
| H | -1.716403 | 2.494197 | -2.030694 |
| H | -1.020870 | 1.129869 | -3.625696 |
| H | -0.715950 | -1.064663 | -3.829869 |
| H | -1.049186 | -2.842227 | -2.533568 |
| H | -3.366674 | -4.674332 | -1.034879 |
| Si | -2.214359 | -3.991982 | -0.363455 |
| H | -2.387729 | -4.129720 | 1.114295 |
| H | -0.963137 | -4.692887 | -0.791833 |
| H | 2.471708 | -1.578104 | -1.857037 |
| H | 2.688001 | -1.421405 | 0.824234 |
| H | 2.170174 | 1.120645 | 1.554004 |
| H | 1.820106 | 0.863650 | -2.777969 |
| H | 1.633232 | 2.534205 | -0.678310 |
| H | -4.315101 | 3.367226 | -0.072774 |
| H | -1.978433 | 3.980988 | 0.000172 |

3

SCF (B3PW91) Energy = -1328.051587
Enthalpy 0K = -1327.539478
Enthalpy 298K = -1327.496862
Free Energy 298K = -1327.616356

| | | | |
|----|-----------|-----------|----------|
| U | 0.059813 | 0.078533 | 2.375749 |
| C | 2.217806 | 0.334027 | 4.149986 |
| H | 2.819538 | 1.217931 | 4.355702 |
| C | 2.720601 | -0.450179 | 3.076596 |
| C | 2.233756 | -1.619754 | 2.434930 |
| C | 1.089777 | -2.455263 | 2.538696 |
| H | 1.107955 | -3.230484 | 1.774264 |
| C | -0.098461 | -2.487686 | 3.317866 |
| C | -0.574721 | -1.648088 | 4.363760 |
| C | -0.062518 | -0.536272 | 5.072757 |
| C | 1.087107 | 0.275373 | 4.988361 |
| H | 1.043169 | 1.118366 | 5.673975 |
| H | -0.778648 | -0.155084 | 5.797072 |
| H | -1.581142 | -1.900404 | 4.693106 |
| Si | -1.272262 | -3.902092 | 2.887395 |
| H | 2.863263 | -1.936770 | 1.604759 |
| Si | 4.383292 | 0.156441 | 2.419729 |
| C | -1.463978 | 2.074825 | 1.244266 |
| C | -2.435796 | 1.237934 | 1.866241 |
| C | -2.271422 | 1.354757 | 3.263322 |
| C | -1.220004 | 2.280218 | 3.507320 |
| C | -0.723372 | 2.730181 | 2.261207 |
| H | 0.068218 | 3.453215 | 2.110013 |
| H | -0.870625 | 2.597293 | 4.481190 |
| H | -2.857369 | 0.847201 | 4.018467 |
| H | -3.187444 | 0.647391 | 1.359481 |
| H | -1.357454 | 2.236156 | 0.181109 |

| | | | |
|----|-----------|-----------|-----------|
| C | -1.012052 | -0.840151 | 0.340246 |
| O | -1.577050 | -1.305853 | -0.603454 |
| U | -0.021991 | -0.076012 | -2.354620 |
| C | 0.135945 | 2.490235 | -3.296763 |
| H | 1.618566 | 1.903140 | -4.672142 |
| C | -1.052243 | 2.457697 | -2.517514 |
| C | -2.196129 | 1.622075 | -2.413679 |
| C | -2.682908 | 0.452461 | -3.055327 |
| H | -2.825603 | 1.939022 | -1.583455 |
| C | -2.180116 | -0.331679 | -4.128767 |
| C | -1.049496 | -0.272882 | -4.967243 |
| C | 0.100032 | 0.538886 | -5.051723 |
| C | 0.612197 | 1.650715 | -4.342720 |
| H | -1.005532 | -1.115854 | -5.652881 |
| H | 0.816132 | 0.157799 | -5.776119 |
| H | -2.781765 | -1.215648 | -4.334442 |
| Si | -4.345491 | -0.154337 | -2.398358 |
| H | -1.070467 | 3.232942 | -1.753108 |
| C | 2.473834 | -1.235284 | -1.845608 |
| C | 1.502202 | -2.072227 | -1.223411 |
| C | 0.761417 | -2.727635 | -2.240189 |
| C | 1.257720 | -2.277622 | -3.486414 |
| C | 2.309150 | -1.352109 | -3.242651 |
| H | 2.894906 | -0.844527 | -3.997927 |
| H | 0.908130 | -2.594708 | -4.460205 |
| H | -0.030083 | -3.450730 | -2.088821 |
| H | 1.396040 | -2.233656 | -0.160232 |
| H | 3.225574 | -0.644716 | -1.339011 |
| C | 1.050219 | 0.842689 | -0.319298 |
| O | 1.615171 | 1.308237 | 0.624485 |
| H | 4.569502 | -0.254552 | 0.992569 |
| H | 4.486572 | 1.644395 | 2.527652 |
| H | 5.512657 | -0.435841 | 3.206653 |
| H | -2.694461 | -3.482150 | 3.087397 |
| H | -1.073259 | -4.329586 | 1.467553 |
| H | -1.022858 | -5.091553 | 3.763236 |
| H | -4.448645 | -1.642297 | -2.506317 |
| H | -4.531655 | 0.256593 | -0.971173 |
| H | -5.474969 | 0.437864 | -3.185181 |
| Si | 1.309630 | 3.904746 | -2.866334 |
| H | 2.731847 | 3.485012 | -3.066643 |
| H | 1.059913 | 5.094297 | -3.741965 |
| H | 1.110840 | 4.332035 | -1.446398 |

3-4-TS

SCF (B3PW91) Energy = -1328.050851
Enthalpy 0K = -1327.539328
Enthalpy 298K = -1327.497318
Free Energy 298K = -1327.616378
Negative frequency = -69.5 cm⁻¹

| | | | |
|---|-----------|-----------|----------|
| U | 0.058009 | 0.108579 | 2.494350 |
| C | 2.156102 | 0.287619 | 4.309291 |
| H | 2.751457 | 1.160552 | 4.572465 |
| C | 2.689438 | -0.449237 | 3.213711 |
| C | 2.225388 | -1.598045 | 2.522387 |
| C | 1.080831 | -2.437445 | 2.557580 |
| H | 1.120831 | -3.171266 | 1.754383 |
| C | -0.137536 | -2.495401 | 3.284252 |
| C | -0.651323 | -1.696860 | 4.346806 |
| C | -0.160653 | -0.611380 | 5.109442 |

| | | | |
|----|-----------|-----------|-----------|
| C | 1.001688 | 0.192454 | 5.109030 |
| H | 0.931361 | 1.007442 | 5.825219 |
| H | -0.901585 | -0.251074 | 5.819228 |
| H | -1.669958 | -1.955357 | 4.629566 |
| Si | -1.300300 | -3.889207 | 2.754190 |
| H | 2.880117 | -1.882569 | 1.700403 |
| Si | 4.361562 | 0.198370 | 2.614533 |
| C | -1.380179 | 2.124336 | 1.303332 |
| C | -2.382373 | 1.298387 | 1.886519 |
| C | -2.273822 | 1.417375 | 3.289300 |
| C | -1.220671 | 2.331120 | 3.574894 |
| C | -0.672160 | 2.773323 | 2.348197 |
| H | 0.130279 | 3.490346 | 2.226060 |
| H | -0.909487 | 2.649772 | 4.561480 |
| H | -2.897527 | 0.920392 | 4.021244 |
| H | -3.109795 | 0.704730 | 1.348352 |
| H | -1.225819 | 2.276003 | 0.243759 |
| C | -0.765189 | -0.713842 | 0.253570 |
| O | -1.418855 | -1.267321 | -0.598717 |
| U | -0.011655 | -0.092283 | -2.402152 |
| C | 0.118100 | 2.469855 | -3.372264 |
| H | 1.532744 | 1.898303 | -4.819472 |
| C | -1.032810 | 2.435429 | -2.536194 |
| C | -2.175637 | 1.603501 | -2.393716 |
| C | -2.685002 | 0.436087 | -3.022743 |
| H | -2.772790 | 1.916771 | -1.538498 |
| C | -2.222106 | -0.350556 | -4.113684 |
| C | -1.131130 | -0.288978 | -5.003661 |
| C | 0.005659 | 0.530888 | -5.139811 |
| C | 0.542375 | 1.640933 | -4.447279 |
| H | -1.117164 | -1.129596 | -5.693662 |
| H | 0.688093 | 0.161583 | -5.901909 |
| H | -2.830778 | -1.235819 | -4.291879 |
| Si | -4.318909 | -0.175965 | -2.306865 |
| H | -1.016581 | 3.207608 | -1.768662 |
| C | 2.563462 | -1.171279 | -2.113053 |
| C | 1.698695 | -1.965524 | -1.304994 |
| C | 0.857344 | -2.721596 | -2.164132 |
| C | 1.178789 | -2.370813 | -3.493895 |
| C | 2.228176 | -1.409152 | -3.462198 |
| H | 2.700469 | -0.957950 | -4.324607 |
| H | 0.717597 | -2.774226 | -4.386186 |
| H | 0.108620 | -3.439555 | -1.854798 |
| H | 1.736909 | -2.043971 | -0.227322 |
| H | 3.350875 | -0.520957 | -1.755301 |
| C | 1.113529 | 0.808379 | -0.416501 |
| O | 1.622332 | 1.185010 | 0.595391 |
| H | 4.601977 | -0.214803 | 1.198229 |
| H | 4.418105 | 1.688646 | 2.724362 |
| H | 5.470081 | -0.361131 | 3.452491 |
| H | -2.725092 | -3.458817 | 2.900623 |
| H | -1.030637 | -4.278586 | 1.336972 |
| H | -1.097870 | -5.097568 | 3.615361 |
| H | -4.420747 | -1.665609 | -2.397912 |
| H | -4.465523 | 0.243474 | -0.876769 |
| H | -5.481242 | 0.401168 | -3.057452 |
| Si | 1.320672 | 3.867097 | -2.974762 |
| H | 2.731503 | 3.440337 | -3.235931 |
| H | 1.051971 | 5.074497 | -3.820957 |
| H | 1.188272 | 4.280373 | -1.542029 |

4

| | | | |
|-----------------------|--------------|-----------|-----------|
| SCF (B3PW91) Energy = | -1328.069475 | | |
| Enthalpy 0K = | -1327.556450 | | |
| Enthalpy 298K = | -1327.514034 | | |
| Free Energy 298K = | -1327.637663 | | |
| U | -0.168548 | 0.346168 | 0.114506 |
| C | -0.041886 | 0.197801 | 2.849076 |
| Si | 1.419117 | 0.311201 | 4.042496 |
| C | -0.365912 | -1.116357 | 2.426833 |
| C | -1.273825 | -1.720673 | 1.518563 |
| C | -2.274528 | -1.282303 | 0.610407 |
| Si | -3.060619 | -2.654005 | -0.424201 |
| C | -2.837632 | 0.007972 | 0.366629 |
| C | -2.645895 | 1.295343 | 0.908678 |
| C | -1.763406 | 1.895014 | 1.839616 |
| C | -0.653028 | 1.464172 | 2.584764 |
| H | -0.136923 | 2.298817 | 3.057179 |
| H | -1.884393 | 2.975363 | 1.872301 |
| H | -3.270745 | 2.035130 | 0.413459 |
| H | -3.568733 | 0.016404 | -0.439909 |
| H | -1.059623 | -2.782904 | 1.417617 |
| H | 0.333264 | -1.857001 | 2.810594 |
| C | 1.566312 | 1.832843 | -1.473149 |
| C | 0.809105 | 1.050646 | -2.385178 |
| C | -0.525559 | 1.531918 | -2.372694 |
| C | -0.592858 | 2.602482 | -1.448141 |
| C | 0.702666 | 2.788000 | -0.889254 |
| H | 0.982241 | 3.545502 | -0.167306 |
| H | -1.469703 | 3.195645 | -1.224796 |
| H | -1.342142 | 1.160415 | -2.979712 |
| H | 1.188840 | 0.262889 | -3.021628 |
| H | 2.620403 | 1.715873 | -1.256836 |
| C | 0.962234 | -1.697162 | -1.005330 |
| O | 1.011188 | -2.707999 | -1.745268 |
| U | 3.444360 | -3.533265 | -1.351906 |
| C | 6.122946 | -3.255342 | -1.576577 |
| H | 6.509418 | -5.291204 | -1.661514 |
| C | 5.590819 | -1.947995 | -1.796603 |
| C | 4.609085 | -1.467783 | -2.704539 |
| C | 3.695529 | -2.032806 | -3.631717 |
| H | 4.416835 | -0.403630 | -2.583517 |
| C | 3.344699 | -3.330226 | -4.083923 |
| C | 3.919084 | -4.616367 | -3.835210 |
| C | 2.307112 | -1.489045 | -0.248084 |
| C | 5.014486 | -5.089021 | -3.091498 |
| C | 5.904110 | -4.527683 | -2.144703 |
| H | 3.384851 | -5.428763 | -4.325809 |
| H | 5.109600 | -6.171132 | -3.143630 |
| Si | 1.895722 | -3.382280 | -5.295554 |
| H | 3.018355 | -1.267281 | -4.005747 |
| Si | 6.400233 | -0.613929 | -0.730949 |
| H | 6.847893 | -3.296912 | -0.765569 |
| C | 3.932969 | -5.650251 | 0.392788 |
| C | 3.594388 | -4.562434 | 1.229421 |
| C | 2.222366 | -4.262478 | 1.019273 |
| C | 1.711258 | -5.181123 | 0.064537 |
| C | 2.766903 | -6.032574 | -0.331460 |
| H | 2.697329 | -6.850889 | -1.037582 |
| H | 0.693490 | -5.214732 | -0.303517 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.652395 | -3.509428 | 1.546446 |
| H | 4.258083 | -4.052775 | 1.917115 |
| H | 4.901986 | -6.127801 | 0.329834 |
| O | 2.259066 | -0.474616 | 0.488064 |
| H | 5.509767 | 0.580549 | -0.624296 |
| H | 6.697674 | -1.147280 | 0.634827 |
| H | 7.699005 | -0.173754 | -1.334759 |
| H | 1.037148 | -4.580184 | -5.038979 |
| H | 1.075886 | -2.138160 | -5.183478 |
| H | 2.393999 | -3.485262 | -6.705368 |
| H | -3.355884 | -2.161888 | -1.805669 |
| H | -2.154502 | -3.839518 | -0.492518 |
| H | -4.357795 | -3.094195 | 0.183202 |
| H | 0.933957 | 0.457366 | 5.453053 |
| H | 2.255083 | -0.924297 | 3.962910 |
| H | 2.258143 | 1.511181 | 3.735358 |

4-5-TS

SCF (B3PW91) Energy = -1328.059296

Enthalpy 0K = -1327.547788

Enthalpy 298K = -1327.505962

Free Energy 298K = -1327.626619

Negative frequency = -697.8 cm⁻¹

| | | | |
|----|-----------|-----------|-----------|
| U | 0.032682 | 0.353386 | 0.220539 |
| C | -0.516005 | 0.232734 | 2.894289 |
| Si | 0.590133 | 0.434660 | 4.414065 |
| C | -0.655262 | -1.104520 | 2.440978 |
| C | -1.292306 | -1.766912 | 1.360385 |
| C | -2.076864 | -1.403311 | 0.233330 |
| Si | -2.625170 | -2.846564 | -0.859585 |
| C | -2.598535 | -0.145115 | -0.201308 |
| C | -2.607542 | 1.161855 | 0.323470 |
| C | -1.994776 | 1.814642 | 1.419969 |
| C | -1.110047 | 1.454303 | 2.454764 |
| H | -0.772465 | 2.325076 | 3.014076 |
| H | -2.157608 | 2.889477 | 1.387607 |
| H | -3.110852 | 1.863611 | -0.337175 |
| H | -3.114993 | -0.199163 | -1.158393 |
| H | -1.024153 | -2.821755 | 1.351328 |
| H | -0.022679 | -1.798364 | 2.990771 |
| C | 2.104982 | 1.761198 | -0.940685 |
| C | 1.383021 | 1.224684 | -2.038634 |
| C | 0.130897 | 1.886305 | -2.105938 |
| C | 0.079506 | 2.827948 | -1.048759 |
| C | 1.301169 | 2.751114 | -0.324917 |
| H | 1.580030 | 3.364959 | 0.522958 |
| H | -0.737905 | 3.506150 | -0.842035 |
| H | -0.640753 | 1.718799 | -2.847227 |
| H | 1.734144 | 0.462660 | -2.719769 |
| H | 3.093616 | 1.457190 | -0.622115 |
| C | 1.030972 | -1.880463 | -0.821511 |
| O | 0.878316 | -2.948498 | -1.464083 |
| U | 3.390935 | -3.485025 | -1.331538 |
| C | 6.003837 | -3.321680 | -1.996470 |
| H | 6.318213 | -5.371149 | -2.040750 |
| C | 5.479817 | -2.007037 | -2.189032 |
| C | 4.383732 | -1.532403 | -2.958122 |
| C | 3.323077 | -2.109861 | -3.702869 |
| H | 4.239220 | -0.458395 | -2.860590 |
| C | 2.864302 | -3.412375 | -4.024292 |

| | | | |
|----|-----------|-----------|-----------|
| C | 3.415646 | -4.707124 | -3.778511 |
| C | 2.224282 | -1.586368 | -0.033815 |
| C | 4.608587 | -5.187880 | -3.202106 |
| C | 5.661982 | -4.611199 | -2.459057 |
| H | 2.779404 | -5.520332 | -4.124623 |
| H | 4.659234 | -6.273988 | -3.206559 |
| Si | 1.236681 | -3.458691 | -4.985314 |
| H | 2.619256 | -1.339592 | -4.012189 |
| Si | 6.490558 | -0.654859 | -1.341614 |
| H | 6.848475 | -3.353233 | -1.310746 |
| C | 4.384079 | -5.238684 | 0.594961 |
| C | 3.896059 | -4.137824 | 1.332713 |
| C | 2.478999 | -4.125756 | 1.207072 |
| C | 2.095306 | -5.234563 | 0.406861 |
| C | 3.269597 | -5.917119 | 0.020164 |
| H | 3.316960 | -6.812169 | -0.587330 |
| H | 1.081736 | -5.503360 | 0.138395 |
| H | 1.807288 | -3.440435 | 1.706248 |
| H | 4.488405 | -3.432656 | 1.902398 |
| H | 5.421259 | -5.532491 | 0.501516 |
| O | 2.161898 | -0.693190 | 0.871607 |
| H | 5.641803 | 0.548231 | -1.085382 |
| H | 7.049857 | -1.159898 | -0.049087 |
| H | 7.642514 | -0.233486 | -2.201086 |
| H | 0.391522 | -4.608910 | -4.540237 |
| H | 0.491673 | -2.175722 | -4.813118 |
| H | 1.507412 | -3.644077 | -6.448360 |
| H | -2.547041 | -2.482670 | -2.307017 |
| H | -1.801095 | -4.058892 | -0.579868 |
| H | -4.056103 | -3.178451 | -0.559917 |
| H | -0.233738 | 0.486555 | 5.664209 |
| H | 1.537426 | -0.714931 | 4.524708 |
| H | 1.359278 | 1.715805 | 4.330805 |

