

Supporting Information For

Substrate-Dependent Mechanism for the Reactions of a Hyrido(hydrosilylene)ruthenium Complex with Carbonyl Compounds: Insights from Quantum Chemical Calculations

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Cartesian coordinates and electronic energies for all of the calculated structures

| | | | | | | | |
|-----------------------|-----------|-----------|-----------|-----------------------|-----------|-----------|-----------|
| 1 | | | | H | -5.100162 | -1.125106 | 1.459597 |
| SCF done: -657.575703 | | | | H | -2.957421 | -2.238273 | 1.475761 |
| Ru | 0.746901 | -0.256031 | -0.199594 | H | 0.200859 | -0.341057 | -1.723936 |
| Si | -1.276131 | 0.665238 | 0.221396 | | | | |
| H | -1.401809 | 2.056114 | 0.802542 | 2a | | | |
| Si | -4.218928 | 1.684967 | -0.140320 | SCF done: -850.740948 | | | |
| Si | -3.311129 | -0.914791 | -1.627927 | Ru | 1.002763 | 0.016666 | -0.447738 |
| O | -0.188741 | -3.137674 | -0.023892 | Si | -1.154354 | 0.174047 | 0.439218 |
| C | -3.095473 | 0.136487 | -0.036560 | H | -1.278598 | 0.642558 | 1.874186 |
| C | 0.133572 | -2.023455 | -0.081832 | Si | -4.003842 | -0.582212 | 1.559925 |
| C | 2.739043 | 0.574407 | -1.050931 | Si | -3.507712 | -0.800419 | -1.501479 |
| C | 3.049085 | -0.553361 | -0.229966 | O | -2.167502 | 1.773254 | -0.277689 |
| C | 2.648194 | -0.240123 | 1.124244 | O | 0.131009 | -1.543832 | -2.887563 |
| C | 2.114793 | 1.090968 | 1.131917 | C | -2.694329 | -0.973030 | 0.226295 |
| C | 2.149669 | 1.592453 | -0.216596 | C | 0.424632 | -0.935086 | -1.936880 |
| C | 3.090571 | 0.731669 | -2.503766 | C | 2.982109 | 1.035387 | 0.267662 |
| H | 4.086439 | 1.184262 | -2.611264 | C | 3.307867 | -0.127988 | -0.504835 |
| H | 2.376353 | 1.375095 | -3.024499 | C | 2.815599 | -1.283604 | 0.213545 |
| H | 3.106378 | -0.231621 | -3.020480 | C | 2.178125 | -0.829900 | 1.406322 |
| C | 3.778920 | -1.793441 | -0.665656 | C | 2.268439 | 0.615020 | 1.435453 |
| H | 3.575272 | -2.031945 | -1.713452 | C | 3.427052 | 2.437889 | -0.043702 |
| H | 3.491515 | -2.663413 | -0.067946 | H | 4.427435 | 2.630018 | 0.369843 |
| H | 4.865597 | -1.666711 | -0.559329 | H | 2.750865 | 3.185008 | 0.383395 |
| C | 2.910153 | -1.096193 | 2.332384 | H | 3.475806 | 2.613759 | -1.121860 |
| H | 2.192176 | -0.896912 | 3.132970 | C | 4.168928 | -0.158256 | -1.737395 |
| H | 3.915732 | -0.907045 | 2.734491 | H | 4.041994 | 0.746977 | -2.338786 |
| H | 2.849243 | -2.161719 | 2.092847 | H | 3.925608 | -1.011665 | -2.377280 |
| C | 1.722482 | 1.881408 | 2.348655 | H | 5.234888 | -0.235957 | -1.477271 |
| H | 2.572121 | 2.475663 | 2.713939 | C | 3.061922 | -2.717667 | -0.166382 |
| H | 1.400963 | 1.229031 | 3.165300 | H | 2.277866 | -3.376492 | 0.217803 |
| H | 0.904771 | 2.576547 | 2.136258 | H | 4.020494 | -3.070879 | 0.240151 |
| C | 1.830868 | 2.999651 | -0.640830 | H | 3.099354 | -2.849147 | -1.251963 |
| H | 1.030165 | 3.434011 | -0.035189 | C | 1.682402 | -1.689345 | 2.535931 |
| H | 1.515161 | 3.041888 | -1.687042 | H | 2.481298 | -1.865910 | 3.271737 |
| H | 2.712060 | 3.648607 | -0.534470 | H | 1.340061 | -2.666643 | 2.184238 |
| H | -4.722635 | -1.378050 | -1.719454 | H | 0.849599 | -1.220472 | 3.068742 |
| H | -5.609981 | 1.299140 | -0.498668 | C | 1.877247 | 1.475428 | 2.604576 |
| H | -3.022012 | -0.089574 | -2.828844 | H | 0.910536 | 1.178067 | 3.025815 |
| H | -3.717740 | 2.625495 | -1.176276 | H | 1.808677 | 2.531569 | 2.325227 |
| H | -2.430376 | -2.103823 | -1.626527 | H | 2.618602 | 1.403547 | 3.413545 |
| H | -4.252280 | 2.396992 | 1.163350 | H | -4.189979 | -2.070007 | -1.872934 |
| Si | -3.628225 | -0.915916 | 1.483103 | H | -5.277740 | -1.309923 | 1.302538 |
| H | -3.283603 | -0.216625 | 2.749686 | H | -4.547933 | 0.263956 | -1.493376 |

| | | | | | | | |
|-------------------------|-----------|-----------|-----------|-------------------------|-----------|-----------|-----------|
| H | -4.316180 | 0.872065 | 1.590373 | H | -2.117584 | 3.036303 | -2.329359 |
| H | -2.524139 | -0.473965 | -2.558861 | H | -3.375828 | 3.654607 | -1.258153 |
| H | -3.524450 | -0.975394 | 2.912378 | H | -1.869156 | 4.584445 | -1.474445 |
| Si | -2.110896 | -2.785206 | 0.453270 | | | | |
| H | -1.253841 | -2.919762 | 1.661618 | 3a | | | |
| H | -3.295674 | -3.664935 | 0.649974 | SCF done: -850.735721 | | | |
| H | -1.357696 | -3.282069 | -0.722270 | Ru | 1.074894 | 0.240207 | -0.506874 |
| C | -1.896005 | 2.985754 | -0.245725 | Si | -1.233623 | 0.372879 | 0.421733 |
| H | 0.625777 | 1.334542 | -1.317516 | H | -1.069820 | 0.578954 | 1.901277 |
| C | -0.778648 | 3.510537 | 0.595135 | Si | -3.743854 | -0.908465 | 1.717726 |
| H | 0.142591 | 3.010250 | 0.258087 | Si | -3.586183 | -0.734010 | -1.373743 |
| H | -0.676599 | 4.595349 | 0.525848 | O | -2.229469 | 1.672303 | -0.150034 |
| H | -0.926823 | 3.212994 | 1.639856 | O | -0.074275 | -1.114897 | -2.971779 |
| C | -2.691510 | 3.921852 | -1.104009 | C | -2.546337 | -1.024980 | 0.220111 |
| H | -3.480048 | 3.388337 | -1.636506 | C | 0.305657 | -0.605405 | -2.004406 |
| H | -3.121532 | 4.721714 | -0.488665 | C | 3.191715 | 0.783966 | 0.173065 |
| H | -2.017586 | 4.404958 | -1.824577 | C | 3.223836 | -0.508413 | -0.463871 |
| | | | | C | 2.472859 | -1.426008 | 0.360894 |
| | | | | C | 1.970696 | -0.700067 | 1.488008 |
| TS_{23a} | | | | C | 2.392581 | 0.672472 | 1.358313 |
| SCF done: -850.7172855 | | | | C | 3.965558 | 2.000695 | -0.252100 |
| Ru | 0.958073 | 0.207365 | -0.434396 | H | 4.946057 | 2.020206 | 0.243333 |
| Si | -1.290793 | 0.201435 | 0.518176 | H | 3.442220 | 2.923768 | 0.011147 |
| H | -1.208968 | 0.414529 | 2.008285 | H | 4.138175 | 2.013056 | -1.331386 |
| Si | -3.899314 | -0.977768 | 1.772130 | C | 4.053754 | -0.882394 | -1.660956 |
| Si | -3.679900 | -0.793686 | -1.317970 | H | 4.176046 | -0.037978 | -2.344809 |
| O | -2.242900 | 1.646492 | -0.016198 | H | 3.600001 | -1.700976 | -2.226944 |
| O | -0.120941 | -1.192151 | -2.897718 | H | 5.056703 | -1.209334 | -1.353443 |
| C | -2.685953 | -1.109142 | 0.294511 | C | 2.387670 | -2.911652 | 0.149060 |
| C | 0.243665 | -0.657777 | -1.933190 | H | 1.483224 | -3.335683 | 0.591517 |
| C | 3.088649 | 0.862774 | 0.164361 | H | 3.249772 | -3.413942 | 0.609514 |
| C | 3.172757 | -0.406074 | -0.500894 | H | 2.388633 | -3.169503 | -0.913889 |
| C | 2.496302 | -1.383160 | 0.323418 | C | 1.301841 | -1.275274 | 2.702085 |
| C | 1.995039 | -0.714796 | 1.482832 | H | 2.030480 | -1.372322 | 3.519082 |
| C | 2.345324 | 0.681660 | 1.379564 | H | 0.887712 | -2.267162 | 2.508814 |
| C | 3.772091 | 2.130467 | -0.267594 | H | 0.489890 | -0.638106 | 3.066118 |
| H | 4.776382 | 2.196285 | 0.173828 | C | 2.181826 | 1.741455 | 2.393314 |
| H | 3.215616 | 3.018020 | 0.046610 | H | 1.212009 | 1.634975 | 2.888293 |
| H | 3.883892 | 2.177200 | -1.354126 | H | 2.226050 | 2.742288 | 1.955801 |
| C | 3.969969 | -0.706753 | -1.739919 | H | 2.955775 | 1.683142 | 3.171472 |
| H | 4.017730 | 0.158080 | -2.407732 | H | -4.180772 | -2.033719 | -1.794895 |
| H | 3.537100 | -1.536237 | -2.306944 | H | -4.961611 | -1.728285 | 1.470535 |
| H | 5.001973 | -0.986141 | -1.484454 | H | -4.710360 | 0.203783 | -1.134331 |
| C | 2.464669 | -2.863667 | 0.064480 | H | -4.165969 | 0.490923 | 1.966362 |
| H | 1.610602 | -3.341535 | 0.551388 | H | -2.769554 | -0.228815 | -2.500986 |
| H | 3.376276 | -3.345056 | 0.445672 | H | -3.093711 | -1.431233 | 2.950311 |
| H | 2.400690 | -3.084863 | -1.005115 | Si | -1.833131 | -2.790481 | 0.185794 |
| C | 1.388489 | -1.358335 | 2.697041 | H | -0.951156 | -3.044267 | 1.356822 |
| H | 2.155803 | -1.510291 | 3.469616 | H | -2.935696 | -3.785803 | 0.252080 |
| H | 0.954100 | -2.335089 | 2.468724 | H | -1.046600 | -3.063618 | -1.041558 |
| H | 0.601480 | -0.739445 | 3.138826 | C | -2.001610 | 3.014571 | -0.095549 |
| C | 2.138834 | 1.703902 | 2.460544 | H | 1.340224 | 1.313380 | -1.670007 |
| H | 1.172308 | 1.574748 | 2.959152 | C | -1.157537 | 3.613402 | 0.758951 |
| H | 2.180429 | 2.724040 | 2.067866 | H | -1.040977 | 4.691023 | 0.742919 |
| H | 2.915852 | 1.619780 | 3.233619 | H | -0.591843 | 3.063817 | 1.502924 |
| H | -4.310641 | -2.066207 | -1.765819 | H | 0.303098 | 1.667478 | -0.438009 |
| H | -5.124142 | -1.786437 | 1.519395 | C | -2.834817 | 3.751228 | -1.107996 |
| H | -4.775170 | 0.184393 | -1.095295 | H | -2.583757 | 3.419288 | -2.122936 |
| H | -4.315065 | 0.427937 | 2.003710 | H | -3.898510 | 3.534147 | -0.952039 |
| H | -2.826102 | -0.297253 | -2.422425 | H | -2.682183 | 4.831681 | -1.040790 |
| H | -3.269509 | -1.492493 | 3.018081 | | | | |
| Si | -1.978119 | -2.882027 | 0.259787 | TS_{24a} | | | |
| H | -1.078592 | -3.121571 | 1.421045 | SCF done: -850.701736 | | | |
| H | -3.083198 | -3.873447 | 0.350162 | Ru | 1.103260 | 0.047590 | -0.519450 |
| H | -1.211722 | -3.157704 | -0.979434 | Si | -1.188212 | 0.353394 | -0.177730 |
| C | -1.689520 | 2.816091 | -0.248623 | H | -1.505305 | 1.600620 | 0.828187 |
| H | 0.923928 | 1.433249 | -1.493830 | Si | -3.405661 | -0.601719 | 1.929967 |
| C | -0.491328 | 3.152453 | 0.365929 | Si | -3.973014 | -0.866963 | -1.159038 |
| H | -0.021813 | 4.097223 | 0.104363 | O | -2.099453 | 1.536459 | -1.353332 |
| H | -0.308448 | 2.816202 | 1.383635 | O | 0.652297 | -1.716466 | -2.942731 |
| H | 0.239838 | 1.974819 | -0.199386 | C | -2.623278 | -0.892401 | 0.208440 |
| C | -2.290723 | 3.580092 | -1.389937 | | | | |