5

SCF (B3PW91) Energy = -1328.089960

Enthalpy 0K = -1327.576503

Enthalpy 298K = -1327.533948

Free Energy 298K = -1327.658478

| | | | |
|----|-----------|-----------|-----------|
| U | -0.006578 | 0.526233 | 0.439385 |
| C | -0.529943 | 0.640231 | 3.100350 |
| Si | 0.593904 | 0.915828 | 4.594924 |
| C | -0.739819 | -0.720954 | 2.762685 |
| C | -1.382870 | -1.448773 | 1.728929 |
| C | -2.139089 | -1.146951 | 0.566524 |
| Si | -2.679341 | -2.654393 | -0.441178 |
| C | -2.666296 | 0.088833 | 0.069917 |
| C | -2.643302 | 1.427063 | 0.502262 |
| C | -1.948905 | 2.155324 | 1.496034 |
| C | -1.033901 | 1.850365 | 2.528676 |
| H | -0.632551 | 2.750331 | 2.991062 |
| H | -2.064096 | 3.228589 | 1.365602 |
| H | -3.155215 | 2.086587 | -0.194401 |
| H | -3.204340 | -0.020868 | -0.870165 |
| H | -1.114457 | -2.501409 | 1.786809 |
| H | -0.130071 | -1.391977 | 3.364183 |
| C | 1.972887 | 1.691282 | -1.083289 |
| C | 1.139589 | 1.031772 | -2.023573 |
| C | -0.098762 | 1.720120 | -2.073197 |
| C | -0.028373 | 2.805870 | -1.162366 |

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 1.252958 | 2.788993 | -0.550292 | C | 1.478063 | -2.139200 | 2.691674 |
| H | 1.623082 | 3.505973 | 0.172738 | C | 0.149436 | -2.546912 | 2.984717 |
| H | -0.806081 | 3.537028 | -0.986040 | Si | -0.559876 | -3.853072 | 1.817834 |
| H | -0.940190 | 1.475555 | -2.709547 | C | -0.717812 | -2.239842 | 4.082509 |
| H | 1.402905 | 0.157116 | -2.603268 | C | -0.625858 | -1.426476 | 5.224680 |
| H | 2.976499 | 1.396778 | -0.807578 | C | 0.273682 | -0.442029 | 5.697711 |
| C | 1.375103 | -2.105300 | -0.708286 | C | 1.509128 | 0.095395 | 5.272587 |
| O | 1.135477 | -3.089134 | -1.519136 | H | 1.809030 | 0.947393 | 5.880311 |
| U | 3.357026 | -3.811602 | -1.578113 | H | -0.135825 | 0.108328 | 6.541296 |
| C | 6.037687 | -3.407318 | -2.017064 | H | -1.546029 | -1.438124 | 5.804188 |
| H | 6.491216 | -5.416459 | -2.223314 | H | -1.689870 | -2.725157 | 4.011475 |
| C | 5.399241 | -2.128052 | -2.067620 | H | 1.841440 | -2.550649 | 1.752631 |
| C | 4.338093 | -1.636401 | -2.881360 | H | 3.267157 | -1.129429 | 2.547260 |
| C | 3.415175 | -2.191553 | -3.799993 | C | -1.407472 | 2.375212 | 2.255871 |
| H | 4.103756 | -0.592864 | -2.683021 | C | -2.260873 | 1.276531 | 1.978768 |
| C | 3.062759 | -3.480349 | -4.282146 | C | -2.674404 | 0.719262 | 3.214608 |
| C | 3.628120 | -4.769434 | -4.059918 | C | -2.077507 | 1.478360 | 4.255727 |
| C | 1.835463 | -1.452650 | 0.251691 | C | -1.295731 | 2.503536 | 3.662515 |
| C | 4.789209 | -5.240490 | -3.399208 | H | -0.733488 | 3.264007 | 4.191190 |
| C | 5.808265 | -4.661704 | -2.606050 | H | -2.216329 | 1.318406 | 5.316645 |
| H | 3.058832 | -5.583215 | -4.505718 | H | -3.344839 | -0.121086 | 3.343846 |
| H | 4.883492 | -6.321649 | -3.462718 | H | -2.546413 | 0.925108 | 0.995644 |
| Si | 1.526417 | -3.513463 | -5.384625 | H | -0.913651 | 2.996282 | 1.521007 |
| H | 2.693556 | -1.434996 | -4.102127 | C | -0.020858 | -0.156543 | -0.136602 |
| Si | 6.258416 | -0.814820 | -1.012968 | O | -0.606804 | -0.920018 | -1.010276 |
| H | 6.853356 | -3.448939 | -1.297296 | U | 0.078741 | -0.083626 | -3.045992 |
| C | 4.428235 | -5.113505 | 0.630756 | C | 0.276624 | 2.293304 | -4.306421 |
| C | 3.304984 | -4.403330 | 1.123810 | H | 1.024295 | 1.544664 | -6.094374 |
| C | 2.137589 | -5.005246 | 0.588579 | C | -0.521056 | 2.549009 | -3.145790 |
| C | 2.534550 | -6.092164 | -0.228963 | C | -1.714285 | 1.939119 | -2.674815 |
| C | 3.951387 | -6.158865 | -0.205200 | C | -2.507562 | 0.816321 | -3.021735 |
| H | 4.562498 | -6.894394 | -0.711808 | H | -2.050254 | 2.361174 | -1.730019 |
| H | 1.872298 | -6.765162 | -0.760661 | C | -2.460243 | -0.239727 | -3.968065 |
| H | 1.121080 | -4.680488 | 0.764240 | C | -1.591403 | -0.478575 | -5.078938 |
| H | 3.329112 | -3.555949 | 1.797910 | C | 0.767849 | 0.581974 | 0.474052 |
| H | 5.464972 | -4.912924 | 0.869217 | C | -0.552046 | 0.253833 | -5.705065 |
| O | 2.046631 | -0.462456 | 1.051924 | C | 0.196371 | 1.408362 | -5.402890 |
| H | 5.320539 | 0.309054 | -0.719529 | H | -1.784526 | -1.420575 | -5.588695 |
| H | 6.741321 | -1.416163 | 0.268360 | H | -0.156821 | -0.271241 | -6.571313 |
| H | 7.447491 | -0.259021 | -1.733809 | Si | -3.809339 | -1.548160 | -3.758217 |
| H | 0.722172 | -4.744917 | -5.111895 | H | -3.259625 | 0.644565 | -2.254371 |
| H | 0.691304 | -2.297261 | -5.152248 | Si | 0.070624 | 4.042293 | -2.146076 |
| H | 1.916946 | -3.542605 | -6.830901 | H | 1.150307 | 2.939195 | -4.376845 |
| H | -2.664329 | -2.340572 | -1.903048 | C | 2.699219 | -0.608565 | -2.342818 |
| H | -1.790881 | -3.817677 | -0.153080 | C | 2.017492 | -1.841650 | -2.184384 |
| H | -4.083740 | -3.030769 | -0.077453 | C | 1.657762 | -2.317317 | -3.470015 |
| H | -0.219521 | 1.095298 | 5.840237 | C | 2.122021 | -1.376884 | -4.427202 |
| H | 1.499282 | -0.255128 | 4.791791 | C | 2.765274 | -0.320504 | -3.730480 |
| H | 1.404974 | 2.159837 | 4.407561 | H | 3.244037 | 0.539434 | -4.181600 |

5-6-TS

SCF (B3PW91) Energy = -1328.089480

Enthalpy 0K = -1327.576205

Enthalpy 298K = -1327.534421

Free Energy 298K = -1327.656297

Negative frequency = -21.3 cm⁻¹

U 0.044930 0.161245 3.022138

C 2.446215 -0.235336 4.245529

Si 4.013305 0.819388 4.281756

C 2.411294 -1.208625 3.214453

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 1.478063 | -2.139200 | 2.691674 | H | 2.028294 | -1.464101 | -5.501796 |
| C | 0.149436 | -2.546912 | 2.984717 | H | 1.147548 | -3.248654 | -3.686259 |
| Si | -0.559876 | -3.853072 | 1.817834 | H | 1.792540 | -2.322548 | -1.242072 |
| C | -0.717812 | -2.239842 | 4.082509 | H | 3.108658 | -0.003419 | -1.543344 |
| C | -0.625858 | -1.426476 | 5.224680 | O | 1.303098 | 1.309667 | 1.400300 |
| C | 0.273682 | -0.442029 | 5.697711 | H | -0.506339 | 4.003075 | -0.770615 |
| C | 1.509128 | 0.095395 | 5.272587 | H | 1.564051 | 4.059107 | -2.077154 |
| H | 1.809030 | 0.947393 | 5.880311 | H | -0.369842 | 5.311263 | -2.807843 |
| H | -0.135825 | 0.108328 | 6.541296 | H | -3.284503 | -2.890169 | -4.161689 |
| H | -1.546029 | -1.438124 | 5.804188 | H | -4.276535 | -1.589989 | -2.340642 |
| H | -1.689870 | -2.725157 | 4.011475 | H | -4.983543 | -1.238716 | -4.634412 |
| H | 1.841440 | -2.550649 | 1.752631 | | | | |
| H | 3.267157 | -1.129429 | 2.547260 | | | | |
| C | -1.407472 | 2.375212 | 2.255871 | | | | |
| C | -2.260873 | 1.276531 | 1.978768 | | | | |
| C | -2.674404 | 0.719262 | 3.214608 | | | | |
| C | -2.077507 | 1.478360 | 4.255727 | | | | |
| C | -1.295731 | 2.503536 | 3.662515 | | | | |
| H | -0.733488 | 3.264007 | 4.191190 | | | | |
| H | -2.216329 | 1.318406 | 5.316645 | | | | |
| H | -3.344839 | -0.121086 | 3.343846 | | | | |
| H | -2.546413 | 0.925108 | 0.995644 | | | | |
| H | -0.913651 | 2.996282 | 1.521007 | | | | |
| C | -0.020858 | -0.156543 | -0.136602 | | | | |
| O | -0.606804 | -0.920018 | -1.010276 | | | | |
| U | 0.078741 | -0.083626 | -3.045992 | | | | |
| C | 0.276624 | 2.293304 | -4.306421 | | | | |
| H | 1.024295 | 1.544664 | -6.094374 | | | | |
| C | -0.521056 | 2.549009 | -3.145790 | | | | |
| C | -1.714285 | 1.939119 | -2.674815 | | | | |
| C | -2.507562 | 0.816321 | -3.021735 | | | | |
| H | -2.050254 | 2.361174 | -1.730019 | | | | |
| C | -2.460243 | -0.239727 | -3.968065 | | | | |
| C | -1.591403 | -0.478575 | -5.078938 | | | | |
| C | 0.767849 | 0.581974 | 0.474052 | | | | |
| C | -0.552046 | 0.253833 | -5.705065 | | | | |
| C | 0.196371 | 1.408362 | -5.402890 | | | | |
| H | -1.784526 | -1.420575 | -5.588695 | | | | |
| H | -0.156821 | -0.271241 | -6.571313 | | | | |
| Si | -3.809339 | -1.548160 | -3.758217 | | | | |
| H | -3.259625 | 0.644565 | -2.254371 | | | | |
| Si | 0.070624 | 4.042293 | -2.146076 | | | | |
| H | 1.150307 | 2.939195 | -4.376845 | | | | |
| C | 2.699219 | -0.608565 | -2.342818 | | | | |
| C | 2.017492 | -1.841650 | -2.184384 | | | | |
| C | 1.657762 | -2.317317 | -3.470015 | | | | |
| C | 2.122021 | -1.376884 | -4.427202 | | | | |
| C | 2.765274 | -0.320504 | -3.730480 | | | | |
| H | 3.244037 | 0.539434 | -4.181600 | | | | |
| H | 2.028294 | -1.464101 | -5.501796 | | | | |
| H | 1.147548 | -3.248654 | -3.686259 | | | | |
| H | 1.792540 | -2.322548 | -1.242072 | | | | |
| H | 3.108658 | -0.003419 | -1.543344 | | | | |
| O | 1.303098 | 1.309667 | 1.400300 | | | | |
| H | -0.506339 | 4.003075 | -0.770615 | | | | |
| H | 1.564051 | 4.059107 | -2.077154 | | | | |
| H | -0.369842 | 5.311263 | -2.807843 | | | | |
| H | -3.284503 | -2.890169 | -4.161689 | | | | |
| H | -4.276535 | -1.589989 | -2.340642 | | | | |
| H | -4.983543 | -1.238716 | -4.634412 | | | | |

| | | | |
|---|-----------|-----------|----------|
| H | -2.018704 | -3.615888 | 1.588076 |
| H | 0.169882 | -3.841755 | 0.515604 |
| H | -0.417539 | -5.217185 | 2.422107 |
| H | 4.978610 | 0.297949 | 5.302847 |
| H | 4.687697 | 0.800682 | 2.949592 |
| H | 3.681701 | 2.228221 | 4.663410 |

6

SCF (B3PW91) Energy = -1328.093317
Enthalpy 0K = -1327.579157
Enthalpy 298K = -1327.536880
Free Energy 298K = -1327.658972

| | | | |
|----|-----------|-----------|-----------|
| U | 0.262535 | 0.201693 | 3.239064 |
| C | 2.261465 | -0.983662 | 4.648777 |
| Si | 3.918094 | -0.308922 | 5.256953 |
| C | 2.310726 | -1.614352 | 3.380233 |
| C | 1.383538 | -2.170765 | 2.463097 |
| C | -0.020307 | -2.373794 | 2.402583 |
| Si | -0.623628 | -3.158789 | 0.800448 |
| C | -1.054044 | -2.194190 | 3.378296 |
| C | -1.089441 | -1.764507 | 4.715396 |
| C | -0.169551 | -1.170624 | 5.612188 |
| C | 1.187830 | -0.792340 | 5.574604 |
| H | 1.472514 | -0.222324 | 6.457259 |
| H | -0.660888 | -0.811789 | 6.513473 |
| H | -2.103540 | -1.742523 | 5.107427 |
| H | -2.047215 | -2.432313 | 3.002121 |
| H | 1.874494 | -2.377511 | 1.513893 |
| H | 3.287706 | -1.520571 | 2.910689 |
| C | -0.517805 | 2.851836 | 3.154640 |
| C | -1.490360 | 2.170868 | 2.379037 |
| C | -2.267632 | 1.369344 | 3.252732 |
| C | -1.774027 | 1.558361 | 4.570059 |
| C | -0.691407 | 2.475221 | 4.509488 |
| H | -0.119137 | 2.842129 | 5.353085 |
| H | -2.171747 | 1.103716 | 5.467430 |
| H | -3.107236 | 0.745051 | 2.972597 |
| H | -1.617045 | 2.255071 | 1.307751 |
| H | 0.236236 | 3.527385 | 2.773515 |
| C | 0.623608 | 0.755087 | 0.191985 |
| O | -0.015996 | 0.489266 | -0.897986 |
| U | 0.089814 | 0.180925 | -3.116456 |
| C | -0.347696 | 1.937038 | -5.093176 |
| H | 0.363547 | 0.748144 | -6.639787 |
| C | -1.072182 | 2.447298 | -3.966665 |
| C | -2.069460 | 1.852723 | -3.149327 |
| C | -2.622361 | 0.559917 | -2.971235 |
| H | -2.400102 | 2.513960 | -2.350964 |
| C | -2.434780 | -0.737686 | -3.515202 |
| C | -1.648173 | -1.199030 | -4.619187 |
| C | 1.431066 | 1.132618 | 1.049730 |
| C | -0.870390 | -0.569031 | -5.618681 |
| C | -0.345454 | 0.722907 | -5.815684 |
| H | -1.689465 | -2.277856 | -4.759017 |
| H | -0.464579 | -1.286053 | -6.328126 |
| Si | -3.502259 | -2.087154 | -2.732246 |
| H | -3.253295 | 0.545348 | -2.084843 |
| Si | -0.720569 | 4.267313 | -3.588914 |
| H | 0.361670 | 2.651320 | -5.506875 |
| C | 2.817062 | 0.450082 | -2.814433 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.478178 | -0.706683 | -2.068030 |
| C | 2.097500 | -1.723784 | -2.978313 |
| C | 2.206096 | -1.196386 | -4.292572 |
| C | 2.653373 | 0.146658 | -4.190961 |
| H | 2.858046 | 0.812515 | -5.019634 |
| H | 2.014101 | -1.734043 | -5.211978 |
| H | 1.807832 | -2.735434 | -2.719403 |
| H | 2.493736 | -0.779248 | -0.987483 |
| H | 3.166901 | 1.389026 | -2.401488 |
| O | 1.979667 | 1.405653 | 2.187517 |
| H | -1.028893 | 4.565499 | -2.158230 |
| H | 0.715329 | 4.576646 | -3.873130 |
| H | -1.560556 | 5.156589 | -4.451564 |
| H | -2.759269 | -3.385454 | -2.708693 |
| H | -3.894756 | -1.696800 | -1.345640 |
| H | -4.748352 | -2.293400 | -3.536338 |
| H | -2.032921 | -2.747920 | 0.517987 |
| H | 0.247561 | -2.759723 | -0.349313 |
| H | -0.595631 | -4.654736 | 0.885653 |
| H | 4.576142 | -1.281456 | 6.188577 |
| H | 4.839137 | -0.066725 | 4.107193 |
| H | 3.711577 | 0.963344 | 6.018280 |

6-7-TS

SCF (B3PW91) Energy = -1328.090357
Enthalpy 0K = -1327.576718
Enthalpy 298K = -1327.534944
Free Energy 298K = -1327.657733
Negative frequency = -18.7 cm⁻¹

| | | | |
|----|-----------|-----------|-----------|
| U | 0.294994 | -0.028128 | 3.778587 |
| C | 2.214725 | -1.030260 | 5.374726 |
| Si | 3.879963 | -0.331921 | 5.933297 |
| C | 2.274576 | -1.855804 | 4.220050 |
| C | 1.350468 | -2.524663 | 3.379489 |
| C | -0.058913 | -2.663779 | 3.285269 |
| Si | -0.659163 | -3.605223 | 1.759261 |
| C | -1.111098 | -2.268115 | 4.171172 |
| C | -1.161828 | -1.701278 | 5.468586 |
| C | -0.241024 | -1.069319 | 6.322794 |
| C | 1.121305 | -0.695926 | 6.237684 |
| H | 1.401776 | -0.017376 | 7.041233 |
| H | -0.731720 | -0.606676 | 7.175927 |
| H | -2.183472 | -1.606394 | 5.828444 |
| H | -2.105290 | -2.492012 | 3.788769 |
| H | 1.858704 | -2.887321 | 2.488355 |
| H | 3.264867 | -1.867697 | 3.769511 |
| C | -0.597716 | 2.411731 | 2.839828 |
| C | -1.774750 | 1.636703 | 2.982807 |
| C | -2.004207 | 1.439716 | 4.370574 |
| C | -0.965025 | 2.092329 | 5.082945 |
| C | -0.093137 | 2.689759 | 4.135007 |
| H | 0.786822 | 3.280793 | 4.361089 |
| H | -0.867461 | 2.143576 | 6.159992 |
| H | -2.839076 | 0.909154 | 4.809888 |
| H | -2.401066 | 1.281843 | 2.173127 |
| H | -0.152445 | 2.709079 | 1.899191 |
| C | 0.467369 | 0.500571 | -0.327679 |
| O | -0.051577 | 0.533947 | -1.513326 |
| U | 0.081126 | 0.382741 | -3.712073 |
| C | -0.430442 | 2.365364 | -5.449963 |

| | | | |
|----|-----------|-----------|-----------|
| H | 0.427271 | 1.465832 | -7.116418 |
| C | -1.255062 | 2.654240 | -4.314339 |
| C | -2.216555 | 1.867649 | -3.627812 |
| C | -2.645636 | 0.516888 | -3.631541 |
| H | -2.628859 | 2.384293 | -2.763426 |
| C | -2.319107 | -0.672474 | -4.336261 |
| C | -1.495684 | -0.893303 | -5.488611 |
| C | 0.981111 | 0.452981 | 0.774760 |
| C | -0.749588 | -0.065673 | -6.355047 |
| C | -0.304421 | 1.271302 | -6.335975 |
| H | -1.441815 | -1.939500 | -5.784207 |
| H | -0.272239 | -0.638177 | -7.146814 |
| Si | -3.224805 | -2.217697 | -3.734055 |
| H | -3.283262 | 0.325927 | -2.770580 |
| Si | -1.080379 | 4.423497 | -3.673118 |
| H | 0.233140 | 3.184416 | -5.721223 |
| C | 2.837377 | 0.647148 | -3.630948 |
| C | 2.533406 | -0.365015 | -2.687409 |
| C | 2.076187 | -1.503817 | -3.397170 |
| C | 2.108746 | -1.200140 | -4.784009 |
| C | 2.577767 | 0.130390 | -4.928646 |
| H | 2.734836 | 0.650203 | -5.864800 |
| H | 1.843057 | -1.871548 | -5.590586 |
| H | 1.785083 | -2.450614 | -2.957341 |
| H | 2.604059 | -0.274069 | -1.609629 |
| H | 3.231691 | 1.630676 | -3.403307 |
| O | 1.525408 | 0.442552 | 1.959083 |
| H | -1.461068 | 4.494012 | -2.230338 |
| H | 0.330839 | 4.891245 | -3.845991 |
| H | -1.964423 | 5.359028 | -4.438974 |
| H | -2.369592 | -3.428159 | -3.942664 |
| H | -3.567288 | -2.087774 | -2.285520 |
| H | -4.495326 | -2.423424 | -4.499805 |
| H | -1.986504 | -3.075685 | 1.317353 |
| H | 0.332876 | -3.489522 | 0.649353 |
| H | -0.837382 | -5.057924 | 2.079840 |
| H | 4.526516 | -1.235463 | 6.937266 |
| H | 4.801065 | -0.188776 | 4.766218 |
| H | 3.679846 | 1.000982 | 6.583852 |

7

SCF (B3PW91) Energy = -1328.093450

Enthalpy 0K = -1327.579284

Enthalpy 298K = -1327.536724

Free Energy 298K = -1327.661627

| | | | |
|----|-----------|-----------|----------|
| U | -0.057567 | -0.401318 | 3.965960 |
| C | 2.367141 | -1.186215 | 4.853991 |
| Si | 4.120522 | -0.664404 | 4.381015 |
| C | 1.880359 | -2.320208 | 4.151463 |
| C | 0.661656 | -3.037829 | 4.058720 |
| C | -0.637910 | -2.953296 | 4.623794 |
| Si | -1.887970 | -4.181786 | 3.916608 |
| C | -1.154523 | -2.149130 | 5.691639 |
| C | -0.599664 | -1.212558 | 6.591842 |
| C | 0.612310 | -0.499806 | 6.685264 |
| C | 1.794798 | -0.414327 | 5.917764 |
| H | 2.423515 | 0.415648 | 6.234723 |
| H | 0.564074 | 0.281011 | 7.440610 |
| H | -1.341235 | -0.842113 | 7.295513 |
| H | -2.214973 | -2.309051 | 5.877796 |

| | | | |
|----|-----------|-----------|-----------|
| H | 0.703377 | -3.732622 | 3.222261 |
| H | 2.559202 | -2.640319 | 3.363416 |
| C | -1.318649 | 1.709283 | 2.711661 |
| C | -2.313581 | 1.152719 | 3.553032 |
| C | -1.952243 | 1.424722 | 4.899853 |
| C | -0.730661 | 2.144588 | 4.888409 |
| C | -0.336838 | 2.315856 | 3.534698 |
| H | 0.542561 | 2.845923 | 3.187699 |
| H | -0.204716 | 2.517380 | 5.758085 |
| H | -2.523056 | 1.155532 | 5.779122 |
| H | -3.210109 | 0.639859 | 3.224401 |
| H | -1.291949 | 1.650120 | 1.629642 |
| C | -0.148805 | -0.003798 | -0.598415 |
| O | -0.349008 | 0.317631 | -1.835572 |
| U | 0.223481 | 0.592682 | -3.944459 |
| C | -0.109460 | 2.785603 | -5.467078 |
| H | 1.108757 | 2.189107 | -7.041510 |
| C | -1.146218 | 2.858940 | -4.479908 |
| C | -2.155211 | 1.931583 | -4.109269 |
| C | -2.472405 | 0.578381 | -4.386580 |
| H | -2.761096 | 2.291225 | -3.279930 |
| C | -1.929229 | -0.475892 | -5.167435 |
| C | -0.884178 | -0.484504 | -6.148149 |
| C | 0.053319 | -0.322319 | 0.556538 |
| C | -0.056791 | 0.499960 | -6.731678 |
| C | 0.263244 | 1.843411 | -6.451492 |
| H | -0.691558 | -1.471895 | -6.563372 |
| H | 0.604927 | 0.075910 | -7.483165 |
| Si | -2.805580 | -2.137745 | -4.960953 |
| H | -3.243094 | 0.230465 | -3.701535 |
| Si | -1.244102 | 4.524265 | -3.592543 |
| H | 0.523658 | 3.670542 | -5.494289 |
| C | 2.837705 | 0.938703 | -3.106954 |
| C | 2.446800 | -0.321528 | -2.589333 |
| C | 2.302487 | -1.217363 | -3.677722 |
| C | 2.615080 | -0.512340 | -4.871035 |
| C | 2.946650 | 0.820268 | -4.518071 |
| H | 3.254348 | 1.601289 | -5.201663 |
| H | 2.622623 | -0.925389 | -5.871429 |
| H | 2.033368 | -2.265049 | -3.608498 |
| H | 2.257508 | -0.548359 | -1.546492 |
| H | 3.049545 | 1.826584 | -2.522605 |
| O | 0.238317 | -0.651546 | 1.794245 |
| H | -3.259500 | -3.583251 | 3.939752 |
| H | -1.521944 | -4.547551 | 2.515539 |
| H | -1.926601 | -5.434434 | 4.736692 |
| H | 5.133174 | -1.346879 | 5.248056 |
| H | 4.405008 | -1.022781 | 2.958688 |
| H | 4.282522 | 0.811432 | 4.571138 |
| H | -1.862797 | 4.361783 | -2.242283 |
| H | 0.126527 | 5.109363 | -3.451634 |
| H | -2.072815 | 5.497054 | -4.373593 |
| H | -3.914548 | -2.281789 | -5.957199 |
| H | -1.839210 | -3.256715 | -5.193346 |
| H | -3.388765 | -2.252678 | -3.590435 |

8

SCF (B3PW91) Energy = -1214.755619

Enthalpy 0K = -1214.252277

Enthalpy 298K = -1214.211629

Free Energy 298K = -1214.332446
U -0.312263 -0.273923 -0.197973
C -2.043645 1.819909 -0.129859
C -1.438555 1.995729 -1.418637
C -1.259149 1.184818 -2.548384
C -1.475268 -0.178393 -2.868315
C -1.963097 -1.303877 -2.184813
C -2.612052 -1.524426 -0.924389
C -2.983457 -0.633729 0.121489
C -2.751355 0.727411 0.447654
C 2.248483 0.698388 -0.549881
C 2.001609 -0.098780 -1.696616
C 2.327213 -0.166568 0.573288
C 2.130272 -1.505638 0.111836
C 1.926895 -1.457947 -1.291578
C -0.041045 -1.012168 1.993825
O 0.075606 -1.404518 3.160292
H -3.461431 -1.145705 0.955321
H -3.098123 0.939826 1.457694
Si -2.046023 3.379370 0.925735
H -2.130503 3.033225 2.380611
H -0.980374 2.975653 -1.544715
H -0.713676 1.701880 -3.335432
H -1.045733 -0.442137 -3.832519
H -1.810899 -2.220960 -2.752349
H -4.482907 -3.595586 -1.267562
Si -3.147370 -3.306645 -0.648370
H -3.264078 -3.600474 0.816338
H -2.163910 -4.258821 -1.256815
H 1.768916 -2.307766 -1.944091
H 2.189423 -2.402114 0.713550
H 2.567262 0.128658 1.585378
H 1.893934 0.266470 -2.710285
H 2.375654 1.773948 -0.537813
H -3.214495 4.265239 0.609581
H -0.805151 4.184100 0.688373
U 0.278062 -2.144415 5.336157
C 2.606689 -0.896574 5.915097
C 1.954653 -1.132763 7.168474
C 1.464039 -2.277526 7.835205
C 1.223825 -3.624871 7.485718
C 1.355250 -4.408849 6.319324
C 1.965537 -4.221462 5.037042
C 2.675310 -3.119438 4.487505
C 2.939425 -1.773163 4.848527
C -1.906010 -0.971610 6.567289
C -1.940247 -2.324882 6.997251
C -2.176387 -0.950347 5.176237
C -2.385232 -2.290595 4.747291
C -2.243968 -3.139141 5.873871
H 2.993119 -3.300607 3.462611
H 3.402266 -1.249120 4.014657
Si 3.198563 0.886782 5.693496
H 3.365421 1.196304 4.241762
H 1.818218 -0.230647 7.761941
H 1.042489 -2.030349 8.806487
H 0.669140 -4.148374 8.260676
H 0.871745 -5.377674 6.429153
H 3.074015 -6.657564 4.227384
Si 1.916636 -5.756673 3.930736

H 1.984287 -5.355376 2.493528
H 0.657224 -6.522315 4.184623
H -2.370477 -4.215049 5.882789
H -2.626933 -2.601989 3.738659
H -2.232439 -0.069051 4.549406
H -1.792093 -2.672482 8.011405
H -1.730144 -0.108187 7.197461
H 4.513412 1.094784 6.377205
H 2.209495 1.829027 6.303016

8-9-TS

SCF (B3PW91) Energy = -1214.752519
Enthalpy 0K = -1214.249163
Enthalpy 298K = -1214.209486
Free Energy 298K = -1214.326402
Negative frequency = -69.8754 cm⁻¹
U 0.136574 -0.095837 0.137665
U -0.071964 -0.003187 5.732780
C 2.791803 -0.247704 -0.458608
C 2.668299 0.921759 0.338773
C 1.790935 2.030728 0.434675
C 0.655813 2.508529 -0.281140
C 0.041861 2.053744 -1.489443
C 0.271267 1.010784 -2.415378
C 1.066663 -0.149099 -2.438892
C 2.067095 -0.705978 -1.597152
Si 4.157380 -1.436429 0.098006
Si -0.110964 4.096172 0.406740
C -1.559781 -2.244151 0.434391
C -2.127973 -1.192496 1.201950
C -2.612363 -0.205144 0.308676
C -2.336288 -0.642660 -1.014006
C -1.689490 -1.904811 -0.934868
H 3.732202 -2.849440 -0.146485
H 5.409578 -1.193032 -0.685209
H 4.458489 -1.235432 1.546624
H 0.134867 4.195019 1.876618
H -1.582037 4.104552 0.139449
H 0.489387 5.295967 -0.255281
H 3.337754 0.904647 1.196490
H 1.996612 2.606493 1.334816
H -0.834088 2.638514 -1.765052
H -0.462716 1.015500 -3.217379
H 0.796800 -0.820199 -3.250696
H 2.356689 -1.702532 -1.925477
H -1.119862 -3.151870 0.830044
H -2.173441 -1.141976 2.283075
H -3.127497 0.706779 0.585518
H -2.602251 -0.121536 -1.924377
H -1.375893 -2.510920 -1.775846
C 1.141233 2.187166 4.583419
C 2.203754 1.268516 4.850120
C 2.362927 1.184388 6.257748
C 1.406652 2.044833 6.856888
C 0.650811 2.662968 5.827217
C -0.239232 -2.540458 6.668658
C 0.208647 -1.796008 7.809669
C -0.280821 -0.695534 8.535709
C -1.324304 0.247892 8.367615
C -2.304609 0.503202 7.400059

| | | | |
|----|-----------|-----------|----------|
| C | -2.752550 | -0.167127 | 6.213461 |
| C | -2.394299 | -1.417433 | 5.633787 |
| C | -1.370643 | -2.382336 | 5.819269 |
| Si | 0.827005 | -4.041912 | 6.276777 |
| Si | -4.208001 | 0.675091 | 5.366768 |
| H | 1.146890 | -2.167372 | 8.219786 |
| H | 0.372423 | -0.434721 | 9.365746 |
| H | -1.275075 | 1.038671 | 9.113632 |
| H | -2.811928 | 1.450836 | 7.573555 |
| H | -2.964924 | -1.640761 | 4.733205 |
| H | -1.400097 | -3.124330 | 5.022843 |
| H | 2.271477 | -3.751421 | 6.547018 |
| H | 0.450640 | -5.224551 | 7.119527 |
| H | 0.666202 | -4.440935 | 4.843228 |
| H | -4.148210 | 2.158481 | 5.565392 |
| H | -5.524231 | 0.204380 | 5.910171 |
| H | -4.206265 | 0.382880 | 3.897177 |
| H | 2.822115 | 0.777501 | 4.111317 |
| H | 3.100243 | 0.588944 | 6.781980 |
| H | 1.279135 | 2.206759 | 7.919826 |
| H | -0.141903 | 3.387503 | 5.966997 |
| H | 0.811954 | 2.514339 | 3.607300 |
| C | 0.346283 | -0.448334 | 3.480538 |
| O | 0.620878 | -0.772369 | 2.314092 |

9

SCF (B3PW91) Energy = -1214.782966

Enthalpy 0K = -1214.278882

Enthalpy 298K = -1214.238743

Free Energy 298K = -1214.355316

| | | | |
|----|-----------|-----------|-----------|
| U | 8.139769 | 9.415989 | 3.379330 |
| U | 10.702851 | 5.789952 | 1.506579 |
| C | 9.721413 | 11.515288 | 2.634672 |
| C | 10.527858 | 10.748269 | 3.516654 |
| C | 10.375963 | 10.118245 | 4.778162 |
| C | 9.339154 | 9.953195 | 5.736866 |
| C | 8.041964 | 10.550689 | 5.834645 |
| C | 7.330694 | 11.506326 | 5.082598 |
| C | 7.503568 | 12.183803 | 3.851859 |
| C | 8.438311 | 12.128945 | 2.808151 |
| Si | 10.545145 | 11.942780 | 0.991457 |
| Si | 9.786861 | 8.854923 | 7.204286 |
| C | 6.321684 | 8.299905 | 1.624406 |
| C | 6.300128 | 7.454661 | 2.765846 |
| C | 5.696356 | 8.171202 | 3.830454 |
| C | 5.353121 | 9.458821 | 3.348526 |
| C | 5.740122 | 9.539049 | 1.983315 |
| H | 9.527729 | 12.003699 | -0.104334 |
| H | 11.220299 | 13.278824 | 1.054205 |
| H | 11.581663 | 10.920430 | 0.647241 |
| H | 10.826620 | 7.854569 | 6.810355 |
| H | 8.572810 | 8.140571 | 7.709336 |
| H | 10.338215 | 9.666458 | 8.336362 |
| H | 11.472985 | 10.454800 | 3.064745 |
| H | 11.247822 | 9.506347 | 5.000555 |
| H | 7.461913 | 10.188092 | 6.681363 |
| H | 6.348928 | 11.697036 | 5.510281 |
| H | 6.622771 | 12.762786 | 3.583536 |
| H | 8.101585 | 12.677603 | 1.929799 |
| H | 6.712855 | 8.044479 | 0.647892 |

| | | | |
|----|-----------|-----------|-----------|
| H | 6.651542 | 6.432952 | 2.812654 |
| H | 5.509447 | 7.792774 | 4.828227 |
| H | 4.857003 | 10.237382 | 3.912170 |
| H | 5.591696 | 10.389538 | 1.329473 |
| C | 12.315692 | 6.921081 | 3.436266 |
| C | 12.688240 | 7.572686 | 2.230214 |
| C | 13.353561 | 6.631601 | 1.408960 |
| C | 13.395660 | 5.395646 | 2.109581 |
| C | 12.758029 | 5.575677 | 3.362055 |
| C | 9.602234 | 5.764450 | -0.996212 |
| C | 10.900649 | 5.193931 | -1.201578 |
| C | 11.600878 | 4.109787 | -0.651157 |
| C | 11.420876 | 3.265648 | 0.469767 |
| C | 10.450227 | 3.090425 | 1.475946 |
| C | 9.136241 | 3.606465 | 1.711916 |
| C | 8.346175 | 4.528001 | 0.970900 |
| C | 8.538697 | 5.404614 | -0.127251 |
| Si | 9.193190 | 7.152956 | -2.206257 |
| Si | 8.257909 | 2.829501 | 3.190561 |
| H | 11.481588 | 5.710210 | -1.964592 |
| H | 12.589086 | 3.993470 | -1.090281 |
| H | 12.308404 | 2.668643 | 0.667585 |
| H | 10.791384 | 2.409192 | 2.253265 |
| H | 7.375620 | 4.706429 | 1.429540 |
| H | 7.673660 | 6.054424 | -0.241237 |
| H | 10.396936 | 8.006315 | -2.456252 |
| H | 8.747551 | 6.606060 | -3.528032 |
| H | 8.088139 | 8.005361 | -1.667096 |
| H | 9.251513 | 2.465242 | 4.248320 |
| H | 7.536686 | 1.577896 | 2.793725 |
| H | 7.250049 | 3.777688 | 3.758038 |
| H | 12.501196 | 8.609245 | 1.980303 |
| H | 13.779827 | 6.823209 | 0.431896 |
| H | 13.860113 | 4.484490 | 1.757229 |
| H | 12.648955 | 4.825459 | 4.135857 |
| H | 11.813426 | 7.374120 | 4.280038 |
| C | 9.327581 | 7.260122 | 2.976063 |
| O | 9.509639 | 7.949659 | 1.894373 |

9_{CO}

SCF (B3PW91) Energy = -1328.042597

Enthalpy 0K = -1327.532864

Enthalpy 298K = -1327.488552

Free Energy 298K = -1327.617393

| | | | |
|----|-----------|-----------|----------|
| U | 8.158531 | 9.416162 | 3.439478 |
| U | 10.723603 | 5.812583 | 1.518263 |
| C | 9.663102 | 11.489465 | 2.481955 |
| C | 10.513514 | 10.812688 | 3.395061 |
| C | 10.415242 | 10.275478 | 4.703985 |
| C | 9.411849 | 10.169552 | 5.706731 |
| C | 8.107902 | 10.752463 | 5.800460 |
| C | 7.348409 | 11.626212 | 4.996679 |
| C | 7.458431 | 12.193467 | 3.706448 |
| C | 8.361018 | 12.065839 | 2.638658 |
| Si | 10.436239 | 11.819891 | 0.792667 |
| Si | 9.938466 | 9.221422 | 7.249881 |
| C | 6.256301 | 8.183301 | 1.859281 |
| C | 6.390629 | 7.344237 | 2.997400 |
| C | 5.845984 | 8.028692 | 4.114069 |
| C | 5.382216 | 9.290196 | 3.667010 |

| | | | |
|----|-----------|-----------|-----------|
| C | 5.636669 | 9.387081 | 2.271588 |
| H | 9.388048 | 11.808676 | -0.275106 |
| H | 11.101815 | 13.161773 | 0.757054 |
| H | 11.473288 | 10.787872 | 0.480864 |
| H | 10.981887 | 8.206688 | 6.905028 |
| H | 8.759802 | 8.538449 | 7.867276 |
| H | 10.519816 | 10.145664 | 8.275310 |
| H | 11.452940 | 10.507867 | 2.938217 |
| H | 11.306817 | 9.699658 | 4.944501 |
| H | 7.565066 | 10.450598 | 6.694454 |
| H | 6.378888 | 11.834302 | 5.443963 |
| H | 6.553111 | 12.722902 | 3.418469 |
| H | 7.981771 | 12.524414 | 1.726714 |
| H | 6.567889 | 7.944993 | 0.850175 |
| H | 6.799194 | 6.342804 | 3.009838 |
| H | 5.776730 | 7.643702 | 5.124284 |
| H | 4.895136 | 10.040803 | 4.274827 |
| H | 5.377091 | 10.223700 | 1.634815 |
| C | 12.383423 | 7.023532 | 3.356038 |
| C | 12.716749 | 7.630690 | 2.115918 |
| C | 13.360148 | 6.660618 | 1.311442 |
| C | 13.431910 | 5.452815 | 2.058729 |
| C | 12.832233 | 5.678239 | 3.321377 |
| C | 9.739441 | 5.854825 | -1.024797 |
| C | 11.018725 | 5.231503 | -1.193615 |
| C | 11.665679 | 4.129455 | -0.618323 |
| C | 11.421947 | 3.288270 | 0.493384 |
| C | 10.393525 | 3.122633 | 1.442663 |
| C | 9.074241 | 3.654392 | 1.602059 |
| C | 8.352999 | 4.622190 | 0.850335 |
| C | 8.623403 | 5.519113 | -0.213711 |
| Si | 9.433442 | 7.279923 | -2.224289 |
| Si | 8.065163 | 2.811116 | 2.952510 |
| H | 11.646207 | 5.733230 | -1.928814 |
| H | 12.668106 | 3.989536 | -1.016694 |
| H | 12.288102 | 2.675585 | 0.733127 |
| H | 10.672754 | 2.420640 | 2.226032 |
| H | 7.363648 | 4.814744 | 1.262124 |
| H | 7.790180 | 6.205677 | -0.348179 |
| H | 10.682549 | 8.080523 | -2.419455 |
| H | 9.010982 | 6.771074 | -3.568820 |
| H | 8.348913 | 8.170946 | -1.707644 |
| H | 8.963505 | 2.310966 | 4.039357 |
| H | 7.314820 | 1.636151 | 2.404947 |
| H | 7.062767 | 3.757511 | 3.533680 |
| H | 12.516187 | 8.655649 | 1.830952 |
| H | 13.749780 | 6.814530 | 0.312963 |
| H | 13.889658 | 4.530515 | 1.727044 |
| H | 12.738142 | 4.957602 | 4.123978 |
| H | 11.906321 | 7.507701 | 4.197330 |
| O | 8.964077 | 5.310958 | 6.166992 |
| C | 9.898653 | 5.038241 | 5.580123 |
| C | 9.389861 | 7.285123 | 3.033815 |
| O | 9.492105 | 7.944594 | 1.924602 |