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|----|-----------|-----------|-----------|-----------------------|-----------|-----------|-----------|
| C | 0.778886 | -1.038177 | -2.004193 | C | 3.149241 | -0.789419 | -2.467829 |
| C | 3.081405 | 1.007304 | 0.208683 | H | 2.382709 | -1.355932 | -3.004103 |
| C | 3.340013 | -0.352194 | -0.165383 | H | 4.109641 | -1.300485 | -2.627814 |
| C | 2.625837 | -1.213528 | 0.757473 | H | 3.222497 | 0.195167 | -2.938884 |
| C | 1.908150 | -0.384812 | 1.662941 | C | 1.676808 | -2.994916 | -0.693174 |
| C | 2.169599 | 0.998810 | 1.314138 | H | 2.478771 | -3.741115 | -0.594735 |
| C | 3.739898 | 2.221361 | -0.385291 | H | 1.381500 | -2.968665 | -1.745144 |
| H | 4.680728 | 2.445886 | 0.137358 | H | 0.822446 | -3.357666 | -0.116975 |
| H | 3.101588 | 3.106181 | -0.308529 | C | 1.776254 | -2.037074 | 2.360226 |
| H | 3.975112 | 2.075286 | -1.442993 | H | 0.951733 | -2.713922 | 2.123174 |
| C | 4.333496 | -0.813328 | -1.195693 | H | 1.456557 | -1.401570 | 3.191200 |
| H | 4.442803 | -0.085304 | -2.004752 | H | 2.612133 | -2.653871 | 2.721947 |
| H | 4.035092 | -1.764075 | -1.647895 | H | -5.247938 | -1.726983 | -0.243440 |
| H | 5.326199 | -0.960494 | -0.746354 | H | -3.482393 | -3.470032 | 1.272519 |
| C | 2.742379 | -2.711124 | 0.815785 | H | -4.644755 | 0.019335 | 1.276685 |
| H | 1.862899 | -3.166616 | 1.279930 | H | -2.257722 | -1.872853 | 2.594994 |
| H | 3.620541 | -3.014532 | 1.404053 | H | -4.625196 | 0.407541 | -1.126143 |
| H | 2.852428 | -3.147812 | -0.181528 | H | -1.094312 | -3.347427 | 1.095593 |
| C | 1.173589 | -0.841073 | 2.892599 | Si | -2.319591 | -2.126086 | -1.833801 |
| H | 1.848420 | -0.855048 | 3.761095 | H | -0.948751 | -2.658374 | -2.011775 |
| H | 0.772299 | -1.850989 | 2.775070 | H | -3.273454 | -3.262463 | -1.935570 |
| H | 0.339468 | -0.178750 | 3.143124 | H | -2.604402 | -1.181231 | -2.944426 |
| C | 1.750939 | 2.191198 | 2.129384 | C | -2.055771 | 2.822434 | 0.474647 |
| H | 0.743128 | 2.070525 | 2.539218 | H | 0.616943 | 1.451652 | 1.188899 |
| H | 1.757990 | 3.109770 | 1.534843 | C | -2.748194 | 3.190376 | 1.785001 |
| H | 2.431236 | 2.347728 | 2.979557 | H | -2.367843 | 2.577070 | 2.608754 |
| H | -4.809768 | -2.089773 | -1.014943 | H | -2.567325 | 4.243756 | 2.028427 |
| H | -4.375868 | -1.679974 | 2.257622 | H | -3.829760 | 3.033048 | 1.707838 |
| H | -4.883025 | 0.298413 | -1.034141 | C | -2.552758 | 3.645102 | -0.711357 |
| H | -4.131046 | 0.692423 | 1.999777 | H | -2.023001 | 3.365883 | -1.627187 |
| H | -3.374254 | -0.879047 | -2.513926 | H | -3.626000 | 3.486716 | -0.865341 |
| H | -2.359547 | -0.590320 | 2.986055 | H | -2.381574 | 4.712625 | -0.530780 |
| Si | -1.876163 | -2.673502 | 0.221360 | | | | |
| H | -0.823514 | -2.822377 | 1.254572 | | | | |
| H | -2.968651 | -3.625223 | 0.559439 | 5b | | | |
| H | -1.329876 | -3.045265 | -1.103086 | SCF done: -850.735512 | | | |
| C | -2.135718 | 2.527973 | -0.493396 | Ru | -0.788157 | 0.121589 | 0.146193 |
| H | 0.936291 | 1.256611 | -1.573142 | Si | 1.387464 | -0.958292 | -0.346980 |
| C | -3.464746 | 2.959754 | 0.062910 | H | 1.459767 | -2.276188 | 0.368879 |
| H | -4.132795 | 2.115285 | 0.223839 | Si | 4.372432 | -1.618383 | -0.655547 |
| H | -3.351724 | 3.537616 | 0.983574 | Si | 3.498534 | 1.279207 | -1.276370 |
| H | -3.924504 | 3.613717 | -0.693994 | O | 0.188502 | 1.554651 | -1.169936 |
| C | -1.037691 | 3.552637 | -0.572896 | O | 0.134374 | 0.702980 | 2.956086 |
| H | -0.064106 | 3.058002 | -0.647656 | C | 3.168631 | -0.216648 | -0.126697 |
| H | -1.191322 | 4.111829 | -1.507134 | C | -0.144604 | 0.521613 | 1.840570 |
| H | -1.062289 | 4.251255 | 0.267286 | C | -3.168471 | -0.018419 | -0.260821 |
| | | | | C | -2.792353 | -0.676007 | 0.944050 |
| | | | | C | -1.892222 | -1.762092 | 0.604766 |
| | | | | C | -1.772559 | -1.791502 | -0.836982 |
| | | | | C | -2.500700 | -0.685047 | -1.355740 |
| | | | | C | -4.239416 | 1.028100 | -0.374870 |
| | | | | H | -5.231113 | 0.554167 | -0.376266 |
| | | | | H | -4.159671 | 1.606601 | -1.297690 |
| | | | | H | -4.218993 | 1.730799 | 0.464111 |
| | | | | C | -3.356390 | -0.401299 | 2.310592 |
| | | | | H | -3.631566 | 0.650790 | 2.430223 |
| | | | | H | -2.645466 | -0.650149 | 3.102952 |
| | | | | H | -4.261030 | -1.001787 | 2.479338 |
| | | | | C | -1.447470 | -2.850601 | 1.541584 |
| | | | | H | -0.482852 | -3.270445 | 1.244284 |
| | | | | H | -2.180065 | -3.669634 | 1.556100 |
| | | | | H | -1.344125 | -2.481952 | 2.566273 |
| | | | | C | -1.141913 | -2.882814 | -1.651039 |
| | | | | H | -1.891039 | -3.652507 | -1.885086 |
| | | | | H | -0.323067 | -3.375596 | -1.120170 |
| | | | | H | -0.745885 | -2.507757 | -2.598656 |
| | | | | C | -2.653438 | -0.362616 | -2.815562 |
| | | | | H | -1.715579 | -0.513686 | -3.358255 |
| | | | | H | -2.962557 | 0.673951 | -2.975345 |
| | | | | H | -3.414588 | -1.004801 | -3.280122 |
| | | | | H | 4.971798 | 1.458774 | -1.426470 |
| | | | | H | 5.784868 | -1.163115 | -0.548538 |