9_{co}-10-TS

| | |
|-----------------------|--------------|
| SCF (B3PW91) Energy = | -1328.031412 |
| Enthalpy 0K = | -1327.520801 |
| Enthalpy 298K = | -1327.478176 |
| Free Energy 298K = | -1327.600173 |

| | | | |
|----------------------|-----------|----------------------------|-----------|
| Negative frequency = | | -205.5292 cm ⁻¹ | |
| U | 8.148497 | 9.327663 | 3.509866 |
| U | 10.747603 | 5.777268 | 1.474174 |
| C | 9.709206 | 11.408022 | 2.706162 |
| C | 10.509170 | 10.709812 | 3.647025 |
| C | 10.336368 | 10.163511 | 4.944722 |
| C | 9.283428 | 10.041129 | 5.889121 |
| C | 7.955396 | 10.577110 | 5.903719 |
| C | 7.240888 | 11.472033 | 5.084351 |
| C | 7.444464 | 12.091446 | 3.828966 |
| C | 8.412210 | 12.008096 | 2.818099 |
| Si | 10.561329 | 11.767399 | 1.061213 |
| Si | 9.741134 | 9.179666 | 7.504439 |
| C | 6.420740 | 8.347179 | 1.590751 |
| C | 6.303991 | 7.441582 | 2.677402 |
| C | 5.653667 | 8.114018 | 3.742921 |
| C | 5.368631 | 9.434246 | 3.313315 |
| C | 5.845839 | 9.580072 | 1.983532 |
| H | 9.566535 | 11.758456 | -0.056734 |
| H | 11.213943 | 13.115767 | 1.073656 |
| H | 11.620611 | 10.748073 | 0.786842 |
| H | 10.978459 | 8.360787 | 7.330727 |
| H | 8.618668 | 8.310866 | 7.977881 |
| H | 10.001864 | 10.197660 | 8.571987 |
| H | 11.462919 | 10.393215 | 3.229234 |
| H | 11.214134 | 9.588501 | 5.233866 |
| H | 7.364563 | 10.246250 | 6.756799 |
| H | 6.238527 | 11.652732 | 5.465801 |
| H | 6.560052 | 12.633575 | 3.501530 |
| H | 8.088399 | 12.504263 | 1.904451 |
| H | 6.865869 | 8.138159 | 0.626527 |
| H | 6.635585 | 6.413251 | 2.692414 |
| H | 5.392533 | 7.684197 | 4.702388 |
| H | 4.851401 | 10.191371 | 3.886575 |
| H | 5.761798 | 10.468964 | 1.371429 |
| C | 12.557239 | 7.198157 | 3.012363 |
| C | 12.936382 | 7.470289 | 1.673390 |
| C | 13.466449 | 6.279840 | 1.121235 |
| C | 13.422111 | 5.272721 | 2.124755 |
| C | 12.865941 | 5.843265 | 3.293810 |
| C | 9.566630 | 5.859294 | -0.962025 |
| C | 10.841282 | 5.261646 | -1.229595 |
| C | 11.542223 | 4.155565 | -0.723891 |
| C | 11.395452 | 3.276292 | 0.375038 |
| C | 10.449999 | 3.078078 | 1.398671 |
| C | 9.138291 | 3.585166 | 1.660218 |
| C | 8.346312 | 4.539038 | 0.971544 |
| C | 8.521684 | 5.477087 | -0.078284 |
| Si | 9.145443 | 7.284031 | -2.125230 |
| Si | 8.279712 | 2.766297 | 3.130035 |
| H | 11.415142 | 5.794046 | -1.986382 |
| H | 12.518635 | 4.048768 | -1.190977 |
| H | 12.288895 | 2.676077 | 0.529698 |
| H | 10.798419 | 2.366406 | 2.144867 |
| H | 7.387199 | 4.703464 | 1.457931 |
| H | 7.658671 | 6.135719 | -0.141714 |
| H | 10.371199 | 8.084689 | -2.432598 |
| H | 8.594560 | 6.776266 | -3.421903 |
| H | 8.115629 | 8.175209 | -1.507192 |
| H | 9.285582 | 2.396999 | 4.172993 |

| | | | |
|---|-----------|----------|----------|
| H | 7.583321 | 1.509505 | 2.704931 |
| H | 7.255876 | 3.684625 | 3.714626 |
| H | 12.843070 | 8.423338 | 1.166695 |
| H | 13.856906 | 6.159862 | 0.118754 |
| H | 13.778251 | 4.256608 | 2.018829 |
| H | 12.717610 | 5.340685 | 4.241848 |
| H | 12.115760 | 7.899921 | 3.705464 |
| O | 9.612879 | 5.813812 | 5.708450 |
| C | 10.071778 | 6.626097 | 5.039798 |
| C | 9.248359 | 7.075829 | 3.084082 |
| O | 9.688534 | 7.899860 | 2.177124 |

10

SCF (B3PW91) Energy = -1328.089833

Enthalpy 0K = -1327.575867

Enthalpy 298K = -1327.533755

Free Energy 298K = -1327.653534

| | | | |
|----|-----------|-----------|-----------|
| U | 8.148007 | 9.271388 | 3.507225 |
| U | 10.708596 | 5.846316 | 1.467428 |
| C | 9.696759 | 11.354055 | 2.721538 |
| C | 10.509259 | 10.670986 | 3.661867 |
| C | 10.351966 | 10.110279 | 4.956457 |
| C | 9.310841 | 9.961349 | 5.906532 |
| C | 7.972968 | 10.467878 | 5.929878 |
| C | 7.230636 | 11.348313 | 5.118086 |
| C | 7.400733 | 11.935346 | 3.844178 |
| C | 8.371679 | 11.886293 | 2.825312 |
| Si | 10.552282 | 11.763448 | 1.089283 |
| Si | 9.783196 | 9.088367 | 7.520297 |
| C | 6.441100 | 8.136780 | 1.686743 |
| C | 6.314899 | 7.328246 | 2.845880 |
| C | 5.647164 | 8.086917 | 3.838864 |
| C | 5.359929 | 9.362439 | 3.291844 |
| C | 5.853106 | 9.396036 | 1.960684 |
| H | 9.555666 | 11.785035 | -0.026559 |
| H | 11.202145 | 13.111273 | 1.145414 |
| H | 11.613464 | 10.754155 | 0.787573 |
| H | 11.139434 | 8.481726 | 7.409795 |
| H | 8.768002 | 8.057604 | 7.895926 |
| H | 9.803046 | 10.107934 | 8.619279 |
| H | 11.472729 | 10.386352 | 3.244121 |
| H | 11.246019 | 9.557907 | 5.240499 |
| H | 7.399105 | 10.134929 | 6.793718 |
| H | 6.227709 | 11.508166 | 5.506082 |
| H | 6.491848 | 12.428450 | 3.506934 |
| H | 8.021024 | 12.357100 | 1.908929 |
| H | 6.908223 | 7.848228 | 0.755438 |
| H | 6.680553 | 6.318938 | 2.964357 |
| H | 5.380840 | 7.743372 | 4.831114 |
| H | 4.832307 | 10.163514 | 3.791385 |
| H | 5.767294 | 10.226040 | 1.270704 |
| C | 12.956945 | 7.481213 | 1.500733 |
| C | 13.445766 | 6.230550 | 1.051782 |
| C | 13.372601 | 5.313813 | 2.135925 |
| C | 12.844772 | 6.000098 | 3.255942 |
| C | 12.582713 | 7.335713 | 2.859614 |
| C | 9.639930 | 5.908158 | -1.011550 |
| C | 10.902895 | 5.262322 | -1.187789 |
| C | 11.532152 | 4.139892 | -0.614973 |
| C | 11.298071 | 3.287798 | 0.484617 |

| | | | |
|----|-----------|----------|-----------|
| C | 10.299399 | 3.175196 | 1.475168 |
| C | 8.988768 | 3.717894 | 1.638699 |
| C | 8.272824 | 4.681555 | 0.885958 |
| C | 8.534846 | 5.579038 | -0.180368 |
| Si | 9.321832 | 7.320317 | -2.223823 |
| Si | 8.049095 | 2.986764 | 3.105949 |
| H | 11.543451 | 5.757671 | -1.914940 |
| H | 12.526369 | 3.987359 | -1.028815 |
| H | 12.157319 | 2.657463 | 0.699200 |
| H | 10.584619 | 2.478320 | 2.261600 |
| H | 7.293153 | 4.889402 | 1.310175 |
| H | 7.696477 | 6.257313 | -0.316017 |
| H | 10.601331 | 8.028827 | -2.537214 |
| H | 8.752074 | 6.806919 | -3.509599 |
| H | 8.344653 | 8.292632 | -1.642725 |
| H | 8.979137 | 2.745575 | 4.251163 |
| H | 7.437011 | 1.670638 | 2.733850 |
| H | 6.947651 | 3.902383 | 3.531288 |
| H | 13.831999 | 6.016282 | 0.064077 |
| H | 13.695016 | 4.281181 | 2.116390 |
| H | 12.678886 | 5.587678 | 4.243757 |
| H | 12.167044 | 8.112528 | 3.485922 |
| H | 12.900125 | 8.392812 | 0.918122 |
| O | 10.358068 | 6.286193 | 5.632380 |
| C | 10.041316 | 6.724610 | 4.576007 |
| C | 9.388136 | 6.954499 | 3.451158 |
| O | 9.670869 | 7.805127 | 2.364043 |

10CO

SCF (B3PW91) Energy = -1441.349751

Enthalpy 0K = -1440.830159

Enthalpy 298K = -1440.783802

Free Energy 298K = -1440.918002

| | | | |
|----|-----------|-----------|-----------|
| U | 8.154393 | 9.299135 | 3.475630 |
| U | 10.705304 | 5.830145 | 1.490185 |
| C | 9.735063 | 11.364072 | 2.721543 |
| C | 10.530427 | 10.667080 | 3.666891 |
| C | 10.350479 | 10.101961 | 4.956477 |
| C | 9.297575 | 9.962219 | 5.895093 |
| C | 7.964652 | 10.481102 | 5.904768 |
| C | 7.240985 | 11.374363 | 5.089532 |
| C | 7.432873 | 11.966872 | 3.821539 |
| C | 8.415515 | 11.912438 | 2.814034 |
| Si | 10.610521 | 11.774181 | 1.100022 |
| Si | 9.743357 | 9.084229 | 7.513627 |
| C | 6.464299 | 8.243889 | 1.593422 |
| C | 6.334036 | 7.387766 | 2.717714 |
| C | 5.654765 | 8.101579 | 3.736532 |
| C | 5.367163 | 9.397439 | 3.241215 |
| C | 5.870110 | 9.488167 | 1.916280 |
| H | 9.628351 | 11.793048 | -0.028620 |
| H | 11.256709 | 13.123419 | 1.162941 |
| H | 11.677331 | 10.766972 | 0.812611 |
| H | 11.093542 | 8.461247 | 7.417243 |
| H | 8.712177 | 8.067871 | 7.883964 |
| H | 9.767779 | 10.106816 | 8.609847 |
| H | 11.494103 | 10.370514 | 3.258050 |
| H | 11.234522 | 9.538009 | 5.248828 |
| H | 7.377080 | 10.150425 | 6.760244 |
| H | 6.235771 | 11.543860 | 5.467325 |

| | | | | | | | |
|------------------------------|----------------------------|-----------|-----------|----|-----------|-----------|-----------|
| H | 6.533334 | 12.471400 | 3.476234 | C | 7.406987 | 11.899399 | 3.694676 |
| H | 8.080293 | 12.390476 | 1.895560 | C | 8.265303 | 11.687544 | 2.588979 |
| H | 6.942360 | 7.997788 | 0.654947 | Si | 10.265148 | 11.372931 | 0.667715 |
| H | 6.710003 | 6.378998 | 2.801074 | Si | 10.208204 | 9.432176 | 7.367629 |
| H | 5.385187 | 7.716405 | 4.712424 | C | 6.333363 | 8.136075 | 1.893240 |
| H | 4.833115 | 10.175564 | 3.769551 | C | 6.392077 | 7.240483 | 2.993962 |
| H | 5.786465 | 10.346054 | 1.261150 | C | 5.762793 | 7.863156 | 4.101064 |
| C | 12.907430 | 7.518882 | 1.600618 | C | 5.336495 | 9.148896 | 3.694795 |
| C | 13.413733 | 6.322671 | 1.038503 | C | 5.686533 | 9.317283 | 2.326220 |
| C | 13.393197 | 5.321821 | 2.047921 | H | 9.150257 | 11.358362 | -0.327565 |
| C | 12.878176 | 5.899140 | 3.233743 | H | 10.978632 | 12.683268 | 0.548507 |
| C | 12.573882 | 7.255018 | 2.952777 | H | 11.241495 | 10.287100 | 0.348217 |
| C | 9.573690 | 5.886806 | -0.963872 | H | 11.075003 | 8.259890 | 7.038156 |
| C | 10.851347 | 5.277523 | -1.168929 | H | 9.077614 | 9.019294 | 8.250032 |
| C | 11.519833 | 4.164940 | -0.621977 | H | 11.053574 | 10.412006 | 8.124673 |
| C | 11.327006 | 3.293901 | 0.471614 | H | 11.412127 | 10.252418 | 2.873791 |
| C | 10.354772 | 3.146531 | 1.482126 | H | 11.398754 | 9.708845 | 4.966632 |
| C | 9.036961 | 3.660276 | 1.682280 | H | 7.752935 | 10.532291 | 6.844639 |
| C | 8.281156 | 4.609687 | 0.951346 | H | 6.427175 | 11.729392 | 5.517881 |
| C | 8.496289 | 5.523773 | -0.111801 | H | 6.461466 | 12.338709 | 3.385232 |
| Si | 9.196311 | 7.294632 | -2.162126 | H | 7.804608 | 12.010316 | 1.657701 |
| Si | 8.141037 | 2.898104 | 3.161563 | H | 6.706510 | 7.949683 | 0.894356 |
| H | 11.463453 | 5.794800 | -1.905373 | H | 6.837146 | 6.254284 | 2.992404 |
| H | 12.510402 | 4.044252 | -1.054648 | H | 5.648846 | 7.433133 | 5.087821 |
| H | 12.205168 | 2.681676 | 0.660180 | H | 4.812105 | 9.869654 | 4.308543 |
| H | 10.673897 | 2.449284 | 2.254974 | H | 5.469116 | 10.184577 | 1.716129 |
| H | 7.304541 | 4.784529 | 1.395775 | C | 12.880753 | 7.610633 | 1.993975 |
| H | 7.636153 | 6.180673 | -0.220277 | C | 13.479805 | 6.558334 | 1.259054 |
| H | 10.445707 | 8.052452 | -2.482058 | C | 13.607934 | 5.438147 | 2.123941 |
| H | 8.632911 | 6.771530 | -3.446752 | C | 13.087533 | 5.799059 | 3.388716 |
| H | 8.191370 | 8.227411 | -1.564641 | C | 12.631702 | 7.138230 | 3.307054 |
| H | 9.099366 | 2.663407 | 4.285202 | C | 9.866875 | 6.059688 | -0.821077 |
| H | 7.546721 | 1.573169 | 2.791935 | C | 11.118813 | 5.423138 | -1.070328 |
| H | 7.033369 | 3.792672 | 3.614602 | C | 11.774402 | 4.290749 | -0.559252 |
| H | 13.783762 | 6.200146 | 0.028958 | C | 11.543538 | 3.352573 | 0.471166 |
| H | 13.734190 | 4.301440 | 1.935145 | C | 10.491604 | 3.087310 | 1.376843 |
| H | 12.753301 | 5.394838 | 4.184469 | C | 9.157536 | 3.570331 | 1.523346 |
| H | 12.158053 | 7.970911 | 3.647900 | C | 8.458446 | 4.629956 | 0.888363 |
| H | 12.806922 | 8.471714 | 1.095130 | C | 8.744556 | 5.657551 | -0.040758 |
| O | 10.250376 | 6.287798 | 5.656585 | Si | 9.540774 | 7.563149 | -1.911267 |
| C | 9.974637 | 6.725005 | 4.586976 | Si | 8.138325 | 2.620573 | 2.791895 |
| C | 9.358698 | 6.958554 | 3.443223 | H | 11.753506 | 5.978667 | -1.758387 |
| O | 9.672384 | 7.805422 | 2.363542 | H | 12.782329 | 4.198442 | -0.958537 |
| C | 12.429446 | 4.086861 | 6.650307 | H | 12.417739 | 2.737679 | 0.669931 |
| O | 12.007495 | 3.829685 | 7.673404 | H | 10.755262 | 2.307119 | 2.088885 |
| 10_{co}-11-TS | | | | H | 7.465972 | 4.777001 | 1.310408 |
| SCF (B3PW91) Energy = | -1441.325917 | | | H | 7.918481 | 6.362144 | -0.098527 |
| Enthalpy 0K = | -1440.806126 | | | H | 10.812792 | 8.298124 | -2.191959 |
| Enthalpy 298K = | -1440.761321 | | | H | 8.944986 | 7.160378 | -3.225360 |
| Free Energy 298K = | -1440.887702 | | | H | 8.572766 | 8.488073 | -1.241418 |
| Negative frequency = | -250.9400 cm ⁻¹ | | | H | 9.009415 | 2.124545 | 3.903648 |
| U | 8.139518 | 9.245172 | 3.654170 | H | 7.489040 | 1.421289 | 2.169849 |
| U | 10.846100 | 5.747420 | 1.707401 | H | 7.052342 | 3.480043 | 3.356680 |
| C | 9.578057 | 11.153280 | 2.413238 | H | 13.804646 | 6.605709 | 0.227864 |
| C | 10.497338 | 10.602039 | 3.346489 | H | 14.047956 | 4.484455 | 1.864118 |
| C | 10.481379 | 10.238318 | 4.714650 | H | 13.050359 | 5.167822 | 4.267965 |
| C | 9.554086 | 10.244997 | 5.788838 | H | 12.164696 | 7.692699 | 4.108172 |
| C | 8.228342 | 10.750958 | 5.890962 | H | 12.663677 | 8.601679 | 1.615072 |
| C | 7.381031 | 11.508759 | 5.045602 | O | 8.409064 | 7.205193 | 5.715283 |
| | | | | C | 9.077121 | 6.585073 | 4.914017 |

| | | | |
|---|-----------|----------|----------|
| C | 9.647702 | 6.343732 | 3.745861 |
| O | 9.525237 | 7.464603 | 2.845051 |
| C | 9.931126 | 4.802564 | 5.772612 |
| O | 10.739889 | 4.039813 | 6.023117 |