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| 4a | | | | | | | |
| SCF done: -850.779005 | | | | | | | |
| Ru | 1.043397 | 0.438963 | 0.003934 | | | | |
| Si | -1.240059 | 0.158267 | 0.028866 | | | | |
| H | -0.974660 | 2.959398 | 0.590024 | | | | |
| Si | -2.326139 | -2.536809 | 1.267222 | | | | |
| Si | -4.333018 | -0.565705 | -0.049101 | | | | |
| O | -2.323188 | 1.430428 | 0.208412 | | | | |
| O | 0.748327 | 2.776726 | -1.902955 | | | | |
| C | -2.533482 | -1.250416 | -0.138411 | | | | |
| C | 0.812251 | 1.874713 | -1.169509 | | | | |
| C | 2.952793 | -0.002207 | 1.223001 | | | | |
| C | 3.339971 | 0.343475 | -0.108919 | | | | |
| C | 2.838938 | -0.683999 | -1.000410 | | | | |
| C | 2.155075 | -1.655552 | -0.211331 | | | | |
| C | 2.195570 | -1.224168 | 1.165962 | | | | |
| C | 3.371088 | 0.711026 | 2.478544 | | | | |
| H | 4.321178 | 0.305191 | 2.854331 | | | | |
| H | 2.626851 | 0.598875 | 3.271533 | | | | |
| H | 3.512646 | 1.781517 | 2.306835 | | | | |
| C | 4.244760 | 1.477758 | -0.503150 | | | | |
| H | 4.157681 | 2.321149 | 0.187658 | | | | |
| H | 4.017715 | 1.848838 | -1.506974 | | | | |
| H | 5.295526 | 1.155099 | -0.502257 | | | | |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|----------|----------|
| H | 2.938023 | 1.057687 | -2.632334 | C | 0.658240 | 2.577962 | 1.390444 |
| H | 4.128078 | -2.027609 | -2.063810 | H | 1.348772 | 3.370248 | 1.065309 |
| H | 2.973552 | 2.552759 | -0.727871 | H | -0.077187 | 3.031382 | 2.064013 |
| H | 4.211535 | -2.817064 | 0.208961 | H | 1.231351 | 1.845225 | 1.960379 |
| Si | 3.577628 | 0.244818 | 1.679335 | | | | |
| H | 3.212169 | -0.857428 | 2.607774 | | | | |
| H | 5.035955 | 0.503289 | 1.832969 | | | | |
| H | 2.865334 | 1.475144 | 2.104652 | | | | |
| H | 1.334778 | -1.302564 | -1.803128 | | | | |
| C | -0.453537 | 2.395457 | -0.444233 | | | | |
| C | 0.279636 | 3.215805 | 0.605609 | | | | |
| H | 0.632111 | 4.143001 | 0.129464 | | | | |
| H | -0.379240 | 3.501798 | 1.431540 | | | | |
| H | 1.147940 | 2.688396 | 0.999293 | | | | |
| C | -1.683664 | 3.070917 | -1.019892 | | | | |
| H | -2.429406 | 3.305947 | -0.255027 | | | | |
| H | -1.366784 | 4.024603 | -1.469023 | | | | |
| H | -2.131001 | 2.461632 | -1.804825 | | | | |

TS_{56b}

SCF done: -850.708927

| | | | |
|----|-----------|-----------|-----------|
| Ru | -0.994938 | 0.067814 | 0.305787 |
| Si | 1.466217 | -0.657877 | -0.383864 |
| H | 1.456752 | -1.913026 | 0.445614 |
| Si | 4.311358 | -1.510588 | -1.128634 |
| Si | 3.722233 | 1.522482 | -1.069006 |
| O | 0.699512 | 1.076955 | -0.582084 |
| O | -0.130206 | -0.412134 | 3.157102 |
| C | 3.317166 | -0.139533 | -0.215770 |
| C | -0.390258 | -0.172883 | 2.046123 |
| C | -3.210865 | 0.378453 | -0.499635 |
| C | -3.157282 | -0.422749 | 0.691056 |
| C | -2.478270 | -1.669156 | 0.361573 |
| C | -2.056619 | -1.589178 | -0.993273 |
| C | -2.486108 | -0.309078 | -1.517334 |
| C | -3.969428 | 1.666273 | -0.641646 |
| H | -5.025881 | 1.468354 | -0.870993 |
| H | -3.574499 | 2.291604 | -1.446501 |
| H | -3.940979 | 2.254446 | 0.280751 |
| C | -3.907921 | -0.151793 | 1.965860 |
| H | -3.980321 | 0.920759 | 2.169563 |
| H | -3.421538 | -0.617426 | 2.827578 |
| H | -4.931318 | -0.549029 | 1.908723 |
| C | -2.368706 | -2.869775 | 1.259360 |
| H | -1.486181 | -3.471317 | 1.022825 |
| H | -3.250684 | -3.516377 | 1.150085 |
| H | -2.300411 | -2.584476 | 2.313039 |
| C | -1.413894 | -2.686289 | -1.792851 |
| H | -2.176480 | -3.310396 | -2.280187 |
| H | -0.806301 | -3.343471 | -1.163480 |
| H | -0.765561 | -2.289821 | -2.579833 |
| C | -2.300110 | 0.129928 | -2.943158 |
| H | -1.276233 | -0.044033 | -3.290878 |
| H | -2.518014 | 1.193637 | -3.073322 |
| H | -2.971159 | -0.424985 | -3.613343 |
| H | 5.197180 | 1.638257 | -1.245319 |
| H | 5.748004 | -1.444033 | -0.754600 |
| H | 3.103164 | 1.603144 | -2.416044 |
| H | 4.204435 | -1.344554 | -2.601921 |
| H | 3.289103 | 2.694061 | -0.267891 |
| H | 3.804959 | -2.863613 | -0.778753 |
| Si | 3.915955 | -0.123946 | 1.601369 |
| H | 3.816343 | -1.482727 | 2.195739 |
| H | 5.337041 | 0.308762 | 1.673326 |
| H | 3.118700 | 0.806119 | 2.439390 |
| H | 1.239760 | -1.054607 | -1.795190 |
| C | -0.049140 | 1.963260 | 0.197886 |
| C | -0.724295 | 2.995782 | -0.685142 |
| H | -1.527538 | 3.500470 | -0.137582 |
| H | -0.000632 | 3.763710 | -0.999049 |
| H | -1.142060 | 2.539787 | -1.585337 |

6b

SCF done: -850.733596

| | | | |
|----|-----------|-----------|-----------|
| Ru | -1.158558 | -0.270880 | -0.273078 |
| Si | 2.373372 | -1.157216 | -0.553882 |
| H | 3.015444 | -2.441000 | -0.165806 |
| Si | 3.137269 | 1.852896 | -1.081737 |
| Si | 3.254794 | 0.678176 | 1.827032 |
| O | 0.891581 | -1.036054 | 0.299293 |
| O | -1.170568 | -0.925212 | -3.223480 |
| C | 3.486608 | 0.284776 | -0.034307 |
| C | -1.075680 | -0.737716 | -2.074043 |
| C | -3.005251 | 0.001406 | 1.096335 |
| C | -3.292078 | 0.325878 | -0.280510 |
| C | -2.575610 | 1.552999 | -0.610072 |
| C | -1.768475 | 1.885296 | 0.499058 |
| C | -2.025567 | 0.921437 | 1.561131 |
| C | -3.694771 | -1.064447 | 1.898631 |
| H | -4.620153 | -0.672918 | 2.344996 |
| H | -3.068101 | -1.432189 | 2.715812 |
| H | -3.969353 | -1.922404 | 1.277715 |
| C | -4.385129 | -0.286579 | -1.112697 |
| H | -4.517363 | -1.347559 | -0.881501 |
| H | -4.168754 | -0.208959 | -2.182061 |
| H | -5.345884 | 0.216760 | -0.931426 |
| C | -2.720718 | 2.326642 | -1.890055 |
| H | -1.834982 | 2.934843 | -2.095673 |
| H | -3.585581 | 3.003754 | -1.843072 |
| H | -2.870530 | 1.665209 | -2.748521 |
| C | -0.880030 | 3.088036 | 0.638352 |
| H | -1.399455 | 3.897763 | 1.171122 |
| H | -0.571434 | 3.479044 | -0.335265 |
| H | 0.026405 | 2.856463 | 1.206583 |
| C | -1.476085 | 1.033721 | 2.956186 |
| H | -0.400501 | 1.241674 | 2.955287 |
| H | -1.636355 | 0.117274 | 3.531333 |
| H | -1.963942 | 1.851356 | 3.506157 |
| H | 4.398269 | 1.506689 | 2.294885 |
| H | 3.866566 | 3.013829 | -0.506639 |
| H | 2.008983 | 1.444098 | 2.074503 |
| H | 1.690506 | 2.171176 | -1.112624 |
| H | 3.227180 | -0.567456 | 2.634472 |
| H | 3.611702 | 1.651593 | -2.475809 |
| Si | 5.308085 | -0.247530 | -0.323105 |
| H | 5.455224 | -0.896876 | -1.652394 |
| H | 6.201504 | 0.937415 | -0.279016 |
| H | 5.744962 | -1.213432 | 0.717352 |
| C | 2.153193 | -1.140898 | -2.021942 |
| C | -0.205284 | -2.015998 | 0.364519 |
| C | -0.377767 | -2.426280 | 1.816534 |
| H | -1.313180 | -2.983594 | 1.938015 |
| H | 0.444941 | -3.080897 | 2.147280 |
| H | -0.403749 | -1.557424 | 2.478606 |
| C | -0.011700 | -3.226980 | -0.533309 |
| H | 0.765134 | -3.908981 | -0.150663 |
| H | -0.950358 | -3.790950 | -0.569439 |
| H | 0.234029 | -2.956280 | -1.564165 |

2c

SCF done: -1042.476951

| | | | |
|----|-----------|-----------|-----------|
| Ru | -1.420721 | -0.468798 | -0.452994 |
| Si | 0.222419 | 0.823132 | 0.611813 |
| H | 0.271660 | 0.728713 | 2.122346 |
| Si | 1.732744 | 3.341467 | 1.769400 |
| Si | 1.818567 | 2.840087 | -1.299126 |
| O | 2.053184 | 0.123526 | 0.373755 |
| O | -1.153356 | 0.990492 | -3.088635 |

| | | | | | | | |
|----|-----------|-----------|-----------|------------------------|-----------|-----------|-----------|
| C | 0.753814 | 2.653939 | 0.280551 | C | -2.287857 | -3.835208 | 0.159073 |
| C | -1.221032 | 0.448512 | -2.057317 | H | -3.156184 | -4.420708 | 0.492138 |
| C | -2.622963 | -2.372293 | 0.162983 | H | -1.451035 | -4.081104 | 0.818839 |
| C | -3.420251 | -1.597641 | -0.739605 | H | -2.025617 | -4.172797 | -0.847123 |
| C | -3.725197 | -0.338458 | -0.092923 | C | -3.590211 | -2.149472 | -2.230155 |
| C | -3.102838 | -0.338309 | 1.189593 | H | -2.931391 | -2.959326 | -2.556190 |
| C | -2.402721 | -1.595362 | 1.348546 | H | -3.568011 | -1.376260 | -3.003713 |
| C | -2.196307 | -3.798087 | -0.053796 | H | -4.613675 | -2.548810 | -2.193501 |
| H | -2.971416 | -4.494779 | 0.296495 | C | -4.188393 | 0.795809 | -1.150382 |
| H | -1.275197 | -4.034168 | 0.487455 | H | -3.939217 | 1.794471 | -0.782509 |
| H | -2.017324 | -4.007227 | -1.112081 | H | -5.274976 | 0.665942 | -1.047393 |
| C | -3.991742 | -2.070650 | -2.047643 | H | -3.956323 | 0.770089 | -2.219116 |
| H | -3.333517 | -2.795262 | -2.536201 | C | -3.286259 | 0.906042 | 1.937436 |
| H | -4.140209 | -1.241141 | -2.745606 | H | -4.177722 | 0.694586 | 2.544910 |
| H | -4.968088 | -2.555883 | -1.902343 | H | -3.454660 | 1.855656 | 1.423677 |
| C | -4.654880 | 0.713473 | -0.632081 | H | -2.448190 | 1.045936 | 2.627564 |
| H | -4.435407 | 1.700133 | -0.213695 | C | -2.086873 | -1.913456 | 2.715669 |
| H | -5.700699 | 0.476387 | -0.388076 | H | -1.581934 | -1.099334 | 3.245842 |
| H | -4.584651 | 0.795517 | -1.720991 | H | -1.412376 | -2.774326 | 2.701974 |
| C | -3.289771 | 0.686587 | 2.273745 | H | -2.964855 | -2.194147 | 3.314691 |
| H | -4.138817 | 0.418408 | 2.919897 | H | 1.919841 | 4.243980 | -1.834458 |
| H | -3.489684 | 1.680630 | 1.864147 | H | 1.681696 | 5.135781 | 1.382759 |
| H | -2.406933 | 0.765053 | 2.915872 | H | 3.386207 | 2.953865 | -0.448833 |
| C | -1.775669 | -2.072216 | 2.629548 | H | 2.237017 | 3.076258 | 2.499344 |
| H | -1.175390 | -1.289438 | 3.107194 | H | 2.016152 | 1.859766 | -2.095446 |
| H | -1.125430 | -2.937080 | 2.463983 | H | 0.009523 | 3.984211 | 2.666902 |
| H | -2.541708 | -2.380194 | 3.356201 | Si | -0.925245 | 3.633832 | -0.528018 |
| H | 1.622198 | 4.183651 | -1.907035 | H | -2.101078 | 3.422284 | 0.357326 |
| H | 2.326114 | 4.673152 | 1.461960 | H | -0.719574 | 5.102575 | -0.640557 |
| H | 3.268680 | 2.724340 | -0.978374 | H | -1.261301 | 3.113033 | -1.876010 |
| H | 2.845887 | 2.431097 | 2.148644 | C | 2.312751 | -0.868329 | 1.001056 |
| H | 1.505069 | 1.816777 | -2.323181 | H | -0.128028 | -1.808866 | -0.926257 |
| H | 0.850100 | 3.506318 | 2.955681 | C | 1.371583 | -1.683807 | 1.620391 |
| Si | -0.837705 | 3.701661 | 0.064138 | H | 1.569235 | -2.747343 | 1.712084 |
| H | -1.800874 | 3.444767 | 1.167561 | H | 0.749680 | -1.263512 | 2.406503 |
| H | -0.484563 | 5.147360 | 0.114802 | H | 0.291476 | -1.417883 | 0.572618 |
| H | -1.513401 | 3.436351 | -1.227770 | C | 3.552682 | -1.364949 | 0.380853 |
| C | 2.543868 | -0.994744 | 0.681149 | C | 4.160181 | -0.654336 | -0.670232 |
| C | 3.874132 | -1.332747 | 0.153807 | C | 4.163527 | -2.548847 | 0.835844 |
| C | 4.596690 | -2.450101 | 0.616613 | C | 5.330128 | -1.126249 | -1.260506 |
| C | 4.452109 | -0.505369 | -0.831347 | H | 3.700257 | 0.260525 | -1.022504 |
| C | 5.861521 | -2.730495 | 0.107499 | C | 5.332476 | -3.018184 | 0.242988 |
| H | 4.185552 | -3.093110 | 1.386455 | H | 3.734357 | -3.087713 | 1.674807 |
| C | 5.710095 | -0.796857 | -1.344194 | C | 5.919290 | -2.309857 | -0.809214 |
| H | 3.898639 | 0.355133 | -1.186937 | H | 5.782390 | -0.569589 | -2.076756 |
| C | 6.418221 | -1.908427 | -0.875364 | H | 5.793038 | -3.931738 | 0.609087 |
| H | 6.412584 | -3.590345 | 0.476547 | H | 6.834043 | -2.674368 | -1.268790 |
| H | 6.141717 | -0.158330 | -2.109119 | | | | |
| H | 7.403242 | -2.132776 | -1.275181 | | | | |
| H | -0.204131 | -1.395524 | -0.993582 | 3c | | | |
| C | 1.741140 | -1.925704 | 1.527605 | SCF done: -1042.469833 | | | |
| H | 0.779480 | -2.062884 | 1.006369 | Ru | -1.335161 | -0.675743 | -0.420890 |
| H | 2.210337 | -2.892280 | 1.702284 | Si | 0.390735 | 0.764495 | 0.658797 |
| H | 1.505620 | -1.447568 | 2.485685 | H | 0.043285 | 0.799500 | 2.119911 |
| | | | | Si | 1.418850 | 3.505278 | 1.691675 |
| | | | | Si | 2.015655 | 2.716654 | -1.250773 |
| | | | | O | 2.034705 | 0.207442 | 0.563147 |
| | | | | O | -0.586763 | 0.580197 | -3.084728 |
| | | | | C | 0.707280 | 2.598135 | 0.155365 |
| | | | | C | -0.834520 | 0.145522 | -2.041177 |
| | | | | C | -2.907321 | -2.224512 | 0.189416 |
| | | | | C | -3.489595 | -1.324236 | -0.771733 |
| | | | | C | -3.568608 | -0.016891 | -0.161613 |
| | | | | C | -3.024993 | -0.110849 | 1.159079 |
| | | | | C | -2.589430 | -1.469171 | 1.366584 |
| | | | | C | -2.775214 | -3.714852 | 0.041511 |
| | | | | H | -3.661518 | -4.217749 | 0.452270 |
| | | | | H | -1.900300 | -4.097243 | 0.574024 |
| | | | | H | -2.681703 | -4.009991 | -1.006764 |
| | | | | C | -4.094200 | -1.711597 | -2.092691 |
| | | | | H | -3.576214 | -2.565476 | -2.538115 |
| | | | | H | -4.052086 | -0.888917 | -2.812174 |

| | | | | | | | |
|-------------------------|-----------|-----------|-----------|--|--|--|--|
| TS_{23c} | | | | | | | |
| SCF done: -1042.450484 | | | | | | | |
| Ru | -1.142951 | -0.673432 | -0.381937 | | | | |
| Si | 0.306672 | 0.980747 | 0.698080 | | | | |
| H | -0.071164 | 1.067146 | 2.154261 | | | | |
| Si | 1.168855 | 3.788098 | 1.755310 | | | | |
| Si | 2.051544 | 2.956371 | -1.099711 | | | | |
| O | 2.008332 | 0.400842 | 0.769467 | | | | |
| O | -0.315290 | 0.479205 | -3.061630 | | | | |
| C | 0.640995 | 2.811665 | 0.191426 | | | | |
| C | -0.605461 | 0.074028 | -2.013047 | | | | |
| C | -2.601527 | -2.364979 | 0.185068 | | | | |
| C | -3.177738 | -1.607374 | -0.889720 | | | | |
| C | -3.452006 | -0.275596 | -0.395654 | | | | |
| C | -3.037470 | -0.216258 | 0.970845 | | | | |
| C | -2.495110 | -1.504366 | 1.329597 | | | | |

| | | | |
|----|-----------|-----------|-----------|
| H | -5.150252 | -1.989775 | -1.971155 |
| C | -4.271666 | 1.172656 | -0.752979 |
| H | -3.896919 | 2.113222 | -0.342955 |
| H | -5.348708 | 1.123446 | -0.540270 |
| H | -4.155364 | 1.214196 | -1.839604 |
| C | -3.068672 | 0.941338 | 2.228369 |
| H | -3.905824 | 0.744075 | 2.912554 |
| H | -3.209028 | 1.941618 | 1.813073 |
| H | -2.154454 | 0.954379 | 2.830027 |
| C | -2.078165 | -2.023927 | 2.666390 |
| H | -1.465514 | -1.293138 | 3.202589 |
| H | -1.472194 | -2.920975 | 2.513675 |
| H | -2.914655 | -2.296099 | 3.325290 |
| H | 1.811664 | 3.996634 | -1.984416 |
| H | 1.961031 | 4.835138 | 1.300021 |
| H | 3.394770 | 2.744398 | -0.703707 |
| H | 2.508841 | 2.726153 | 2.326825 |
| H | 1.910695 | 1.609973 | -2.227046 |
| H | 0.351676 | 3.735265 | 2.703098 |
| Si | -0.860602 | 3.533721 | -0.391593 |
| H | -1.950935 | 3.404864 | 0.611898 |
| H | -0.563278 | 4.984353 | -0.524413 |
| H | -1.383309 | 3.054707 | -1.694788 |
| C | 2.536833 | -0.988377 | 0.985978 |
| C | 3.821675 | -1.345243 | 0.327514 |
| C | 4.195006 | -2.686718 | 0.141743 |
| C | 4.693952 | -0.339521 | -0.117900 |
| C | 5.412264 | -3.012248 | -0.454152 |
| H | 3.514752 | -3.477632 | 0.443245 |
| C | 5.912538 | -0.666514 | -0.712121 |
| H | 4.414270 | 0.699063 | 0.015686 |
| C | 6.278393 | -2.003133 | -0.881726 |
| H | 5.679038 | -4.056400 | -0.596036 |
| H | 6.577680 | 0.126667 | -1.043784 |
| H | 7.225735 | -2.257020 | -1.349998 |
| H | -0.678996 | -1.899515 | -1.224881 |
| C | 1.956681 | -1.756853 | 1.927392 |
| H | 2.433577 | -2.669932 | 2.261863 |
| H | 1.032738 | -1.474280 | 2.417378 |
| H | 0.046673 | -1.322040 | 0.135516 |