11

SCF (B3PW91) Energy = -1441.394669
Enthalpy 0K = -1440.871192
Enthalpy 298K = -1440.827219
Free Energy 298K = -1440.951862

| | | | |
|----|-----------|-----------|-----------|
| U | 8.038940 | 9.284756 | 3.822479 |
| U | 10.953921 | 5.603087 | 1.703831 |
| C | 9.294301 | 11.329065 | 2.479951 |
| C | 10.315736 | 10.646330 | 3.212382 |
| C | 10.510318 | 10.256767 | 4.553804 |
| C | 9.762688 | 10.278814 | 5.766930 |
| C | 8.462405 | 10.734512 | 6.089032 |
| C | 7.448279 | 11.438157 | 5.388675 |
| C | 7.325340 | 11.967837 | 4.087086 |
| C | 8.077138 | 11.927478 | 2.894521 |
| Si | 9.722968 | 11.631035 | 0.669251 |
| Si | 10.637140 | 9.395079 | 7.186852 |
| C | 6.520557 | 8.319177 | 1.703499 |
| C | 6.300122 | 7.411178 | 2.772322 |
| C | 5.519125 | 8.067743 | 3.753711 |
| C | 5.273997 | 9.386591 | 3.306008 |
| C | 5.889143 | 9.540940 | 2.033269 |
| H | 8.480194 | 11.712599 | -0.160586 |
| H | 10.472896 | 12.915995 | 0.493365 |
| H | 10.591884 | 10.528010 | 0.150611 |
| H | 11.297419 | 8.132145 | 6.722734 |
| H | 9.671539 | 9.070241 | 8.279913 |
| H | 11.721200 | 10.256413 | 7.761353 |
| H | 11.130132 | 10.303544 | 2.578549 |
| H | 11.440800 | 9.697986 | 4.650324 |
| H | 8.141904 | 10.466906 | 7.093263 |
| H | 6.554783 | 11.587163 | 5.989644 |
| H | 6.348697 | 12.419391 | 3.928306 |
| H | 7.518670 | 12.366673 | 2.069754 |
| H | 7.068214 | 8.116133 | 0.791871 |
| H | 6.657302 | 6.391353 | 2.829080 |
| H | 5.191825 | 7.640242 | 4.693152 |
| H | 4.697736 | 10.139970 | 3.827958 |
| H | 5.862500 | 10.429791 | 1.417080 |
| C | 12.803284 | 7.543839 | 2.385198 |
| C | 13.456064 | 6.760162 | 1.403608 |
| C | 13.726610 | 5.486279 | 1.974813 |
| C | 13.241644 | 5.486950 | 3.305103 |
| C | 12.666028 | 6.757554 | 3.558495 |
| C | 9.943269 | 5.887936 | -0.807232 |
| C | 11.212391 | 5.280990 | -1.060320 |
| C | 11.901172 | 4.173553 | -0.543997 |
| C | 11.699312 | 3.243254 | 0.503597 |
| C | 10.659963 | 2.956105 | 1.416946 |
| C | 9.317133 | 3.415978 | 1.579215 |
| C | 8.586599 | 4.451617 | 0.938173 |
| C | 8.838589 | 5.470976 | -0.011954 |
| Si | 9.585917 | 7.374043 | -1.919063 |
| Si | 8.327493 | 2.448745 | 2.862590 |
| H | 11.824535 | 5.842625 | -1.763706 |

| | | | |
|---|-----------|----------|-----------|
| H | 12.908144 | 4.101587 | -0.949244 |
| H | 12.591411 | 2.656044 | 0.706601 |
| H | 10.948946 | 2.191519 | 2.135380 |
| H | 7.598427 | 4.587644 | 1.374673 |
| H | 7.996464 | 6.156696 | -0.066999 |
| H | 10.837952 | 8.155332 | -2.159962 |
| H | 9.060661 | 6.924764 | -3.247042 |
| H | 8.557255 | 8.257128 | -1.289906 |
| H | 9.239194 | 1.917601 | 3.922953 |
| H | 7.632425 | 1.282688 | 2.230611 |
| H | 7.283834 | 3.320210 | 3.485942 |
| H | 13.727997 | 7.080756 | 0.405761 |
| H | 14.240037 | 4.669201 | 1.486044 |
| H | 13.316973 | 4.668638 | 4.011093 |
| H | 12.229564 | 7.082077 | 4.493387 |
| H | 12.478257 | 8.569107 | 2.264821 |
| O | 8.256927 | 7.497666 | 5.276944 |
| C | 8.975912 | 6.442597 | 4.902298 |
| C | 9.648007 | 6.324438 | 3.666511 |
| O | 9.497489 | 7.353721 | 2.863660 |
| C | 9.170521 | 5.354944 | 5.704432 |
| O | 9.342598 | 4.430308 | 6.383401 |

11-12-TS

SCF (B3PW91) Energy = -1441.382900
Enthalpy 0K = -1440.860055
Enthalpy 298K = -1440.816534
Free Energy 298K = -1440.942735
Negative frequency = -82.4147 cm⁻¹

| | | | |
|----|-----------|-----------|----------|
| U | 8.008526 | 9.972013 | 4.330992 |
| U | 11.221202 | 5.176143 | 0.692060 |
| C | 9.696839 | 12.076906 | 4.437223 |
| C | 10.038449 | 11.315837 | 5.585188 |
| C | 9.351872 | 10.633013 | 6.620334 |
| C | 8.002075 | 10.400649 | 6.993346 |
| C | 6.776884 | 10.958010 | 6.500215 |
| C | 6.442552 | 11.935540 | 5.537017 |
| C | 7.124151 | 12.605245 | 4.500414 |
| C | 8.439181 | 12.594130 | 3.984225 |
| Si | 11.168960 | 12.591073 | 3.367562 |
| Si | 7.785040 | 9.235632 | 8.466768 |
| C | 7.281932 | 8.702575 | 1.999643 |
| C | 6.662392 | 7.952428 | 3.033677 |
| C | 5.626715 | 8.739768 | 3.595583 |
| C | 5.606821 | 9.982747 | 2.909042 |
| C | 6.626458 | 9.956493 | 1.920771 |
| H | 10.748811 | 12.693287 | 1.935209 |
| H | 11.685695 | 13.931634 | 3.788612 |
| H | 12.277683 | 11.598156 | 3.499218 |
| H | 8.907899 | 8.251337 | 8.516631 |
| H | 6.482263 | 8.508591 | 8.352289 |
| H | 7.770746 | 10.001160 | 9.753103 |
| H | 11.093233 | 11.048640 | 5.602849 |
| H | 10.047571 | 10.008654 | 7.177531 |
| H | 5.892763 | 10.557545 | 6.992541 |
| H | 5.368141 | 12.093158 | 5.481728 |
| H | 6.440829 | 13.145550 | 3.849635 |
| H | 8.507679 | 13.131086 | 3.040117 |
| H | 8.116859 | 8.367386 | 1.393494 |
| H | 6.935386 | 6.948275 | 3.334572 |

| | | | | | | | |
|-----------------------|-----------|-----------|--------------|----|-----------|-----------|-----------|
| H | 4.947643 | 8.437725 | 4.384009 | C | 6.076124 | 7.552882 | 4.493198 |
| H | 4.914372 | 10.794765 | 3.087343 | C | 6.436081 | 7.632629 | 5.864241 |
| H | 6.846951 | 10.747663 | 1.214262 | C | 5.795595 | 8.764581 | 6.414139 |
| C | 13.202053 | 7.083263 | 0.317928 | C | 5.023344 | 9.377891 | 5.384455 |
| C | 13.524005 | 6.043679 | -0.587822 | H | 8.855855 | 12.314027 | 0.676930 |
| C | 13.944110 | 4.917936 | 0.172898 | H | 11.040556 | 12.832280 | 1.599868 |
| C | 13.879728 | 5.264249 | 1.545547 | H | 10.445808 | 10.539761 | 1.210206 |
| C | 13.417948 | 6.602116 | 1.634043 | H | 10.633429 | 8.843433 | 8.041225 |
| C | 9.434861 | 4.801220 | -1.308288 | H | 8.563579 | 9.514242 | 9.150395 |
| C | 10.600672 | 4.106269 | -1.766451 | H | 10.484956 | 10.976330 | 9.171035 |
| C | 11.443231 | 3.118763 | -1.228756 | H | 10.976052 | 10.758180 | 3.825004 |
| C | 11.599701 | 2.479279 | 0.024002 | H | 10.916144 | 10.102226 | 5.891872 |
| C | 10.946361 | 2.532828 | 1.270270 | H | 7.362869 | 11.232241 | 7.801772 |
| C | 9.737625 | 3.135202 | 1.745306 | H | 6.003251 | 12.283853 | 6.430946 |
| C | 8.791019 | 3.984129 | 1.112937 | H | 6.002064 | 12.836768 | 4.266740 |
| C | 8.664838 | 4.667809 | -0.122021 | H | 7.445556 | 12.610654 | 2.579829 |
| Si | 8.713438 | 5.994241 | -2.581240 | H | 4.741132 | 8.829767 | 3.241297 |
| Si | 9.258673 | 2.616774 | 3.495070 | H | 6.393270 | 6.786979 | 3.797083 |
| H | 10.944465 | 4.440788 | -2.743644 | H | 7.100298 | 6.955788 | 6.386482 |
| H | 12.268851 | 2.889210 | -1.898897 | H | 5.861558 | 9.096238 | 7.442081 |
| H | 12.514991 | 1.893962 | 0.069440 | H | 4.402303 | 10.257360 | 5.495775 |
| H | 11.476848 | 1.967882 | 2.034338 | C | 12.609927 | 7.066707 | 1.877282 |
| H | 8.007836 | 4.307506 | 1.797215 | C | 13.606182 | 6.387319 | 1.133346 |
| H | 7.833572 | 5.368847 | -0.082340 | C | 13.747194 | 5.085572 | 1.685019 |
| H | 9.812610 | 6.658117 | -3.351132 | C | 12.843734 | 4.968978 | 2.775207 |
| H | 7.849896 | 5.269786 | -3.568491 | C | 12.138965 | 6.192510 | 2.892847 |
| H | 7.877044 | 7.034885 | -1.909722 | C | 10.910878 | 5.063704 | -2.156206 |
| H | 10.476192 | 2.278659 | 4.293006 | C | 12.218246 | 4.534925 | -1.901883 |
| H | 8.381051 | 1.402034 | 3.462735 | C | 12.729334 | 3.460004 | -1.139102 |
| H | 8.490004 | 3.705965 | 4.174758 | C | 12.225191 | 2.609872 | -0.134335 |
| H | 13.484936 | 6.101511 | -1.668597 | C | 10.987377 | 2.453081 | 0.532611 |
| H | 14.279355 | 3.971187 | -0.228856 | C | 9.654644 | 2.931575 | 0.313263 |
| H | 14.156211 | 4.628376 | 2.378007 | C | 9.126742 | 3.820063 | -0.659485 |
| H | 13.278026 | 7.167848 | 2.545261 | C | 9.635708 | 4.688321 | -1.657884 |
| H | 12.847528 | 8.072124 | 0.055676 | Si | 10.871938 | 6.430726 | -3.466002 |
| O | 9.522085 | 8.345613 | 4.247582 | Si | 8.362928 | 2.170746 | 1.468865 |
| C | 10.104050 | 7.286927 | 3.699389 | H | 13.007182 | 5.062948 | -2.433910 |
| C | 10.399862 | 6.789475 | 2.435639 | H | 13.808773 | 3.374446 | -1.237414 |
| O | 10.175156 | 7.251930 | 1.254563 | H | 13.015540 | 2.038425 | 0.346484 |
| C | 10.760987 | 6.258359 | 4.341139 | H | 11.072760 | 1.790209 | 1.391298 |
| O | 11.284419 | 5.466828 | 5.025110 | H | 8.066123 | 4.011824 | -0.509856 |
| 12 | | | | H | 8.841669 | 5.334305 | -2.026901 |
| SCF (B3PW91) Energy = | | | -1441.413622 | H | 12.139546 | 7.222682 | -3.403991 |
| Enthalpy 0K = | | | -1440.888463 | H | 10.765953 | 5.837530 | -4.835756 |
| Enthalpy 298K = | | | -1440.844907 | H | 9.699111 | 7.326691 | -3.241993 |
| Free Energy 298K = | | | -1440.971169 | H | 8.983877 | 1.883374 | 2.799163 |
| U | 7.684841 | 9.794637 | 4.639197 | H | 7.851905 | 0.880523 | 0.909221 |
| U | 11.231682 | 5.106843 | 0.515690 | H | 7.209710 | 3.104522 | 1.638276 |
| C | 9.189150 | 11.773880 | 3.397126 | H | 14.179467 | 6.795726 | 0.309729 |
| C | 10.073118 | 11.127430 | 4.311350 | H | 14.447244 | 4.328779 | 1.356513 |
| C | 10.048038 | 10.714386 | 5.658053 | H | 12.739326 | 4.108036 | 3.424532 |
| C | 9.113425 | 10.783988 | 6.733359 | H | 11.397880 | 6.440055 | 3.645236 |
| C | 7.836367 | 11.398926 | 6.836338 | H | 12.272723 | 8.083093 | 1.713749 |
| C | 6.960358 | 12.077149 | 5.958106 | O | 7.404904 | 9.385089 | 2.126335 |
| C | 6.954185 | 12.422959 | 4.589168 | C | 8.251357 | 8.447139 | 2.253575 |
| C | 7.877850 | 12.290805 | 3.524662 | C | 9.102173 | 7.385694 | 1.909954 |
| Si | 9.896061 | 11.864101 | 1.649081 | O | 9.591014 | 6.594698 | 1.011496 |
| Si | 9.723908 | 9.993549 | 8.333383 | C | 9.051450 | 7.799689 | 3.247260 |
| C | 5.186145 | 8.619050 | 4.205189 | O | 9.325182 | 7.832989 | 4.490980 |

CO

SCF (B3PW91) Energy = -113.258297
 Enthalpy 0K = -113.253238
 Enthalpy 298K = -113.250878
 Free Energy 298K = -113.272375
 C -0.033084 0.013350 2.235027
 O -0.050778 0.017223 3.371896

CO₂

SCF (B3PW91) Energy = -188.504221
 Enthalpy 0K = -188.492487
 Enthalpy 298K = -188.489853
 Free Energy 298K = -188.513197
 C -0.034873 0.006908 2.227722
 O -0.050155 0.020640 3.395408
 O -0.019591 -0.006825 1.060037

U(η-C₈H₆{SiH₃-1,4}2)(η-Cp)(η³-CO₂) / small core

SCF (B3PW91) Energy = -1178.804804
 Enthalpy 0K = -1178.544491
 Enthalpy 298K = -1178.522978
 Free Energy 298K = -1178.597061
 U -0.034385 -0.040478 0.151339
 C 1.958136 0.251654 1.887396
 C 0.769995 0.313809 2.663644
 C -0.400472 1.107297 2.551327
 C -0.934917 2.018773 1.616217
 C -0.543004 2.558374 0.363802
 C 0.666864 2.468652 -0.376295
 C 1.909511 1.837730 -0.181338
 C 2.440260 0.924884 0.748668
 H 2.652129 -0.520512 2.217591
 Si 0.768411 -0.888397 4.127531
 H 1.592802 -0.335084 5.249088
 H -0.623006 -1.104785 4.622393
 H 1.376334 -2.195424 3.726314
 H -1.150354 0.847454 3.296026
 H -1.970798 2.246588 1.860204
 Si -1.864892 3.617326 -0.484080
 H -3.216215 3.302678 0.066118
 H -1.848321 3.380101 -1.961432
 H -1.585355 5.071566 -0.258905
 H 0.621364 2.969597 -1.342499
 H 2.574210 1.983198 -1.030070
 H 3.412965 0.549243 0.439639
 C 1.249709 -2.150416 -0.981441
 C -0.112639 -2.324144 -1.331781
 C -0.465227 -1.299328 -2.239803
 C 0.676168 -0.489395 -2.454219
 C 1.738450 -1.021989 -1.684220
 H 1.822326 -2.784879 -0.315101
 H -0.767580 -3.102031 -0.962265
 H -1.443188 -1.151248 -2.679849
 H 0.732655 0.371659 -3.108658
 H 2.751690 -0.646926 -1.656755
 O -1.583102 -1.640374 1.210745
 C -2.540500 -1.100976 0.609387
 O -2.467895 -0.191121 -0.247348

U(η-C₈H₆{SiH₃-1,4}2)(η-Cp)(η³-CO₂) / large core

SCF (B3PW91) Energy = -739.253274
 Enthalpy 0K = -738.993131
 Enthalpy 298K = -738.971622
 Free Energy 298K = -739.045298
 U -0.008259 -0.050556 0.099199
 C 1.961559 0.264206 1.903041
 C 0.760159 0.310761 2.678126
 C -0.413005 1.096011 2.551987
 C -0.948613 2.021567 1.618449
 C -0.556979 2.589716 0.380354
 C 0.665908 2.510290 -0.358615
 C 1.912841 1.886047 -0.153230
 C 2.445911 0.961395 0.777328
 H 2.670818 -0.486479 2.247003
 Si 0.774637 -0.853456 4.169824
 H 1.525266 -0.230424 5.306490
 H -0.619099 -1.138059 4.620393
 H 1.471064 -2.130139 3.817856
 H -1.168578 0.830123 3.288257
 H -1.985172 2.242158 1.864587
 Si -1.859206 3.700611 -0.426616
 H -3.220875 3.356369 0.077206
 H -1.809687 3.550893 -1.914596
 H -1.582855 5.138306 -0.110026
 H 0.633463 3.041550 -1.308073
 H 2.588224 2.047940 -0.989877
 H 3.424892 0.601431 0.470605
 C 1.281954 -2.225570 -1.033479
 C -0.089802 -2.405701 -1.341543
 C -0.469807 -1.402492 -2.271027
 C 0.663614 -0.596133 -2.534857
 C 1.747565 -1.105386 -1.769394
 H 1.876010 -2.849020 -0.376209
 H -0.733212 -3.178058 -0.941249
 H -1.456027 -1.275619 -2.698660
 H 0.707157 0.241043 -3.220532
 H 2.759891 -0.723971 -1.772604
 O -1.667223 -1.632180 1.191643
 C -2.600683 -1.106111 0.546179
 O -2.519722 -0.167985 -0.276571