TS_{24c}

SCF done: -1042.433571

| | | | |
|----|-----------|-----------|-----------|
| Ru | -1.747734 | -0.157107 | -0.521597 |
| Si | 0.519749 | 0.362704 | -0.256741 |
| H | 1.319454 | -0.824517 | 0.565784 |
| Si | 2.599065 | 1.768357 | 1.773675 |
| Si | 2.269330 | 2.841524 | -1.169768 |
| O | 1.741064 | -0.249947 | -1.550209 |
| O | -2.158806 | 2.132646 | -2.463768 |
| C | 1.383566 | 1.995853 | 0.312272 |
| C | -1.957101 | 1.266144 | -1.711469 |
| C | -3.196114 | -1.904030 | -0.050393 |
| C | -3.948220 | -0.685141 | -0.099169 |
| C | -3.519057 | 0.150686 | 1.006510 |
| C | -2.486364 | -0.536925 | 1.699604 |
| C | -2.265541 | -1.808119 | 1.035211 |
| C | -3.419095 | -3.108649 | -0.922104 |
| H | -4.175942 | -3.772974 | -0.480947 |
| H | -2.502074 | -3.691317 | -1.048393 |
| H | -3.767427 | -2.824391 | -1.918780 |
| C | -5.116571 | -0.400970 | -1.001885 |
| H | -5.014448 | -0.908145 | -1.965600 |
| H | -5.220022 | 0.669491 | -1.203479 |
| H | -6.057545 | -0.741289 | -0.546081 |
| C | -4.152712 | 1.455358 | 1.401675 |
| H | -3.469816 | 2.072761 | 1.991931 |
| H | -5.054766 | 1.288342 | 2.008014 |
| H | -4.451863 | 2.040162 | 0.526311 |
| C | -1.859014 | -0.130446 | 3.003800 |
| H | -2.403506 | -0.575864 | 3.849325 |

| | | | |
|----|-----------|-----------|-----------|
| H | -1.870201 | 0.953997 | 3.141254 |
| H | -0.818929 | -0.463216 | 3.078558 |
| C | -1.394037 | -2.915373 | 1.560242 |
| H | -0.462699 | -2.530379 | 1.987859 |
| H | -1.128509 | -3.628245 | 0.774002 |
| H | -1.907020 | -3.480379 | 2.352630 |
| H | 2.359078 | 4.303163 | -0.904730 |
| H | 3.200940 | 3.076305 | 2.149389 |
| H | 3.654437 | 2.345353 | -1.357265 |
| H | 3.700932 | 0.832923 | 1.455320 |
| H | 1.514719 | 2.651444 | -2.431638 |
| H | 1.874411 | 1.247473 | 2.964265 |
| Si | 0.015163 | 3.216061 | 0.913957 |
| H | -0.799798 | 2.631761 | 2.005103 |
| H | 0.690741 | 4.422879 | 1.463533 |
| H | -0.868712 | 3.646827 | -0.192897 |
| C | 2.144633 | -1.289951 | -0.830941 |
| H | -1.224967 | -0.956815 | -1.821235 |
| C | 1.417773 | -2.588145 | -1.073793 |
| H | 0.337010 | -2.418139 | -1.079945 |
| H | 1.707658 | -2.918728 | -2.081044 |
| H | 1.690416 | -3.368664 | -0.360970 |
| C | 3.561493 | -1.346888 | -0.394141 |
| C | 4.508401 | -0.552582 | -1.059208 |
| C | 3.990179 | -2.231860 | 0.610808 |
| C | 5.859188 | -0.643838 | -0.726400 |
| H | 4.174429 | 0.115835 | -1.843545 |
| C | 5.336097 | -2.304094 | 0.954697 |
| H | 3.264878 | -2.837738 | 1.146096 |
| C | 6.275070 | -1.512948 | 0.283605 |
| H | 6.585794 | -0.033012 | -1.254515 |
| H | 5.655937 | -2.976438 | 1.745689 |
| H | 7.326749 | -1.576408 | 0.549036 |

4c

SCF done: -1042.5066505

| | | | |
|----|-----------|-----------|-----------|
| Ru | -1.525576 | -0.358417 | -0.482633 |
| Si | 0.315488 | 0.981642 | -0.268533 |
| H | 1.490149 | -1.350175 | -1.234445 |
| Si | 1.788551 | 2.881061 | 1.745852 |
| Si | 1.313031 | 3.787576 | -1.213647 |
| O | 1.901420 | 0.599011 | -0.671191 |
| O | -3.000704 | 1.602181 | -2.274632 |
| C | 0.573267 | 2.795312 | 0.260141 |
| C | -2.394886 | 0.884647 | -1.587753 |
| C | -2.107533 | -2.568649 | -0.058440 |
| C | -3.298678 | -1.774714 | -0.053188 |
| C | -3.215768 | -0.850461 | 1.063834 |
| C | -1.969729 | -1.062374 | 1.715664 |
| C | -1.261041 | -2.113761 | 1.006556 |
| C | -1.836182 | -3.741611 | -0.958326 |
| H | -2.231436 | -4.667137 | -0.516060 |
| H | -0.764329 | -3.885099 | -1.120050 |
| H | -2.304476 | -3.616075 | -1.938240 |
| C | -4.507015 | -1.985199 | -0.922742 |
| H | -4.232799 | -2.384831 | -1.903209 |
| H | -5.054216 | -1.052390 | -1.088020 |
| H | -5.204109 | -2.696837 | -0.457740 |
| C | -4.315382 | 0.066660 | 1.522396 |
| H | -3.919106 | 0.928924 | 2.066605 |
| H | -5.008942 | -0.458857 | 2.194441 |
| H | -4.903072 | 0.448037 | 0.682061 |
| C | -1.533734 | -0.442557 | 3.014288 |
| H | -1.911070 | -1.027701 | 3.865494 |
| H | -1.909995 | 0.578123 | 3.125344 |
| H | -0.444010 | -0.407512 | 3.102582 |
| C | -0.006395 | -2.794073 | 1.483624 |
| C | 0.680638 | -2.097339 | 1.972302 |
| H | 0.539726 | -3.263956 | 0.660666 |
| H | -0.243047 | -3.584432 | 2.211182 |
| H | 1.057653 | 5.239486 | -1.016252 |