2 Cp*

SCF (B3PW91) Energy = -860.535076
 Enthalpy 0K = -860.140938
 Enthalpy 298K = -860.111765
 Free Energy 298K = -860.200737
 U -0.335881 -0.218945 -0.348165
 C -2.616313 1.243270 -0.496502
 C -2.032158 1.410360 -1.792714
 C -1.559700 0.539738 -2.794805
 C -1.327962 -0.849066 -2.910661
 C -1.492368 -1.970387 -2.065578
 C -2.145646 -2.202224 -0.814492
 C -2.800149 -1.323176 0.091504
 C -2.984946 0.075546 0.229655
 C 1.818890 1.484286 -0.601137
 C 1.905939 0.618985 -1.733170
 C 2.090101 0.709343 0.568009

| | | | | | | | |
|-----------------------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| C | 2.337232 | -0.645582 | 0.153221 | Si | 4.135021 | 1.025927 | 2.436485 |
| C | 2.213980 | -0.698700 | -1.266829 | C | -2.063841 | 1.951237 | 1.927106 |
| C | -0.134790 | -0.807533 | 2.012792 | C | -2.772798 | 0.865073 | 2.529862 |
| O | -0.048600 | -1.089683 | 3.144636 | C | -2.544084 | 0.921056 | 3.929962 |
| H | -3.142162 | -1.835745 | 0.988941 | C | -1.693699 | 2.048987 | 4.196748 |
| H | -3.412476 | 0.305955 | 1.203897 | C | -1.394083 | 2.678222 | 2.957497 |
| Si | -3.140552 | 2.860762 | 0.323912 | C | -0.636333 | 3.960567 | 2.765890 |
| H | -3.172008 | 2.708933 | 1.811011 | C | -1.392088 | 2.612794 | 5.551897 |
| H | -1.890885 | 2.454352 | -2.067653 | C | -3.248235 | 0.092377 | 4.962784 |
| H | -1.158242 | 1.085941 | -3.645194 | C | -3.690274 | -0.083987 | 1.815998 |
| H | -0.785720 | -1.099516 | -3.819864 | C | -2.251132 | 2.436363 | 0.526050 |
| H | -1.040273 | -2.865906 | -2.489524 | C | -0.497844 | -0.270268 | 0.193192 |
| H | -3.293060 | -4.753341 | -0.957569 | O | -1.160211 | -0.646917 | -0.808632 |
| Si | -2.165842 | -4.018062 | -0.298318 | U | 0.382432 | 0.063488 | -2.861179 |
| H | -2.333775 | -4.141755 | 1.181499 | C | 1.205679 | 2.679498 | -3.037070 |
| H | -0.892803 | -4.687733 | -0.715145 | H | 2.847102 | 2.066716 | -4.223561 |
| C | 2.520573 | -1.885893 | -2.134069 | C | -0.126782 | 2.772732 | -2.567672 |
| C | 2.856184 | -1.754481 | 1.022926 | C | -1.384239 | 2.186181 | -2.864240 |
| C | 2.335089 | 1.272260 | 1.938489 | C | -1.903514 | 1.254120 | -3.797437 |
| C | 1.877123 | 1.048475 | -3.169260 | H | -2.112009 | 2.456866 | -2.105577 |
| C | 1.632383 | 2.974179 | -0.641586 | C | -1.315566 | 0.659687 | -4.955693 |
| H | -4.506831 | 3.279008 | -0.127032 | C | -0.053498 | 0.732095 | -5.565238 |
| H | -2.191135 | 3.959013 | -0.042996 | C | 1.218538 | 1.248382 | -5.220768 |
| H | 2.511040 | -2.736286 | 0.686077 | C | 1.762766 | 1.992340 | -4.155795 |
| H | 3.954160 | -1.771579 | 1.006054 | H | 0.001649 | 0.105415 | -6.450956 |
| H | 2.544709 | -1.641505 | 2.063520 | H | 1.989566 | 0.903274 | -5.906392 |
| H | 2.180255 | 0.531298 | 2.725333 | H | -1.986234 | -0.013596 | -5.487589 |
| H | 3.369975 | 1.630331 | 2.021255 | Si | -3.732004 | 0.842671 | -3.581905 |
| H | 1.679768 | 2.120179 | 2.156849 | H | -0.194070 | 3.355892 | -1.652012 |
| H | 2.320416 | -2.829617 | -1.618730 | C | 2.457758 | -1.674838 | -3.574606 |
| H | 1.932263 | -1.883675 | -3.056631 | C | 2.154298 | -1.993152 | -2.220304 |
| H | 3.579270 | -1.896165 | -2.424725 | C | 0.859490 | -2.599478 | -2.188130 |
| H | 1.480218 | 0.268971 | -3.825121 | C | 0.359764 | -2.646617 | -3.522661 |
| H | 1.275022 | 1.948610 | -3.317084 | C | 1.359637 | -2.102085 | -4.382695 |
| H | 2.893537 | 1.277487 | -3.515052 | C | 1.369367 | -2.211777 | -5.876433 |
| H | 1.176309 | 3.353580 | 0.277492 | C | -0.909257 | -3.322227 | -3.957458 |
| H | 2.595858 | 3.487547 | -0.757327 | C | 0.233043 | -3.298036 | -1.021965 |
| H | 0.996956 | 3.286345 | -1.475507 | C | 3.130931 | -1.921312 | -1.086452 |
| 4 Cp* | | | | C | 3.781897 | -1.178160 | -4.076109 |
| SCF (B3PW91) Energy = | | | | C | 0.722530 | 0.543976 | -0.265523 |
| Enthalpy 0K = | | | | O | 1.152186 | 1.256728 | 0.676565 |
| Enthalpy 298K = | | | | H | 5.379150 | 0.803413 | 3.245162 |
| Free Energy 298K = | | | | H | 4.398610 | 0.530615 | 1.052460 |
| -1720.398934 | | | | H | 3.884466 | 2.499978 | 2.415397 |
| U | -0.076213 | 0.242210 | 2.781775 | H | -0.352821 | -5.031577 | 4.038290 |
| C | 2.128913 | 0.790650 | 4.338560 | H | -2.244325 | -3.669938 | 3.415254 |
| H | 2.581773 | 1.763071 | 4.528239 | H | -0.599517 | -4.327110 | 1.736468 |
| C | 2.679731 | 0.109343 | 3.216189 | H | -4.001019 | -0.577573 | -3.971458 |
| C | 2.348761 | -1.123977 | 2.605978 | H | -4.161199 | 1.058847 | -2.166933 |
| C | 1.340265 | -2.114512 | 2.711386 | H | -4.582415 | 1.712092 | -4.458178 |
| H | 1.422454 | -2.835223 | 1.900649 | Si | 2.478505 | 3.677319 | -2.061993 |
| C | 0.200899 | -2.341871 | 3.533215 | H | 1.923062 | 4.091904 | -0.740467 |
| C | -0.252637 | -1.661157 | 4.701764 | H | 3.735042 | 2.889104 | -1.864865 |
| C | 0.197583 | -0.554215 | 5.452556 | H | 2.854003 | 4.915604 | -2.820251 |
| C | 1.164389 | 0.460239 | 5.311186 | H | -1.305421 | -2.895912 | -4.883753 |
| H | 1.055586 | 1.235693 | 6.064466 | H | -0.743422 | -4.392487 | -4.138449 |
| H | -0.458769 | -0.360352 | 6.298160 | H | -1.692779 | -3.241850 | -3.198635 |
| H | -1.173564 | -2.071729 | 5.112203 | H | -0.857378 | -3.230579 | -1.035864 |
| Si | -0.788237 | -3.902247 | 3.155058 | H | 0.504011 | -4.361868 | -1.030789 |
| H | 2.966664 | -1.315844 | 1.732758 | H | 0.562042 | -2.883213 | -0.068119 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|----------|-----------|-----------|
| H | 2.623125 | -1.981083 | -0.123241 | U | 3.450241 | -3.551759 | -1.310158 |
| H | 3.839913 | -2.758268 | -1.135927 | C | 5.945355 | -3.587860 | -2.373859 |
| H | 3.716067 | -0.997415 | -1.092208 | H | 6.152874 | -5.648017 | -2.373327 |
| H | 3.683958 | -0.630699 | -5.017388 | C | 5.486719 | -2.252647 | -2.572995 |
| H | 4.268551 | -0.513819 | -3.356298 | C | 4.324219 | -1.755176 | -3.219083 |
| H | 4.468506 | -2.015446 | -4.258252 | C | 3.144680 | -2.308625 | -3.779103 |
| H | 0.360742 | -2.213254 | -6.297164 | H | 4.273354 | -0.668449 | -3.206962 |
| H | 1.934722 | -1.406660 | -6.353016 | C | 2.562647 | -3.588076 | -3.944212 |
| H | 1.843464 | -3.156609 | -6.173698 | C | 3.044204 | -4.896783 | -3.657310 |
| H | -3.317811 | -0.337993 | 0.820107 | C | 2.248211 | -1.553964 | -0.015167 |
| H | -3.814388 | -1.019865 | 2.368707 | C | 4.285360 | -5.422437 | -3.238398 |
| H | -4.689403 | 0.355334 | 1.697522 | C | 5.471108 | -4.872811 | -2.716424 |
| H | -1.341099 | 2.889448 | 0.126146 | H | 2.313166 | -5.682129 | -3.844164 |
| H | -2.552382 | 1.627517 | -0.140537 | H | 4.276456 | -6.507557 | -3.181967 |
| H | -3.037556 | 3.202222 | 0.495470 | Si | 0.823269 | -3.578770 | -4.680664 |
| H | -2.668586 | 0.000653 | 5.884910 | H | 2.457647 | -1.514026 | -4.058966 |
| H | -4.209441 | 0.550908 | 5.229032 | Si | 6.766131 | -0.966156 | -2.056132 |
| H | -3.461609 | -0.918138 | 4.603396 | H | 6.881871 | -3.644887 | -1.821458 |
| H | 0.071819 | 4.142641 | 3.579301 | C | 4.838665 | -4.901917 | 0.723386 |
| H | -0.069072 | 3.963804 | 1.830386 | C | 4.029643 | -3.947307 | 1.395602 |
| H | -1.320397 | 4.818754 | 2.734208 | C | 2.661781 | -4.341097 | 1.229821 |
| H | -0.446348 | 3.161047 | 5.569354 | C | 2.630535 | -5.540423 | 0.455931 |
| H | -2.180056 | 3.317329 | 5.848891 | C | 3.972299 | -5.897961 | 0.155954 |
| H | -1.344744 | 1.839854 | 6.322979 | C | 4.412771 | -7.212553 | -0.410694 |

4-5-TS Cp*

SCF (B3PW91) Energy = -1721.091347

Enthalpy 0K = -1720.300613

Enthalpy 298K = -1720.242246

Free Energy 298K = -1720.392270

Negative frequency = -635.2516 cm⁻¹

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| U | 0.004440 | 0.443016 | 0.272943 | C | 1.404152 | -6.353821 | 0.158533 |
| C | -0.792007 | -0.104164 | 2.847615 | C | 1.498101 | -3.813058 | 2.006328 |
| Si | 0.149688 | -0.239470 | 4.477331 | C | 4.526610 | -2.826122 | 2.260783 |
| C | -0.986776 | -1.327393 | 2.160515 | C | 6.333967 | -4.988965 | 0.798324 |
| C | -1.561499 | -1.754594 | 0.935327 | O | 2.140494 | -0.682360 | 0.912659 |
| C | -2.200709 | -1.160772 | -0.181977 | H | 6.151026 | 0.387315 | -1.925272 |
| Si | -2.699204 | -2.352640 | -1.561442 | H | 7.401203 | -1.351484 | -0.755638 |
| C | -2.616526 | 0.180896 | -0.429089 | H | 7.861307 | -0.880735 | -3.074824 |
| C | -2.614223 | 1.366156 | 0.328692 | H | -0.024609 | -4.639829 | -4.056868 |
| C | -2.067283 | 1.780617 | 1.565128 | H | 0.183021 | -2.239568 | -4.519992 |
| C | -1.266341 | 1.212439 | 2.572736 | H | 0.890027 | -3.876921 | -6.150180 |
| H | -0.930563 | 1.958351 | 3.291809 | H | -2.373723 | -1.779277 | -2.904100 |
| H | -2.194414 | 2.848727 | 1.714562 | H | -2.031828 | -3.674160 | -1.386402 |
| H | -3.046040 | 2.200870 | -0.218171 | H | -4.183473 | -2.565020 | -1.524887 |
| H | -3.047042 | 0.331484 | -1.418220 | H | -0.798537 | -0.335705 | 5.633880 |
| H | -1.359688 | -2.811156 | 0.773618 | H | 1.016597 | -1.456345 | 4.491868 |
| H | -0.478829 | -2.155949 | 2.644667 | H | 0.995631 | 0.976072 | 4.696656 |
| C | 2.140674 | 1.865946 | -0.767844 | H | 3.679658 | -7.627450 | -1.107167 |
| C | 1.231896 | 1.738582 | -1.863794 | H | 5.370692 | -7.142654 | -0.931374 |
| C | 0.091847 | 2.545541 | -1.588038 | H | 4.538605 | -7.942875 | 0.399384 |
| C | 0.299970 | 3.183180 | -0.326758 | H | 1.545039 | -6.998033 | -0.714154 |
| C | 1.552991 | 2.741384 | 0.193704 | H | 1.150431 | -7.004989 | 1.005350 |
| C | 2.217790 | 3.249672 | 1.441014 | H | 0.534671 | -5.720792 | -0.039000 |
| C | -0.513658 | 4.316369 | 0.217772 | H | 6.763545 | -5.477024 | -0.080595 |
| C | -1.014153 | 2.846179 | -2.555647 | H | 6.797898 | -4.003189 | 0.890275 |
| C | 1.501616 | 1.054956 | -3.169492 | H | 6.640026 | -5.573885 | 1.675536 |
| C | 3.549883 | 1.365152 | -0.719782 | H | 3.850786 | -1.967891 | 2.251009 |
| C | 1.074556 | -1.860601 | -0.804931 | H | 4.628969 | -3.160161 | 3.301666 |
| O | 0.913451 | -2.981705 | -1.354581 | H | 5.510936 | -2.473457 | 1.938681 |
| | | | | H | 0.571121 | -3.865567 | 1.429651 |
| | | | | H | 1.353163 | -4.414603 | 2.913415 |
| | | | | H | 1.650944 | -2.779025 | 2.316294 |
| | | | | H | 3.884530 | 1.192682 | 0.305467 |
| | | | | H | 3.669189 | 0.419928 | -1.252526 |
| | | | | H | 4.226010 | 2.098530 | -1.177744 |
| | | | | H | 1.489651 | 3.523071 | 2.210541 |

| | | | |
|---|-----------|----------|-----------|
| H | 2.890349 | 2.504718 | 1.875459 |
| H | 2.818634 | 4.144238 | 1.230780 |
| H | 0.615514 | 0.550412 | -3.566567 |
| H | 1.834443 | 1.778640 | -3.925151 |
| H | 2.282708 | 0.302699 | -3.060567 |
| H | -1.957800 | 3.069388 | -2.050498 |
| H | -0.762695 | 3.719782 | -3.171436 |
| H | -1.194470 | 2.012862 | -3.240317 |
| H | -0.448036 | 4.389364 | 1.306571 |
| H | -0.143495 | 5.266301 | -0.190421 |
| H | -1.569307 | 4.241035 | -0.056247 |

6 Cp*

SCF (B3PW91) Energy = -1721.137636
Enthalpy 0K = -1720.346593
Enthalpy 298K = -1720.286825
Free Energy 298K = -1720.444481

| | | | |
|----|-----------|-----------|-----------|
| U | 0.058319 | 0.238857 | 3.354805 |
| C | 2.319373 | -0.885048 | 4.458334 |
| Si | 4.052096 | -0.183414 | 4.720644 |
| C | 2.140838 | -1.578856 | 3.233594 |
| C | 1.072342 | -2.160328 | 2.511251 |
| C | -0.319074 | -2.373609 | 2.719940 |
| Si | -1.196220 | -3.238721 | 1.293689 |
| C | -1.143071 | -2.188552 | 3.874531 |
| C | -0.946651 | -1.658904 | 5.160627 |
| C | 0.085482 | -0.953579 | 5.822163 |
| C | 1.419178 | -0.586706 | 5.522732 |
| H | 1.847514 | 0.047175 | 6.297808 |
| H | -0.251357 | -0.530032 | 6.764655 |
| H | -1.869040 | -1.648377 | 5.737381 |
| H | -2.180576 | -2.474990 | 3.712458 |
| H | 1.384519 | -2.397903 | 1.496701 |
| H | 3.024690 | -1.521515 | 2.601471 |
| C | -1.054425 | 2.724303 | 2.864447 |
| C | -2.061908 | 1.786203 | 2.482149 |
| C | -2.557506 | 1.162408 | 3.666210 |
| C | -1.849991 | 1.712918 | 4.780621 |
| C | -0.910382 | 2.664713 | 4.281568 |
| C | -0.025180 | 3.549757 | 5.112126 |
| C | -2.205689 | 1.516528 | 6.223429 |
| C | -3.750395 | 0.256276 | 3.748427 |
| C | -2.623233 | 1.615967 | 1.099505 |
| C | -0.381703 | 3.709073 | 1.958650 |
| C | 0.740261 | 0.729340 | -0.124391 |
| O | 0.319796 | 0.383026 | -1.289360 |
| U | 0.319601 | 0.185728 | -3.524688 |
| C | -0.211217 | 2.116196 | -5.300258 |
| H | 0.315745 | 1.024966 | -6.985762 |
| C | -0.832836 | 2.564765 | -4.090700 |
| C | -1.789641 | 1.941691 | -3.248593 |
| C | -2.376209 | 0.659044 | -3.119746 |
| H | -2.034304 | 2.550960 | -2.380745 |
| C | -2.283971 | -0.600787 | -3.764734 |
| C | -1.614685 | -1.001894 | -4.964476 |
| C | 1.155256 | 1.042780 | 0.986443 |
| C | -0.891694 | -0.320323 | -5.969975 |
| C | -0.323310 | 0.962061 | -6.107882 |
| H | -1.717496 | -2.062714 | -5.186542 |
| H | -0.577886 | -0.988719 | -6.767408 |

| | | | |
|----|-----------|-----------|-----------|
| Si | -3.322480 | -1.969410 | -2.980168 |
| H | -2.931730 | 0.600434 | -2.185958 |
| Si | -0.393709 | 4.339138 | -3.612673 |
| H | 0.495970 | 2.831906 | -5.715033 |
| C | 3.029893 | 0.155353 | -3.138620 |
| C | 2.591561 | -1.154400 | -2.767315 |
| C | 2.178798 | -1.836242 | -3.949928 |
| C | 2.380769 | -0.956122 | -5.057434 |
| C | 2.902432 | 0.276288 | -4.554572 |
| C | 3.386198 | 1.424825 | -5.390965 |
| C | 2.307012 | -1.349418 | -6.501692 |
| C | 1.768119 | -3.278776 | -4.041261 |
| C | 2.689241 | -1.755283 | -1.397371 |
| C | 3.633740 | 1.172156 | -2.212465 |
| O | 1.612374 | 1.439201 | 2.141430 |
| H | -0.559399 | 4.538739 | -2.141954 |
| H | 1.019403 | 4.638118 | -4.005467 |
| H | -1.277026 | 5.317115 | -4.324002 |
| H | -2.644272 | -3.293712 | -3.144547 |
| H | -3.542780 | -1.691570 | -1.529584 |
| H | -4.660189 | -2.064866 | -3.647383 |
| H | -2.639966 | -2.845501 | 1.252193 |
| H | -0.551946 | -2.895413 | -0.010753 |
| H | -1.143633 | -4.728748 | 1.450067 |
| H | 4.850886 | -1.063956 | 5.635158 |
| H | 4.785688 | -0.081357 | 3.423543 |
| H | 3.979044 | 1.165063 | 5.367670 |
| H | 2.072085 | -0.503167 | -7.152622 |
| H | 3.273484 | -1.751250 | -6.833443 |
| H | 1.559301 | -2.126852 | -6.679840 |
| H | 1.069105 | -3.456283 | -4.864208 |
| H | 2.639893 | -3.923409 | -4.213009 |
| H | 1.289032 | -3.629065 | -3.122372 |
| H | 1.952648 | -2.550164 | -1.247541 |
| H | 3.681040 | -2.201400 | -1.248491 |
| H | 2.535051 | -1.011387 | -0.611499 |
| H | 2.804113 | 1.533910 | -6.310723 |
| H | 3.333547 | 2.375485 | -4.852838 |
| H | 4.433432 | 1.277700 | -5.684986 |
| H | 3.530217 | 2.190673 | -2.599692 |
| H | 3.175741 | 1.147853 | -1.219446 |
| H | 4.707884 | 0.988113 | -2.082129 |
| H | -3.047389 | 0.618282 | 0.950156 |
| H | -3.428742 | 2.339675 | 0.916851 |
| H | -1.858193 | 1.764500 | 0.333020 |
| H | 0.621358 | 3.962400 | 2.308929 |
| H | -0.276975 | 3.316760 | 0.944429 |
| H | -0.966487 | 4.636555 | 1.904399 |
| H | 0.283163 | 3.063659 | 6.043116 |
| H | 0.882666 | 3.835013 | 4.572786 |
| H | -0.542021 | 4.477945 | 5.389254 |
| H | -1.350743 | 1.677929 | 6.885794 |
| H | -2.982053 | 2.233719 | 6.521254 |
| H | -2.600152 | 0.516420 | 6.422293 |
| H | -3.685502 | -0.431417 | 4.596154 |
| H | -4.672079 | 0.839809 | 3.873808 |
| H | -3.872052 | -0.346384 | 2.844049 |