| | | | | | | | |
|------------------------|-----------|-----------|-----------|-------------------------|-----------|-----------|-----------|
| H | 1.780274 | 4.253400 | 2.318462 | H | -2.831392 | -1.610199 | 2.434509 |
| H | 2.776257 | 3.583997 | -1.336139 | H | -2.036243 | 0.457248 | -2.078846 |
| H | 3.176061 | 2.546195 | 1.351071 | C | 0.897144 | -1.676535 | 0.414284 |
| H | 0.667430 | 3.380759 | -2.488970 | C | 2.342611 | -1.927393 | 0.108685 |
| H | 1.362017 | 1.941306 | 2.818034 | C | 3.311499 | -2.063019 | 1.117382 |
| Si | -1.096193 | 3.586230 | 0.780228 | C | 2.720707 | -2.169683 | -1.223205 |
| H | -1.744922 | 2.805514 | 1.864127 | C | 4.623753 | -2.414074 | 0.801164 |
| H | -0.837178 | 4.956393 | 1.295273 | H | 3.043286 | -1.887049 | 2.154846 |
| H | -2.030161 | 3.689217 | -0.365392 | C | 4.031462 | -2.527944 | -1.537255 |
| C | 2.328163 | -0.643974 | -1.260099 | H | 1.962561 | -2.097443 | -1.995852 |
| H | -0.728732 | -0.839896 | -1.808862 | C | 4.989438 | -2.649449 | -0.526503 |
| C | 2.703520 | -0.372885 | -2.719959 | H | 5.360959 | -2.509250 | 1.594091 |
| H | 1.831701 | -0.006971 | -3.273257 | H | 4.302956 | -2.726847 | -2.570898 |
| H | 3.499363 | 0.377188 | -2.773768 | H | 6.009567 | -2.933305 | -0.770320 |
| H | 3.060551 | -1.291107 | -3.198905 | C | 0.357941 | -2.373262 | 1.658286 |
| C | 3.489032 | -1.217515 | -0.467501 | H | 0.502981 | -3.455836 | 1.536589 |
| C | 4.450360 | -0.387528 | 0.122655 | H | 0.873095 | -2.074934 | 2.575049 |
| C | 3.639461 | -2.605976 | -0.364389 | H | -0.707917 | -2.182418 | 1.774564 |
| C | 5.537078 | -0.937734 | 0.804002 | | | | |
| H | 4.336950 | 0.689540 | 0.053181 | | | | |
| C | 4.729153 | -3.158265 | 0.311374 | | | | |
| H | 2.898693 | -3.261156 | -0.818861 | | | | |
| C | 5.681370 | -2.323830 | 0.899493 | | | | |
| H | 6.273233 | -0.281657 | 1.261397 | | | | |
| H | 4.829650 | -4.238119 | 0.383427 | | | | |
| H | 6.528201 | -2.750195 | 1.430590 | | | | |
| 5d | | | | | | | |
| SCF done: -1042.470738 | | | | | | | |
| Ru | 0.198753 | 0.598715 | 0.237430 | | | | |
| Si | -2.138812 | 0.468956 | -0.585001 | | | | |
| H | -2.848879 | 1.747519 | -0.246499 | | | | |
| Si | -5.031111 | -0.370594 | -1.190604 | | | | |
| Si | -2.948518 | -2.627366 | -0.895896 | | | | |
| O | 0.094346 | -1.425459 | -0.560157 | | | | |
| O | -0.838662 | 0.504862 | 3.064928 | | | | |
| C | -3.459202 | -0.907297 | -0.222787 | | | | |
| C | -0.484479 | 0.459352 | 1.956759 | | | | |
| C | 2.337357 | 1.638313 | -0.227998 | | | | |
| C | 1.607330 | 2.339815 | 0.771433 | | | | |
| C | 0.373282 | 2.816932 | 0.174417 | | | | |
| C | 0.399361 | 2.453529 | -1.226813 | | | | |
| C | 1.567094 | 1.675175 | -1.450990 | | | | |
| C | 3.742201 | 1.132136 | -0.100388 | | | | |
| H | 4.452021 | 1.926380 | -0.373700 | | | | |
| H | 3.933959 | 0.281188 | -0.756922 | | | | |
| H | 3.975620 | 0.821805 | 0.921106 | | | | |
| C | 2.091916 | 2.672163 | 2.155612 | | | | |
| H | 2.802829 | 1.927001 | 2.524111 | | | | |
| H | 1.269230 | 2.730553 | 2.873504 | | | | |
| H | 2.601687 | 3.645576 | 2.159839 | | | | |
| C | -0.579967 | 3.794104 | 0.805142 | | | | |
| H | -1.597372 | 3.668433 | 0.425025 | | | | |
| H | -0.268835 | 4.827187 | 0.596368 | | | | |
| H | -0.617244 | 3.673347 | 1.891666 | | | | |
| C | -0.539695 | 2.957468 | -2.283014 | | | | |
| H | -0.149074 | 3.892874 | -2.708289 | | | | |
| H | -1.534611 | 3.171644 | -1.884282 | | | | |
| H | -0.656224 | 2.244608 | -3.103646 | | | | |
| C | 2.010447 | 1.129938 | -2.778456 | | | | |
| H | 1.156880 | 0.878123 | -3.414474 | | | | |
| H | 2.618069 | 0.229687 | -2.660992 | | | | |
| H | 2.618037 | 1.870598 | -3.317654 | | | | |
| H | -4.176844 | -3.451343 | -1.091056 | | | | |
| H | -6.145032 | -1.326574 | -0.947948 | | | | |
| H | -2.273579 | -2.520091 | -2.212420 | | | | |
| H | -4.767313 | -0.335918 | -2.653396 | | | | |
| H | -2.084524 | -3.379215 | 0.045793 | | | | |
| H | -5.486832 | 0.980489 | -0.770101 | | | | |
| Si | -3.933774 | -1.041090 | 1.620493 | | | | |
| H | -4.289339 | 0.291262 | 2.176904 | | | | |
| H | -5.113288 | -1.934097 | 1.787825 | | | | |
| | | | | TS_{56d} | | | |
| | | | | SCF done: -1042.443674 | | | |
| Ru | 0.529350 | -0.870018 | -0.335657 | | | | |
| Si | -1.918362 | -0.308932 | 0.544289 | | | | |
| H | -2.501237 | -1.636811 | 0.148822 | | | | |
| Si | -4.705840 | 0.333754 | 1.632761 | | | | |
| Si | -3.048320 | 2.699498 | 0.536384 | | | | |
| O | -0.539822 | 0.948654 | 0.141211 | | | | |
| O | -0.796590 | -1.856404 | -2.861614 | | | | |
| C | -3.440770 | 0.845752 | 0.276143 | | | | |
| C | -0.331288 | -1.395589 | -1.897270 | | | | |
| C | 2.754823 | -1.188494 | 0.479936 | | | | |
| C | 2.368126 | -2.174044 | -0.488082 | | | | |
| C | 1.284892 | -2.960467 | 0.087646 | | | | |
| C | 0.980424 | -2.417468 | 1.369706 | | | | |
| C | 1.869992 | -1.300339 | 1.594272 | | | | |
| C | 3.926645 | -0.260225 | 0.363812 | | | | |
| H | 4.831159 | -0.734041 | 0.771221 | | | | |
| H | 3.766341 | 0.673090 | 0.908950 | | | | |
| H | 4.133546 | 0.002359 | -0.677088 | | | | |
| C | 3.110858 | -2.505798 | -1.752288 | | | | |
| H | 3.544147 | -1.611032 | -2.208978 | | | | |
| H | 2.456811 | -2.972374 | -2.494349 | | | | |
| H | 3.933621 | -3.206442 | -1.550330 | | | | |
| C | 0.712716 | -4.223134 | -0.494882 | | | | |
| H | -0.316446 | -4.390215 | -0.163559 | | | | |
| H | 1.307415 | -5.092977 | -0.182848 | | | | |
| H | 0.708844 | -4.203491 | -1.588228 | | | | |
| C | 0.016159 | -2.989988 | 2.368418 | | | | |
| H | 0.500035 | -3.767922 | 2.975908 | | | | |
| H | -0.850784 | -3.446718 | 1.880928 | | | | |
| H | -0.355720 | -2.224874 | 3.055619 | | | | |
| C | 1.929216 | -0.489483 | 2.857708 | | | | |
| H | 0.931241 | -0.320136 | 3.274802 | | | | |
| H | 2.389620 | 0.486901 | 2.687851 | | | | |
| H | 2.520013 | -1.008676 | 3.625493 | | | | |
| H | -4.322507 | 3.447494 | 0.726580 | | | | |
| H | -6.053489 | 0.869250 | 1.308967 | | | | |
| H | -2.221417 | 2.908346 | 1.751806 | | | | |
| H | -4.297324 | 0.865170 | 2.959386 | | | | |
| H | -2.357541 | 3.303715 | -0.629081 | | | | |
| H | -4.809343 | -1.145226 | 1.739642 | | | | |
| Si | -4.293195 | 0.571272 | -1.415119 | | | | |
| H | -4.844474 | -0.806405 | -1.503569 | | | | |
| H | -5.416038 | 1.530729 | -1.587883 | | | | |
| H | -3.355172 | 0.765112 | -2.548860 | | | | |
| H | -1.650918 | -0.343581 | 2.003102 | | | | |
| C | 0.351316 | 1.194031 | -0.900241 | | | | |
| C | 1.484236 | 2.071070 | -0.469226 | | | | |
| C | 2.494042 | 2.426496 | -1.382597 | | | | |
| C | 1.548598 | 2.608061 | 0.828661 | | | | |
| C | 3.532589 | 3.278470 | -1.009845 | | | | |

| | | | | | | | |
|---|-----------|----------|-----------|---|-----------|-----------|-----------|
| H | 2.471096 | 2.028823 | -2.393006 | C | -0.644926 | 0.653565 | -2.494421 |
| C | 2.590513 | 3.459984 | 1.199825 | H | -1.598175 | 1.190159 | -2.616829 |
| H | 0.763557 | 2.366977 | 1.536746 | H | 0.074802 | 1.110957 | -3.178372 |
| C | 3.588840 | 3.800818 | 0.284707 | H | -0.773018 | -0.377860 | -2.826721 |
| H | 4.299803 | 3.536544 | -1.735505 | | | | |
| H | 2.611630 | 3.871242 | 2.206190 | | | | |
| H | 4.395263 | 4.469404 | 0.573213 | | | | |
| C | -0.284571 | 1.586201 | -2.225195 | | | | |
| H | 0.411600 | 1.437820 | -3.055298 | | | | |
| H | -1.173813 | 0.988852 | -2.430796 | | | | |
| H | -0.577448 | 2.645008 | -2.215627 | | | | |

6d

SCF done: -1042.466326

| | | | |
|----|-----------|-----------|-----------|
| Ru | 1.293504 | -0.644005 | -0.310799 |
| Si | -2.083925 | -1.272676 | -0.275677 |
| H | -2.086904 | -1.834428 | -1.645968 |
| Si | -5.009438 | -2.157589 | 0.052055 |
| Si | -3.892288 | 0.050422 | 1.938295 |
| O | -0.860986 | -0.078888 | -0.109518 |
| O | 1.280012 | -2.485890 | -2.705947 |
| C | -3.827733 | -0.642735 | 0.151674 |
| C | 1.182846 | -1.742890 | -1.809315 |
| C | 3.019812 | 0.580138 | 0.718775 |
| C | 3.506854 | -0.463231 | -0.151680 |
| C | 3.152115 | -1.742689 | 0.450462 |
| C | 2.348287 | -1.479808 | 1.587096 |
| C | 2.262845 | -0.035033 | 1.749636 |
| C | 3.315884 | 2.042030 | 0.566793 |
| H | 4.286594 | 2.284333 | 1.022730 |
| H | 2.556998 | 2.666818 | 1.043400 |
| H | 3.364046 | 2.335618 | -0.485502 |
| C | 4.480381 | -0.273171 | -1.281574 |
| H | 4.297376 | 0.666359 | -1.811592 |
| H | 4.410435 | -1.083170 | -2.013399 |
| H | 5.515739 | -0.249690 | -0.911145 |
| C | 3.627835 | -3.087195 | -0.023932 |
| H | 2.952973 | -3.888864 | 0.289831 |
| H | 4.622851 | -3.309613 | 0.386268 |
| H | 3.704951 | -3.130861 | -1.113983 |
| C | 1.787403 | -2.485341 | 2.552414 |
| H | 2.417210 | -2.565874 | 3.450345 |
| H | 1.723102 | -3.481195 | 2.104901 |
| H | 0.781982 | -2.207849 | 2.886058 |
| C | 1.597791 | 0.644800 | 2.912291 |
| H | 0.634736 | 0.181081 | 3.152713 |
| H | 1.416527 | 1.703266 | 2.712922 |
| H | 2.223885 | 0.575553 | 3.813346 |
| H | -5.302717 | 0.144565 | 2.396987 |
| H | -6.417379 | -1.709765 | 0.191028 |
| H | -3.157719 | -0.847036 | 2.867616 |
| H | -4.710621 | -3.126579 | 1.138226 |
| H | -3.290494 | 1.404054 | 2.012492 |
| H | -4.857189 | -2.855045 | -1.250863 |
| Si | -4.453984 | 0.694651 | -1.071397 |
| H | -4.543275 | 0.136670 | -2.446063 |
| H | -5.808623 | 1.148709 | -0.663589 |
| H | -3.548512 | 1.868269 | -1.089479 |
| H | -1.706164 | -2.306329 | 0.715419 |
| C | -0.119372 | 0.742346 | -1.069333 |
| C | -0.009744 | 2.149147 | -0.566835 |
| C | 0.603960 | 3.136052 | -1.364038 |
| C | -0.503776 | 2.544525 | 0.688727 |
| C | 0.717487 | 4.453907 | -0.924369 |
| H | 1.006555 | 2.870991 | -2.337092 |
| C | -0.389685 | 3.864755 | 1.128099 |
| H | -0.986666 | 1.808463 | 1.319319 |
| C | 0.220951 | 4.830245 | 0.325890 |
| H | 1.196127 | 5.190727 | -1.564816 |
| H | -0.791527 | 4.139442 | 2.100612 |
| H | 0.305309 | 5.858741 | 0.666055 |