7 Cp*

SCF (B3PW91) Energy = -1721.140462

| | | | | | | | |
|--------------------|--------------|-----------|-----------|-----------------------|--------------|-----------|-----------|
| Enthalpy 0K = | -1720.348634 | H | -0.481322 | 2.621531 | -5.811555 | | |
| Enthalpy 298K = | -1720.289036 | H | -1.425731 | 4.407714 | -2.242217 | | |
| Free Energy 298K = | -1720.446873 | H | -0.104063 | 4.628699 | -4.285154 | | |
| U | 0.112660 | 0.165720 | -3.437471 | H | -2.505803 | 4.853159 | -4.364429 |
| O | 0.360539 | 0.560159 | -1.280109 | H | -2.042414 | -3.737996 | -2.498180 |
| C | 0.719753 | 0.672346 | -0.045215 | H | -2.925146 | -2.201917 | -0.814487 |
| C | 1.058133 | 0.751844 | 1.121077 | H | -4.307954 | -2.923295 | -2.669262 |
| O | 1.398143 | 0.844544 | 2.362843 | H | -1.520185 | -1.628484 | 5.574904 |
| U | 1.678328 | 1.399865 | 4.484113 | H | -0.229191 | -2.810836 | 3.869007 |
| C | -0.978131 | 1.824397 | -5.261253 | H | -0.079224 | -3.461666 | 6.199136 |
| C | -0.961829 | 0.605336 | -5.973260 | H | 7.007607 | 0.303153 | 4.515817 |
| C | -1.266298 | -0.740767 | -5.681451 | H | 5.737773 | 0.357402 | 2.452198 |
| C | -1.725253 | -1.453083 | -4.551699 | H | 6.041650 | 2.387772 | 3.776079 |
| C | -2.294553 | -1.081234 | -3.291228 | H | 1.769239 | -0.030600 | -7.192705 |
| Si | -2.915073 | -2.542963 | -2.269016 | H | 3.042899 | -1.237534 | -7.038144 |
| C | -1.529519 | 2.252570 | -4.010471 | H | 1.356793 | -1.717371 | -6.862219 |
| Si | -1.383858 | 4.109603 | -3.706134 | H | 1.087911 | -3.271981 | -5.138799 |
| C | -2.238819 | 1.541902 | -3.008084 | H | 2.738226 | -3.642256 | -4.640318 |
| C | -2.549854 | 0.191212 | -2.717665 | H | 1.449128 | -3.588232 | -3.440860 |
| C | 3.978535 | 1.425706 | 5.882535 | H | 2.070456 | -2.621983 | -1.510406 |
| C | 3.025197 | 1.476310 | 6.922829 | H | 3.741137 | -2.064464 | -1.473233 |
| C | 1.798591 | 0.839891 | 7.205907 | H | 2.461755 | -1.079354 | -0.749635 |
| C | 0.997320 | -0.139707 | 6.577590 | H | 2.247634 | 2.013099 | -6.136665 |
| C | 1.205632 | -1.071018 | 5.510054 | H | 2.964547 | 2.699524 | -4.677618 |
| Si | -0.213563 | -2.293565 | 5.270396 | H | 3.955940 | 1.750531 | -5.782335 |
| C | 2.317733 | -1.280230 | 4.654575 | H | 3.243092 | 2.339089 | -2.497534 |
| C | 3.540649 | -0.629654 | 4.358784 | H | 2.981316 | 1.174607 | -1.196676 |
| C | 4.229398 | 0.534044 | 4.789725 | H | 4.498177 | 1.166603 | -2.106122 |
| Si | 5.816025 | 0.908773 | 3.839008 | H | -1.941288 | 1.893410 | 3.198949 |
| C | 2.839804 | 0.328746 | -3.183439 | H | -2.001480 | 3.500201 | 2.478479 |
| C | 2.520171 | -1.038879 | -2.912587 | H | -0.893583 | 2.279591 | 1.833796 |
| C | 2.109791 | -1.647431 | -4.135338 | H | 2.504170 | 4.196882 | 1.879236 |
| C | 2.181795 | -0.658610 | -5.164524 | H | 1.127040 | 3.297231 | 1.240246 |
| C | 2.625369 | 0.564916 | -4.573584 | H | 0.977458 | 5.025877 | 1.586574 |
| C | 3.412311 | 1.301342 | -2.194064 | H | 3.462770 | 4.776509 | 5.531087 |
| C | 2.701849 | -1.732157 | -1.593868 | H | 3.552286 | 4.816632 | 3.770180 |
| C | 1.825617 | -3.106721 | -4.347767 | H | 2.666242 | 6.070146 | 4.635409 |
| C | 2.071238 | -0.921478 | -6.635528 | H | 2.063474 | 4.354425 | 7.319492 |
| C | 2.959190 | 1.820249 | -5.327752 | H | 0.541158 | 5.236063 | 7.229622 |
| C | -0.269330 | 3.165422 | 3.706589 | H | 0.552313 | 3.562897 | 7.780701 |
| C | 0.964932 | 3.789315 | 3.341602 | H | -1.281666 | 2.411794 | 6.934252 |
| C | 1.630934 | 4.184720 | 4.539403 | H | -2.251072 | 3.610210 | 6.078181 |
| C | 0.803186 | 3.817992 | 5.645162 | H | -2.131808 | 1.967904 | 5.452792 |
| C | -0.368083 | 3.181903 | 5.129384 | | | | |
| C | 1.417154 | 4.084714 | 1.941524 | | | | |
| C | -1.324599 | 2.681407 | 2.755051 | 8 Cp* | | | |
| C | -1.563143 | 2.766180 | 5.938297 | SCF (B3PW91) Energy = | -1607.795469 | | |
| C | 1.004922 | 4.254328 | 7.064730 | Enthalpy 0K = | -1607.013687 | | |
| C | 2.892240 | 4.995954 | 4.623613 | Enthalpy 298K = | -1606.956402 | | |
| H | 4.696633 | 2.240821 | 5.951565 | Free Energy 298K = | -1607.107126 | | |
| H | 3.203576 | 2.315385 | 7.590423 | U | -0.382674 | -0.349465 | -0.208159 |
| H | 1.279074 | 1.316547 | 8.033690 | C | -2.345679 | 1.552680 | -0.172328 |
| H | 0.014601 | -0.218754 | 7.039019 | C | -1.748438 | 1.798940 | -1.451663 |
| H | 2.123741 | -2.052182 | 3.912361 | C | -1.473158 | 1.019094 | -2.582620 |
| H | 3.981198 | -1.062008 | 3.462547 | C | -1.524990 | -0.356299 | -2.913376 |
| H | -0.459901 | 0.705115 | -6.932498 | C | -1.893492 | -1.534475 | -2.246444 |
| H | -2.485106 | 2.169754 | -2.153999 | C | -2.547354 | -1.827544 | -1.006497 |
| H | -1.650562 | -2.529821 | -4.693087 | C | -3.032351 | -0.986289 | 0.033095 |
| H | -0.935730 | -1.408914 | -6.472782 | C | -2.947219 | 0.386527 | 0.379588 |
| H | -2.959486 | 0.114555 | -1.712298 | C | 2.038410 | 0.943691 | -0.564315 |
| | | | | C | 1.871351 | 0.181757 | -1.758530 |

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|----|-----------|-----------|-----------|
| C | 2.258205 | 0.031682 | 0.511033 |
| C | 2.204870 | -1.304974 | -0.024273 |
| C | 1.949978 | -1.206389 | -1.422752 |
| C | -0.006284 | -1.129900 | 1.971524 |
| O | 0.200124 | -1.534362 | 3.127454 |
| H | -3.490650 | -1.550597 | 0.843185 |
| H | -3.346668 | 0.553048 | 1.378371 |
| Si | -2.557478 | 3.111669 | 0.857880 |
| H | -2.701692 | 2.781972 | 2.310574 |
| H | -1.406034 | 2.825976 | -1.573122 |
| H | -0.991080 | 1.600605 | -3.365337 |
| H | -1.065270 | -0.560768 | -3.878424 |
| H | -1.633160 | -2.426140 | -2.815075 |
| H | -4.284050 | -4.012753 | -1.327824 |
| Si | -2.936907 | -3.652442 | -0.772537 |
| H | -2.946966 | -4.023161 | 0.677374 |
| H | -1.927848 | -4.504021 | -1.480112 |
| C | 1.949804 | -2.342041 | -2.404923 |
| C | 2.602486 | -2.560719 | 0.690242 |
| C | 2.757910 | 0.422837 | 1.868211 |
| C | 1.845919 | 0.734971 | -3.150300 |
| C | 2.134150 | 2.439957 | -0.478758 |
| H | -3.777952 | 3.886768 | 0.455966 |
| H | -1.383867 | 4.027691 | 0.686433 |
| U | 0.350516 | -2.194785 | 5.371364 |
| C | 2.801101 | -1.263796 | 6.099836 |
| C | 2.086501 | -1.508838 | 7.314718 |
| C | 1.443918 | -2.630615 | 7.881463 |
| C | 1.049365 | -3.909545 | 7.434239 |
| C | 1.126950 | -4.625078 | 6.219921 |
| C | 1.837835 | -4.444221 | 4.991728 |
| C | 2.694253 | -3.402996 | 4.551679 |
| C | 3.079217 | -2.111217 | 4.994109 |
| C | -1.644640 | -0.699777 | 6.555576 |
| C | -1.826979 | -2.003572 | 7.112707 |
| C | -1.966451 | -0.768105 | 5.167196 |
| C | -2.328381 | -2.123367 | 4.862060 |
| C | -2.236302 | -2.885112 | 6.064308 |
| H | 3.058225 | -3.572220 | 3.540955 |
| H | 3.650742 | -1.604793 | 4.218898 |
| Si | 3.661595 | 0.418442 | 6.071040 |
| H | 3.992430 | 0.818058 | 4.671838 |
| H | 2.032063 | -0.639749 | 7.968341 |
| H | 1.027912 | -2.404100 | 8.859542 |
| H | 0.411124 | -4.410235 | 8.158214 |
| H | 0.528736 | -5.534201 | 6.246570 |
| H | 2.633486 | -6.996501 | 4.176184 |
| Si | 1.677132 | -5.906268 | 3.803373 |
| H | 1.973065 | -5.475103 | 2.405317 |
| H | 0.294162 | -6.473525 | 3.875886 |
| C | -2.653437 | -4.315833 | 6.245614 |
| C | -2.866373 | -2.605445 | 3.549942 |
| C | -2.087800 | 0.398570 | 4.237389 |
| C | -1.851915 | -2.326467 | 8.575513 |
| C | -1.344623 | 0.549985 | 7.333309 |
| H | 4.932967 | 0.366482 | 6.859895 |
| H | 2.783921 | 1.455600 | 6.698490 |
| H | 2.048979 | -3.429305 | 0.323693 |
| H | 3.672863 | -2.766238 | 0.548504 |
| H | 2.412489 | -2.489230 | 1.762209 |

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|---|-----------|-----------|-----------|
| H | 2.518429 | -0.326024 | 2.624777 |
| H | 3.849871 | 0.546367 | 1.853811 |
| H | 2.327356 | 1.370739 | 2.202346 |
| H | 1.781340 | 2.817567 | 0.485703 |
| H | 3.171576 | 2.779823 | -0.598133 |
| H | 1.540090 | 2.930127 | -1.255315 |
| H | 1.246670 | 0.122644 | -3.828667 |
| H | 1.450794 | 1.752979 | -3.179796 |
| H | 2.866362 | 0.768671 | -3.554854 |
| H | 1.650480 | -3.284376 | -1.937202 |
| H | 1.266488 | -2.160058 | -3.240086 |
| H | 2.950251 | -2.496580 | -2.830835 |
| H | -2.897922 | -3.696902 | 3.498957 |
| H | -3.892754 | -2.246049 | 3.400713 |
| H | -2.272916 | -2.254020 | 2.700606 |
| H | -2.526408 | -4.899884 | 5.329976 |
| H | -2.077320 | -4.811302 | 7.032747 |
| H | -3.712047 | -4.381391 | 6.527620 |
| H | -1.565351 | -3.361228 | 8.780167 |
| H | -1.195300 | -1.673223 | 9.155511 |
| H | -2.868066 | -2.190905 | 8.968242 |
| H | -0.806851 | 1.289791 | 6.733475 |
| H | -2.270627 | 1.027377 | 7.678624 |
| H | -0.737519 | 0.344041 | 8.219551 |
| H | -1.595479 | 0.232158 | 3.271694 |
| H | -3.144535 | 0.608224 | 4.030079 |
| H | -1.662128 | 1.306738 | 4.671873 |

8-9-TS Cp*

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|-----------------------|----------------------------|-----------|-----------|
| SCF (B3PW91) Energy = | -1607.783398 | | |
| Enthalpy 0K = | -1607.001841 | | |
| Enthalpy 298K = | -1606.945228 | | |
| Free Energy 298K = | -1607.093103 | | |
| Negative frequency = | -115.5730 cm ⁻¹ | | |
| U | 0.091010 | -0.120924 | 0.160826 |
| U | -0.071312 | 0.076511 | 5.694708 |
| C | 2.543585 | -1.342811 | -0.192250 |
| C | 2.866165 | -0.068304 | 0.341555 |
| C | 2.467079 | 1.278974 | 0.165880 |
| C | 1.592118 | 1.992348 | -0.700652 |
| C | 0.879290 | 1.569052 | -1.863124 |
| C | 0.685197 | 0.342177 | -2.518979 |
| C | 0.960836 | -1.017759 | -2.241325 |
| C | 1.695763 | -1.731619 | -1.264154 |
| Si | 3.366803 | -2.799547 | 0.691803 |
| Si | 1.543968 | 3.865675 | -0.452268 |
| C | -2.346638 | -1.103007 | 0.929212 |
| C | -2.513506 | 0.320293 | 0.901629 |
| C | -2.485058 | 0.735345 | -0.463640 |
| C | -2.309816 | -0.427239 | -1.274631 |
| C | -2.201758 | -1.560805 | -0.411790 |
| H | 2.436777 | -3.970322 | 0.726057 |
| H | 4.597499 | -3.225850 | -0.049753 |
| H | 3.766054 | -2.416690 | 2.077528 |
| H | 2.105622 | 4.229840 | 0.881263 |
| H | 0.142780 | 4.381420 | -0.562341 |
| H | 2.353214 | 4.545137 | -1.512867 |
| H | 3.495268 | -0.151482 | 1.224696 |
| H | 2.891102 | 1.910898 | 0.943054 |
| H | 0.319228 | 2.371255 | -2.342036 |

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|----|-----------|-----------|-----------|
| H | 0.015202 | 0.442373 | -3.367883 |
| H | 0.434644 | -1.684428 | -2.920510 |
| H | 1.585016 | -2.808624 | -1.377713 |
| C | -2.492310 | -1.977452 | 2.132064 |
| C | -2.896932 | 1.189681 | 2.063687 |
| C | -2.784274 | 2.117891 | -0.966579 |
| C | -2.490984 | -0.491333 | -2.760048 |
| C | -2.143611 | -2.994431 | -0.854814 |
| C | 1.139251 | 2.388358 | 4.812752 |
| C | 2.210742 | 1.439833 | 4.953428 |
| C | 2.394267 | 1.190333 | 6.344132 |
| C | 1.455491 | 1.988703 | 7.062244 |
| C | 0.666615 | 2.714573 | 6.116678 |
| C | -0.342306 | -2.589654 | 6.243887 |
| C | 0.374323 | -2.032552 | 7.346659 |
| C | 0.082182 | -1.049552 | 8.317135 |
| C | -0.939171 | -0.092819 | 8.512009 |
| C | -2.055930 | 0.361462 | 7.799123 |
| C | -2.700596 | -0.031382 | 6.587023 |
| C | -2.518741 | -1.169229 | 5.748221 |
| C | -1.571213 | -2.218115 | 5.633170 |
| Si | 0.493520 | -4.092667 | 5.479876 |
| Si | -4.246467 | 0.977525 | 6.217048 |
| H | 1.342453 | -2.501234 | 7.518678 |
| H | 0.880050 | -0.952471 | 9.050429 |
| H | -0.736119 | 0.529495 | 9.380476 |
| H | -2.483360 | 1.259151 | 8.245112 |
| H | -3.239368 | -1.209472 | 4.933819 |
| H | -1.796612 | -2.833679 | 4.764963 |
| H | 1.984404 | -3.953011 | 5.517528 |
| H | 0.155291 | -5.346765 | 6.231806 |
| H | 0.048807 | -4.289974 | 4.064696 |
| H | -4.016449 | 2.434830 | 6.479444 |
| H | -5.398954 | 0.555048 | 7.078597 |
| H | -4.665452 | 0.805388 | 4.790752 |
| C | 3.143654 | 0.995642 | 3.870577 |
| C | 3.483103 | 0.357988 | 6.956135 |
| C | 1.456322 | 2.213641 | 8.542787 |
| C | -0.345602 | 3.773757 | 6.446124 |
| C | 0.757477 | 3.125807 | 3.563667 |
| C | 0.266828 | -0.400422 | 3.374210 |
| O | 0.546868 | -1.040634 | 2.340573 |
| H | -0.320493 | 3.298976 | 3.497081 |
| H | 1.249145 | 4.108089 | 3.533586 |
| H | 1.053730 | 2.579219 | 2.666575 |
| H | 3.586710 | 0.020495 | 4.088749 |
| H | 2.629014 | 0.910448 | 2.913011 |
| H | 3.967230 | 1.712727 | 3.746560 |
| H | 3.169656 | -0.083611 | 7.906600 |
| H | 3.788022 | -0.462133 | 6.299457 |
| H | 4.377854 | 0.962000 | 7.156975 |
| H | 0.481902 | 2.546452 | 8.907711 |
| H | 1.737024 | 1.316295 | 9.100034 |
| H | 2.184268 | 2.995471 | 8.797874 |
| H | -0.902106 | 3.540644 | 7.358592 |
| H | 0.138347 | 4.747534 | 6.600180 |
| H | -1.076436 | 3.903522 | 5.642492 |
| H | -2.297102 | 2.322980 | -1.923979 |
| H | -3.863622 | 2.250177 | -1.116654 |
| H | -2.461913 | 2.890345 | -0.262861 |

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|---|-----------|-----------|-----------|
| H | -1.864775 | -1.256081 | -3.228190 |
| H | -3.533270 | -0.746533 | -2.992025 |
| H | -2.280256 | 0.464856 | -3.244729 |
| H | -1.590972 | -3.111577 | -1.791720 |
| H | -1.666767 | -3.635572 | -0.108199 |
| H | -3.153004 | -3.392044 | -1.022492 |
| H | -1.907606 | -2.898045 | 2.050748 |
| H | -2.166599 | -1.459132 | 3.034412 |
| H | -3.542712 | -2.264700 | 2.270703 |
| H | -2.582824 | 2.227706 | 1.918213 |
| H | -3.987745 | 1.195884 | 2.189868 |
| H | -2.442902 | 0.839657 | 2.993672 |

10 Cp*

| | | | |
|-----------------------|-----------|--------------|-----------|
| SCF (B3PW91) Energy = | | -1721.105584 | |
| Enthalpy 0K = | | -1720.312935 | |
| Enthalpy 298K = | | -1720.254249 | |
| Free Energy 298K = | | -1720.403656 | |
| U | 8.070090 | 9.321015 | 3.480272 |
| U | 10.749567 | 5.979725 | 1.238776 |
| C | 9.639931 | 11.044820 | 1.694227 |
| C | 10.450346 | 10.854963 | 2.842236 |
| C | 10.287747 | 10.764313 | 4.236849 |
| C | 9.228033 | 11.039915 | 5.155467 |
| C | 7.950250 | 11.626998 | 4.924312 |
| C | 7.160154 | 11.929048 | 3.796817 |
| C | 7.226764 | 11.695462 | 2.409470 |
| C | 8.256157 | 11.286531 | 1.528435 |
| Si | 10.575070 | 10.794557 | 0.076382 |
| Si | 9.733632 | 10.918206 | 6.969655 |
| C | 5.703774 | 7.836472 | 3.203933 |
| C | 6.408009 | 7.206315 | 4.271305 |
| C | 6.429090 | 8.105828 | 5.379794 |
| C | 5.675651 | 9.264028 | 5.017423 |
| C | 5.257246 | 9.113658 | 3.662527 |
| H | 9.823609 | 11.428390 | -1.050158 |
| H | 11.925554 | 11.431223 | 0.181954 |
| H | 10.797190 | 9.355127 | -0.281510 |
| H | 10.667390 | 9.772712 | 7.182746 |
| H | 8.522318 | 10.748940 | 7.831616 |
| H | 10.427300 | 12.173128 | 7.404253 |
| H | 11.460776 | 10.548491 | 2.573809 |
| H | 11.185016 | 10.388084 | 4.723376 |
| H | 7.394311 | 11.797400 | 5.843187 |
| H | 6.170739 | 12.269139 | 4.091753 |
| H | 6.283707 | 11.879415 | 1.902229 |
| H | 7.913460 | 11.236017 | 0.497511 |
| C | 5.236477 | 7.186760 | 1.933716 |
| C | 6.816082 | 5.767892 | 4.337922 |
| C | 6.924339 | 7.779989 | 6.760818 |
| C | 5.157286 | 10.283520 | 5.984549 |
| C | 4.280894 | 9.990319 | 2.936524 |
| C | 13.296316 | 7.102966 | 1.543361 |
| C | 13.557073 | 5.857769 | 0.907122 |
| C | 13.253966 | 4.815110 | 1.840423 |
| C | 12.809439 | 5.419194 | 3.051352 |
| C | 12.849180 | 6.836345 | 2.871674 |
| C | 8.922032 | 6.549807 | -0.829101 |
| C | 10.199656 | 6.357449 | -1.420811 |
| C | 11.116758 | 5.285541 | -1.425542 |

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|----|-----------|-----------|-----------|
| C | 11.211602 | 4.044990 | -0.757642 |
| C | 10.546895 | 3.393845 | 0.294357 |
| C | 9.379517 | 3.651904 | 1.073003 |
| C | 8.368259 | 4.639864 | 0.917257 |
| C | 8.190759 | 5.794457 | 0.124362 |
| Si | 7.965810 | 8.035960 | -1.476133 |
| Si | 9.003335 | 2.320148 | 2.356253 |
| H | 10.524573 | 7.183270 | -2.050202 |
| H | 11.986721 | 5.487906 | -2.044158 |
| H | 12.131574 | 3.527669 | -1.020860 |
| H | 11.099987 | 2.519390 | 0.630652 |
| H | 7.567033 | 4.540156 | 1.645090 |
| H | 7.276359 | 6.303491 | 0.420183 |
| H | 8.841709 | 8.909705 | -2.312562 |
| H | 6.814092 | 7.583035 | -2.321474 |
| H | 7.379000 | 8.855495 | -0.365530 |
| H | 10.275379 | 1.799104 | 2.949703 |
| H | 8.291818 | 1.158861 | 1.731564 |
| H | 8.138109 | 2.866616 | 3.443546 |
| C | 14.284157 | 5.689602 | -0.392432 |
| C | 13.611234 | 3.367874 | 1.685313 |
| C | 12.559468 | 4.679116 | 4.334975 |
| C | 12.714333 | 7.878637 | 3.939363 |
| C | 13.656285 | 8.455226 | 1.002616 |
| O | 10.002137 | 6.569925 | 5.673957 |
| C | 9.914390 | 6.948952 | 4.541617 |
| C | 9.516554 | 7.086755 | 3.300758 |
| O | 9.794283 | 7.949856 | 2.249725 |
| H | 12.939863 | 2.712979 | 2.247024 |
| H | 13.597363 | 3.046520 | 0.641171 |
| H | 14.626341 | 3.188670 | 2.063989 |
| H | 12.087130 | 3.707308 | 4.159287 |
| H | 13.507775 | 4.482992 | 4.852708 |
| H | 11.918207 | 5.232756 | 5.023193 |
| H | 12.480257 | 7.436879 | 4.909228 |
| H | 13.658272 | 8.427657 | 4.046203 |
| H | 11.933022 | 8.606100 | 3.704402 |
| H | 13.075885 | 9.247866 | 1.480029 |
| H | 14.716583 | 8.675710 | 1.185506 |
| H | 13.492820 | 8.533823 | -0.076331 |
| H | 14.050610 | 4.740147 | -0.880881 |
| H | 14.058938 | 6.494338 | -1.098007 |
| H | 15.368724 | 5.704984 | -0.221513 |
| H | 7.570262 | 5.598034 | 5.108625 |
| H | 5.944395 | 5.146196 | 4.582813 |
| H | 7.238088 | 5.413347 | 3.398291 |
| H | 7.166479 | 8.682858 | 7.328048 |
| H | 6.157161 | 7.237378 | 7.328978 |
| H | 7.822376 | 7.157811 | 6.740323 |
| H | 4.150712 | 7.029076 | 1.964947 |
| H | 5.441599 | 7.785637 | 1.039388 |
| H | 5.694260 | 6.204897 | 1.796406 |
| H | 4.339585 | 11.032961 | 3.260597 |
| H | 4.432737 | 9.968779 | 1.853287 |
| H | 3.252101 | 9.653742 | 3.123275 |
| H | 4.969988 | 11.254690 | 5.519451 |
| H | 4.200499 | 9.939828 | 6.399864 |
| H | 5.833907 | 10.434181 | 6.829153 |

11-12-TS Cp*

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|-----------------------|---------------------------|-----------|-----------|
| SCF (B3PW91) Energy = | -1834.425780 | | |
| Enthalpy 0K = | -1833.624570 | | |
| Enthalpy 298K = | -1833.564380 | | |
| Free Energy 298K = | -1833.722009 | | |
| Negative frequency = | -90.6932 cm ⁻¹ | | |
| U | 8.018902 | 10.046843 | 4.447073 |
| U | 11.236199 | 4.934685 | 0.784785 |
| C | 9.263177 | 12.119482 | 3.262665 |
| C | 10.307485 | 11.500869 | 4.003995 |
| C | 10.480415 | 10.999073 | 5.316165 |
| C | 9.691908 | 10.823119 | 6.481823 |
| C | 8.371386 | 11.259960 | 6.808545 |
| C | 7.426473 | 12.106637 | 6.178968 |
| C | 7.291886 | 12.689704 | 4.903142 |
| C | 7.991187 | 12.626493 | 3.678845 |
| Si | 9.688426 | 12.499005 | 1.461929 |
| Si | 10.538939 | 9.871052 | 7.876693 |
| C | 6.131741 | 8.966872 | 2.767272 |
| C | 6.300756 | 7.995271 | 3.799470 |
| C | 5.770491 | 8.533038 | 5.009111 |
| C | 5.234253 | 9.825348 | 4.717459 |
| C | 5.459390 | 10.094470 | 3.332221 |
| H | 8.449378 | 12.461028 | 0.623126 |
| H | 10.284079 | 13.866531 | 1.330979 |
| H | 10.675345 | 11.506614 | 0.939127 |
| H | 11.645617 | 9.026717 | 7.334789 |
| H | 9.545427 | 9.003730 | 8.585601 |
| H | 11.117067 | 10.809677 | 8.890807 |
| H | 11.155457 | 11.225570 | 3.379793 |
| H | 11.426619 | 10.465254 | 5.381785 |
| H | 8.022734 | 10.916170 | 7.780985 |
| H | 6.537667 | 12.248508 | 6.787830 |
| H | 6.325086 | 13.173923 | 4.785808 |
| H | 7.415544 | 13.065907 | 2.866643 |
| C | 6.481105 | 8.776665 | 1.317639 |
| C | 6.808467 | 6.599128 | 3.612609 |
| C | 5.655414 | 7.801654 | 6.316690 |
| C | 4.385686 | 10.643371 | 5.643828 |
| C | 4.907378 | 11.258728 | 2.563939 |
| C | 12.513597 | 6.937956 | -0.632045 |
| C | 13.055566 | 5.734469 | -1.164921 |
| C | 13.874183 | 5.133920 | -0.151664 |
| C | 13.828145 | 5.965826 | 1.003867 |
| C | 12.995962 | 7.085694 | 0.704205 |
| C | 9.249197 | 3.776245 | -0.651744 |
| C | 10.438301 | 3.192363 | -1.191625 |
| C | 11.556739 | 2.535754 | -0.648371 |
| C | 12.062186 | 2.267627 | 0.644838 |
| C | 11.625353 | 2.504470 | 1.963666 |
| C | 10.403192 | 2.965525 | 2.543072 |
| C | 9.208159 | 3.465788 | 1.963259 |
| C | 8.736211 | 3.807692 | 0.673370 |
| Si | 8.079892 | 4.476768 | -1.954779 |
| Si | 10.329612 | 2.791420 | 4.418618 |
| H | 10.531932 | 3.323518 | -2.268038 |
| H | 12.282696 | 2.281855 | -1.418175 |
| H | 13.076096 | 1.877883 | 0.613012 |
| H | 12.382528 | 2.240063 | 2.699676 |
| H | 8.497195 | 3.800249 | 2.717672 |
| H | 7.795253 | 4.349677 | 0.745014 |

| | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 8.855688 | 5.063140 | -3.094408 | C | 6.669357 | 12.310994 | 5.427811 |
| H | 7.194889 | 3.409099 | -2.524019 | C | 6.817170 | 12.418913 | 4.026827 |
| H | 7.202196 | 5.532481 | -1.363068 | C | 7.832446 | 12.085695 | 3.102225 |
| H | 11.702835 | 2.843932 | 5.007562 | Si | 10.042631 | 11.402337 | 1.559043 |
| H | 9.721823 | 1.475338 | 4.803342 | Si | 9.140286 | 10.713304 | 8.416284 |
| H | 9.477479 | 3.863688 | 5.021744 | C | 5.136485 | 8.607133 | 3.690183 |
| C | 12.968093 | 5.283858 | -2.593207 | C | 5.803238 | 7.641818 | 4.506027 |
| C | 14.810616 | 3.981541 | -0.359627 | C | 5.715876 | 8.068091 | 5.867916 |
| C | 14.625366 | 5.776343 | 2.262906 | C | 5.021614 | 9.307232 | 5.891123 |
| C | 12.853709 | 8.326644 | 1.532141 | C | 4.664793 | 9.642970 | 4.539361 |
| C | 11.676711 | 7.946375 | -1.363855 | H | 9.072874 | 11.396518 | 0.422081 |
| O | 9.306668 | 8.282780 | 4.042128 | H | 10.985112 | 12.551074 | 1.340771 |
| C | 10.090116 | 7.316723 | 3.587225 | H | 10.878837 | 10.159695 | 1.516711 |
| C | 10.340124 | 6.664709 | 2.383956 | H | 10.130545 | 9.595033 | 8.439210 |
| O | 9.825770 | 6.828158 | 1.214468 | H | 7.908651 | 10.304410 | 9.165634 |
| C | 11.078671 | 6.635755 | 4.261130 | H | 9.738387 | 11.871280 | 9.158450 |
| O | 11.879811 | 6.154800 | 4.967631 | H | 10.867403 | 10.677560 | 4.005167 |
| H | 14.097367 | 6.150359 | 3.144589 | H | 10.583120 | 10.411513 | 6.137850 |
| H | 14.855054 | 4.722447 | 2.445223 | H | 6.845904 | 11.797351 | 7.426521 |
| H | 15.583163 | 6.310074 | 2.206280 | H | 5.673639 | 12.609227 | 5.747809 |
| H | 15.031114 | 3.456990 | 0.573882 | H | 5.909373 | 12.767529 | 3.541351 |
| H | 14.415920 | 3.249027 | -1.068752 | H | 7.508103 | 12.241624 | 2.075392 |
| H | 15.767520 | 4.338870 | -0.762716 | C | 4.883329 | 8.475374 | 2.217747 |
| H | 13.024831 | 4.195822 | -2.683842 | C | 6.270553 | 6.292679 | 4.048913 |
| H | 12.039238 | 5.607133 | -3.071123 | C | 6.174948 | 7.274330 | 7.055246 |
| H | 13.796654 | 5.701903 | -3.179803 | C | 4.531310 | 10.015533 | 7.118224 |
| H | 10.909734 | 8.378260 | -0.714168 | C | 3.748278 | 10.758194 | 4.133655 |
| H | 12.295469 | 8.771327 | -1.740404 | C | 13.785567 | 6.280137 | 2.062529 |
| H | 11.168267 | 7.506009 | -2.226513 | C | 14.147344 | 6.038233 | 0.704521 |
| H | 13.046056 | 8.137780 | 2.590803 | C | 14.304419 | 4.627615 | 0.537559 |
| H | 13.574879 | 9.084171 | 1.197290 | C | 14.026584 | 3.997192 | 1.791698 |
| H | 11.856003 | 8.765497 | 1.444608 | C | 13.708885 | 5.019280 | 2.734591 |
| H | 7.361948 | 6.239683 | 4.484254 | C | 10.036294 | 6.021269 | -0.972595 |
| H | 5.967763 | 5.911997 | 3.450535 | C | 11.106085 | 5.305183 | -1.598559 |
| H | 7.470510 | 6.523515 | 2.747596 | C | 11.604867 | 3.983105 | -1.529138 |
| H | 6.622844 | 9.733100 | 0.804912 | C | 11.422531 | 2.877703 | -0.674788 |
| H | 7.395449 | 8.189846 | 1.185135 | C | 10.639054 | 2.606536 | 0.473178 |
| H | 5.677127 | 8.247870 | 0.789519 | C | 9.536760 | 3.257093 | 1.112722 |
| H | 4.806853 | 12.152024 | 3.186487 | C | 8.890696 | 4.492711 | 0.847590 |
| H | 5.531989 | 11.522377 | 1.705647 | C | 9.095093 | 5.620213 | 0.013099 |
| H | 3.908755 | 11.022405 | 2.174147 | Si | 9.748050 | 7.752645 | -1.685889 |
| H | 5.636974 | 8.485886 | 7.170464 | Si | 8.755198 | 2.245641 | 2.506841 |
| H | 4.731414 | 7.210385 | 6.357658 | H | 11.663332 | 5.906217 | -2.315075 |
| H | 6.486134 | 7.105891 | 6.469770 | H | 12.443083 | 3.834035 | -2.204499 |
| H | 4.424074 | 11.709964 | 5.406615 | H | 12.156430 | 2.095972 | -0.858072 |
| H | 3.334878 | 10.334070 | 5.570399 | H | 10.923953 | 1.668648 | 0.945836 |
| H | 4.682620 | 10.522796 | 6.689476 | H | 8.114911 | 4.712447 | 1.578711 |
| | | | | H | 8.430707 | 6.431158 | 0.305925 |
| | | | | H | 11.063378 | 8.380622 | -2.027411 |
| | | | | H | 8.955756 | 7.654158 | -2.952689 |
| | | | | H | 9.007485 | 8.594762 | -0.707085 |
| | | | | H | 9.797910 | 1.397917 | 3.165633 |
| | | | | H | 7.699588 | 1.330894 | 1.968134 |
| | | | | H | 8.124263 | 3.145187 | 3.518088 |
| | | | | C | 14.481094 | 7.087317 | -0.317599 |
| | | | | C | 14.894318 | 3.951267 | -0.662800 |
| | | | | C | 14.206953 | 2.535631 | 2.086115 |
| | | | | C | 13.442149 | 4.836598 | 4.200294 |
| | | | | C | 13.643521 | 7.623820 | 2.712580 |
| | | | | O | 8.066791 | 8.747752 | 2.344779 |

12 Cp*
SCF (B3PW91) Energy = -1834.459589
Enthalpy 0K = -1833.656374
Enthalpy 298K = -1833.596016
Free Energy 298K = -1833.754219

| | | | |
|---|-----------|-----------|----------|
| U | 7.470066 | 9.831383 | 4.623380 |
| U | 11.576532 | 5.043404 | 1.015672 |
| C | 9.151600 | 11.575809 | 3.209212 |
| C | 9.918518 | 11.115546 | 4.314503 |
| C | 9.747931 | 10.959678 | 5.707758 |
| C | 8.706380 | 11.195597 | 6.645593 |
| C | 7.423454 | 11.794621 | 6.504506 |

| | | | | | | | |
|---|-----------|----------|-----------|---|-----------|-----------|----------|
| C | 8.866186 | 7.993587 | 2.989831 | H | 13.919446 | 1.908182 | 1.236905 |
| C | 9.895197 | 7.068297 | 3.232175 | H | 15.256964 | 2.311199 | 2.313614 |
| O | 10.811545 | 6.268560 | 2.794237 | H | 7.082705 | 5.908705 | 4.672064 |
| C | 9.231585 | 7.655209 | 4.321608 | H | 5.448129 | 5.566977 | 4.102141 |
| O | 8.934975 | 7.942949 | 5.526613 | H | 6.614374 | 6.316269 | 3.011070 |
| H | 13.178124 | 3.802927 | 4.441059 | H | 4.590148 | 9.429195 | 1.770481 |
| H | 14.332443 | 5.087491 | 4.790265 | H | 5.772501 | 8.124768 | 1.687011 |
| H | 12.625544 | 5.477880 | 4.544170 | H | 4.069892 | 7.763544 | 2.026122 |
| H | 12.964394 | 7.583358 | 3.566450 | H | 3.852641 | 11.634456 | 4.778797 |
| H | 14.616432 | 7.981288 | 3.073105 | H | 3.924131 | 11.081962 | 3.104221 |
| H | 13.257610 | 8.379463 | 2.021793 | H | 2.700871 | 10.435087 | 4.197485 |
| H | 14.266270 | 6.754694 | -1.337244 | H | 4.410814 | 11.089433 | 6.952920 |
| H | 13.926739 | 8.015049 | -0.150388 | H | 3.550179 | 9.624363 | 7.418088 |
| H | 15.548323 | 7.340587 | -0.278425 | H | 5.206235 | 9.884337 | 7.968057 |
| H | 14.500582 | 2.941233 | -0.807587 | H | 6.224400 | 7.888344 | 7.958401 |
| H | 14.715530 | 4.516844 | -1.580966 | H | 5.481014 | 6.449005 | 7.261102 |
| H | 15.982364 | 3.859355 | -0.548369 | H | 7.168258 | 6.846794 | 6.892412 |
| H | 13.615703 | 2.213795 | 2.947861 | | | | |

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