2e

SCF done: -1234.206812

| | | | |
|----|-----------|-----------|-----------|
| Ru | -1.575108 | -0.384354 | -0.619551 |
| Si | -0.282559 | 1.030119 | 0.711005 |
| H | -0.091795 | 0.649936 | 2.158819 |
| Si | 0.718450 | 3.543015 | 2.349856 |
| Si | 0.612160 | 3.743599 | -0.746383 |
| O | 1.653026 | 0.875810 | 0.164368 |
| O | -2.260782 | 1.715366 | -2.685359 |
| C | -0.216858 | 2.963380 | 0.791969 |
| C | -1.971039 | 0.936179 | -1.865581 |
| C | -1.864043 | -2.695778 | -0.469516 |
| C | -2.996215 | -2.131096 | -1.143694 |
| C | -3.685125 | -1.274005 | -0.202787 |
| C | -2.970836 | -1.303249 | 1.032670 |
| C | -1.829821 | -2.177945 | 0.865526 |
| C | -0.940727 | -3.740257 | -1.033399 |
| H | -1.328835 | -4.750579 | -0.838411 |
| H | 0.056583 | -3.678853 | -0.588196 |
| H | -0.826617 | -3.633102 | -2.115776 |
| C | -3.481648 | -2.497759 | -2.518849 |
| H | -2.650361 | -2.753567 | -3.182898 |
| H | -4.030480 | -1.674014 | -2.985489 |
| H | -4.157457 | -3.365136 | -2.485688 |
| C | -4.998025 | -0.584262 | -0.453563 |
| H | -5.122551 | 0.291648 | 0.189714 |
| H | -5.841512 | -1.261821 | -0.256945 |
| H | -5.085619 | -0.245834 | -1.490496 |
| C | -3.412550 | -0.695829 | 2.335323 |
| H | -4.025640 | -1.405757 | 2.910368 |
| H | -4.012435 | 0.205737 | 2.181035 |
| H | -2.559562 | -0.421221 | 2.963568 |
| C | -0.919302 | -2.633191 | 1.972519 |
| H | -0.664491 | -1.817300 | 2.656660 |
| H | 0.018593 | -3.040386 | 1.583759 |
| H | -1.396043 | -3.423207 | 2.572024 |
| H | 0.128061 | 5.139444 | -0.934148 |
| H | 0.957298 | 5.013030 | 2.333614 |
| H | 2.088148 | 3.815800 | -0.575916 |
| H | 2.048638 | 2.883693 | 2.461193 |
| H | 0.326326 | 2.989640 | -1.989224 |
| H | -0.045747 | 3.224527 | 3.586446 |
| Si | -2.024189 | 3.596650 | 0.914096 |
| H | -2.793215 | 2.812625 | 1.917320 |
| H | -2.019397 | 5.013898 | 1.372188 |
| H | -2.730313 | 3.535149 | -0.385884 |
| C | 2.553661 | 0.001415 | 0.085632 |
| C | 2.787905 | -0.954430 | 1.188868 |
| C | 3.156343 | -2.288147 | 0.929793 |
| C | 2.611560 | -0.533810 | 2.519570 |
| C | 3.333214 | -3.182941 | 1.983448 |
| H | 3.273525 | -2.625199 | -0.094798 |
| C | 2.815725 | -1.425354 | 3.568533 |
| H | 2.338291 | 0.495856 | 2.719689 |
| C | 3.170064 | -2.751425 | 3.302429 |
| H | 3.599057 | -4.215328 | 1.775669 |
| H | 2.694820 | -1.088284 | 4.593814 |
| H | 3.318800 | -3.448059 | 4.122875 |
| C | 3.361341 | -0.039187 | -1.145552 |
| C | 4.696476 | -0.488046 | -1.146947 |
| C | 2.782135 | 0.419842 | -2.345324 |
| C | 5.436218 | -0.474698 | -2.326293 |
| H | 5.158307 | -0.816358 | -0.221592 |
| C | 3.521287 | 0.407685 | -3.523898 |
| H | 1.749743 | 0.751281 | -2.337587 |
| C | 4.848344 | -0.033595 | -3.515591 |

| | | | |
|---|-----------|-----------|-----------|
| H | 6.471026 | -0.804574 | -2.318629 |
| H | 3.064249 | 0.744914 | -4.449503 |
| H | 5.425926 | -0.031343 | -4.436004 |
| H | -0.231128 | -0.613421 | -1.495155 |

| | | | |
|---|-----------|----------|-----------|
| H | -2.301097 | 5.401103 | 0.915152 |
| H | 0.325260 | 4.364538 | -2.335087 |
| H | -0.622094 | 6.073555 | -0.793064 |
| H | 1.398839 | 0.952942 | -1.673867 |

TS_{23a}

SCF done: -1234.163155

| | | | |
|----|-----------|-----------|-----------|
| Ru | 1.907235 | -0.077300 | -0.553078 |
| Si | -0.347371 | -0.703039 | -0.349441 |
| H | -1.090344 | 0.302804 | 0.729201 |
| Si | -2.290421 | -2.684338 | 1.382676 |
| Si | -1.964558 | -3.020299 | -1.731543 |
| O | -1.632530 | 0.133144 | -1.407427 |
| O | 2.340254 | -1.908761 | -2.928370 |
| C | -1.096463 | -2.472354 | -0.104229 |
| C | 2.131763 | -1.227281 | -2.006248 |
| C | 3.399986 | 1.525498 | 0.173997 |
| C | 4.106897 | 0.289098 | 0.008129 |
| C | 3.606611 | -0.651853 | 0.991758 |
| C | 2.570423 | -0.005872 | 1.720868 |
| C | 2.424532 | 1.343431 | 1.208697 |
| C | 3.700434 | 2.815772 | -0.536796 |
| C | 4.438172 | 3.406818 | 0.024817 |
| H | 2.802138 | 3.428871 | -0.651283 |
| H | 4.109675 | 2.638395 | -1.535319 |
| C | 5.295885 | 0.063361 | -0.883854 |
| H | 5.246484 | 0.680669 | -1.785539 |
| H | 5.368659 | -0.980509 | -1.203613 |
| H | 6.230807 | 0.312685 | -0.361773 |
| C | 4.188432 | -2.009903 | 1.269290 |
| H | 3.459349 | -2.674079 | 1.741982 |
| H | 5.053527 | -1.936464 | 1.944526 |
| H | 4.532977 | -2.498485 | 0.352454 |
| C | 1.871288 | -0.544921 | 2.937881 |
| H | 2.408966 | -0.253100 | 3.851765 |
| H | 1.815180 | -1.636756 | 2.925098 |
| H | 0.851129 | -0.159126 | 3.027009 |
| C | 1.564098 | 2.419728 | 1.809834 |
| H | 0.636840 | 2.011523 | 2.223080 |
| H | 1.286822 | 3.174498 | 1.068751 |
| H | 2.088324 | 2.934772 | 2.628975 |
| H | -2.076481 | -4.504613 | -1.742932 |
| H | -2.287897 | -4.104328 | 1.828114 |
| H | -3.333395 | -2.467546 | -1.855100 |
| H | -3.689387 | -2.331592 | 1.050251 |
| H | -1.169087 | -2.616334 | -2.917280 |
| H | -1.848001 | -1.861901 | 2.539598 |
| Si | 0.363890 | -3.698918 | 0.200542 |
| H | 1.088132 | -3.374120 | 1.454676 |
| H | -0.208250 | -5.062125 | 0.362984 |
| H | 1.320951 | -3.733833 | -0.925927 |
| C | -2.110869 | 0.917484 | -0.432615 |
| C | -3.433635 | 0.546487 | 0.165993 |
| C | -3.737625 | 0.710512 | 1.525678 |
| C | -4.427398 | 0.080560 | -0.707571 |
| C | -5.015155 | 0.420911 | 2.001446 |
| H | -2.960815 | 1.027682 | 2.215634 |
| C | -5.706841 | -0.201893 | -0.229040 |
| H | -4.188497 | -0.052964 | -1.756924 |
| C | -6.004437 | -0.031767 | 1.124123 |
| H | -5.234878 | 0.536612 | 3.059109 |
| H | -6.469228 | -0.560790 | -0.914717 |
| H | -6.999365 | -0.259129 | 1.496710 |
| C | -1.719072 | 2.346947 | -0.492263 |
| C | -2.269373 | 3.328306 | 0.357801 |
| C | -0.782742 | 2.740836 | -1.467295 |
| C | -1.869128 | 4.655542 | 0.253537 |
| H | -3.019928 | 3.057536 | 1.090466 |
| C | -0.392220 | 4.075280 | -1.572397 |
| H | -0.382789 | 1.992886 | -2.137417 |
| C | -0.925739 | 5.033399 | -0.709218 |

3e

SCF done: -1234.236552

| | | | |
|----|-----------|-----------|-----------|
| Ru | 1.889427 | -0.175833 | 0.428820 |
| Si | 0.108363 | 1.054349 | -0.322678 |
| H | -1.250211 | -1.235579 | 0.543355 |
| Si | -1.773313 | 3.201230 | -1.712867 |
| Si | -0.119189 | 3.956435 | 0.803004 |
| O | -1.507084 | 0.565200 | -0.435570 |
| O | 3.528322 | 2.233956 | 1.248535 |
| C | -0.109055 | 2.887171 | -0.803214 |
| C | 2.841921 | 1.354799 | 0.918396 |
| C | 2.154911 | -2.452331 | 0.917192 |
| C | 3.434273 | -1.801054 | 0.927178 |
| C | 3.701404 | -1.338306 | -0.420330 |
| C | 2.581815 | -1.674395 | -1.236162 |
| C | 1.612393 | -2.359020 | -0.402869 |
| C | 1.546713 | -3.194329 | 2.074326 |
| H | 1.887228 | -4.239356 | 2.085053 |
| H | 0.454543 | -3.206038 | 2.020232 |
| H | 1.826605 | -2.744784 | 3.030834 |
| C | 4.410369 | -1.784445 | 2.070662 |
| H | 3.897817 | -1.749707 | 3.036332 |
| H | 5.075586 | -0.917338 | 2.021336 |
| H | 5.042285 | -2.684198 | 2.062493 |
| C | 4.993033 | -0.730859 | -0.893030 |
| H | 4.844705 | -0.107476 | -1.779338 |
| H | 5.715890 | -1.515617 | -1.156898 |
| H | 5.455208 | -0.106376 | -0.122976 |
| C | 2.494101 | -1.525681 | -2.729725 |
| H | 2.942667 | -2.394943 | -3.232821 |
| H | 3.021677 | -0.634870 | -3.081919 |
| H | 1.456839 | -1.454040 | -3.068564 |
| C | 0.399805 | -3.084727 | -0.916818 |
| H | -0.148676 | -2.507422 | -1.666235 |
| H | -0.302194 | -3.328032 | -0.114889 |
| H | 0.693002 | -4.034846 | -1.386594 |
| H | -0.553323 | 5.336776 | 0.462098 |
| H | -1.730132 | 4.575825 | -2.283616 |
| H | -1.072329 | 3.398411 | 1.794486 |
| H | -2.944098 | 3.127955 | -0.808489 |
| H | 1.227633 | 4.025271 | 1.416514 |
| H | -1.959082 | 2.261417 | -2.846976 |
| Si | 1.322096 | 3.476159 | -1.938905 |
| H | 1.254958 | 2.775250 | -3.249291 |
| H | 1.181789 | 4.933978 | -2.194831 |
| H | 2.654288 | 3.235124 | -1.341123 |
| C | -2.070801 | -0.609296 | 0.170310 |
| C | -2.863196 | -1.410872 | -0.857055 |
| C | -3.467511 | -2.612913 | -0.458329 |
| C | -2.997056 | -0.997322 | -2.185664 |
| C | -4.185345 | -3.385557 | -1.368969 |
| H | -3.383253 | -2.937864 | 0.576185 |
| C | -3.721002 | -1.770971 | -3.098980 |
| H | -2.539288 | -0.067412 | -2.502485 |
| C | -4.315307 | -2.966016 | -2.696364 |
| H | -4.646557 | -4.314002 | -1.042386 |
| H | -3.819229 | -1.432669 | -4.127361 |
| H | -4.877087 | -3.566172 | -3.407105 |
| H | -2.913206 | -0.184731 | 1.366842 |
| C | -2.488584 | -0.480677 | 2.666446 |
| C | -4.107318 | 0.527309 | 1.186474 |
| C | -3.244624 | -0.077999 | 3.771032 |
| H | -1.556841 | -1.021302 | 2.816482 |
| C | -4.858466 | 0.935933 | 2.286639 |
| H | -4.446485 | 0.755856 | 0.180075 |
| C | -4.430300 | 0.631704 | 3.582838 |

| | | | | | | | |
|---|-----------|-----------|----------|---|-----------|----------|----------|
| H | -2.903448 | -0.316757 | 4.774898 | C | -0.872152 | 4.565635 | 2.173356 |
| H | -5.781605 | 1.489020 | 2.134536 | H | 0.586076 | 5.334674 | 0.783525 |
| H | -5.019475 | 0.947646 | 4.439677 | H | -2.328573 | 3.522060 | 3.376984 |
| H | 1.070704 | -0.009238 | 1.822811 | H | -0.824775 | 5.428934 | 2.831434 |

7g

SCF done: -1234.196655

| | | | |
|----|-----------|-----------|-----------|
| Ru | -0.071108 | -0.769087 | 0.452531 |
| Si | 2.255505 | -0.984937 | -0.396686 |
| H | 3.040535 | -1.844867 | 0.550615 |
| Si | 5.126601 | -0.412703 | -1.326629 |
| Si | 2.889536 | 1.424533 | -2.410505 |
| O | 0.038753 | 0.782607 | -1.079206 |
| O | 1.040453 | 0.706450 | 2.829429 |
| C | 3.471848 | 0.448480 | -0.867099 |
| C | 0.638022 | 0.220682 | 1.853162 |
| C | -2.140232 | -2.045114 | 0.579611 |
| C | -1.413179 | -2.065737 | 1.803456 |
| C | -0.136633 | -2.704841 | 1.552245 |
| C | -0.133661 | -3.141440 | 0.171739 |
| C | -1.331927 | -2.683457 | -0.436191 |
| C | -3.571335 | -1.630937 | 0.414549 |
| H | -4.232730 | -2.487733 | 0.608577 |
| H | -3.784453 | -1.274227 | -0.594651 |
| H | -3.852455 | -0.837883 | 1.113008 |
| C | -1.930048 | -1.649996 | 3.153144 |
| H | -2.682480 | -0.859852 | 3.073345 |
| H | -1.129610 | -1.280041 | 3.799816 |
| H | -2.400116 | -2.501284 | 3.665004 |
| C | 0.842691 | -3.141700 | 2.606993 |
| H | 1.862635 | -3.190981 | 2.215893 |
| H | 0.581365 | -4.138871 | 2.987774 |
| H | 0.850368 | -2.454612 | 3.457907 |
| C | 0.858542 | -4.078772 | -0.450012 |
| H | 0.525402 | -5.115695 | -0.300020 |
| H | 1.851641 | -3.988267 | -0.002785 |
| H | 0.959007 | -3.916742 | -1.526453 |
| C | -1.770292 | -3.016448 | -1.834340 |
| H | -0.932319 | -2.986446 | -2.537950 |
| H | -2.534506 | -2.326060 | -2.196069 |
| H | -2.194108 | -4.030306 | -1.873075 |
| H | 4.081928 | 1.919045 | -3.158241 |
| H | 6.157046 | 0.596796 | -1.689911 |
| H | 2.112594 | 0.568380 | -3.341265 |
| H | 4.948831 | -1.322428 | -2.489987 |
| H | 2.088938 | 2.624498 | -2.066902 |
| H | 5.650510 | -1.214967 | -0.190153 |
| Si | 3.822595 | 1.656225 | 0.569495 |
| H | 4.301337 | 0.921105 | 1.770704 |
| H | 4.892334 | 2.615325 | 0.175480 |
| H | 2.623479 | 2.444578 | 0.935735 |
| H | 2.155642 | -1.781085 | -1.661227 |
| C | -1.048183 | 1.182278 | -0.510569 |
| C | -2.321415 | 1.004597 | -1.293454 |
| C | -3.555926 | 1.556316 | -0.908159 |
| C | -2.241713 | 0.362171 | -2.543643 |
| C | -4.679004 | 1.436901 | -1.728134 |
| H | -3.641527 | 2.101207 | 0.024171 |
| C | -3.362301 | 0.249238 | -3.363204 |
| H | -1.279772 | -0.021153 | -2.865166 |
| C | -4.590572 | 0.779878 | -2.956104 |
| H | -5.622637 | 1.871214 | -1.408647 |
| H | -3.274503 | -0.241139 | -4.329393 |
| H | -5.463694 | 0.696265 | -3.597587 |
| C | -0.989841 | 2.325898 | 0.474501 |
| C | -0.138186 | 3.400721 | 0.182138 |
| C | -1.779386 | 2.388444 | 1.633965 |
| C | -0.808898 | 4.511589 | 1.025647 |
| H | 0.476580 | 3.358601 | -0.710351 |
| C | -1.720163 | 3.496911 | 2.476720 |
| H | -2.416540 | 1.547907 | 1.895358 |

TS_{78g}

SCF done: -1234.168500

| | | | |
|----|-----------|-----------|----------|
| Ru | -0.651336 | -0.845188 | 0.57413 |
| Si | 1.725215 | -1.140058 | -0.50777 |
| H | 2.219387 | -2.111719 | 0.52363 |
| Si | 4.505166 | -1.707964 | -1.67179 |
| Si | 3.155321 | 0.945445 | -2.46223 |
| O | 0.616270 | 0.440238 | -0.66706 |
| O | 0.828473 | -0.617097 | 3.19415 |
| C | 3.371545 | -0.294869 | -1.02378 |
| C | 0.299877 | -0.614830 | 2.15729 |
| C | -2.920542 | -1.356137 | -0.00093 |
| C | -2.594282 | -1.679460 | 1.35864 |
| C | -1.606335 | -2.747649 | 1.33290 |
| C | -1.298132 | -3.029403 | -0.03099 |
| C | -2.092379 | -2.146595 | -0.85252 |
| C | -4.006925 | -0.417508 | -0.43212 |
| H | -4.970396 | -0.945360 | -0.47345 |
| H | -3.816457 | 0.005293 | -1.42084 |
| H | -4.119755 | 0.418380 | 0.26339 |
| C | -3.333048 | -1.196349 | 2.57582 |
| H | -3.641611 | -0.151695 | 2.46998 |
| H | -2.719940 | -1.271337 | 3.47851 |
| H | -4.240931 | -1.793062 | 2.74472 |
| C | -1.133489 | -3.533861 | 2.52430 |
| H | -0.128413 | -3.937454 | 2.37014 |
| H | -1.806705 | -4.381362 | 2.71351 |
| H | -1.108355 | -2.924751 | 3.43187 |
| C | -0.425362 | -4.144763 | -0.52799 |
| H | -1.011702 | -5.063849 | -0.66800 |
| H | 0.379706 | -4.373938 | 0.17704 |
| H | 0.035428 | -3.903532 | -1.49043 |
| C | -2.132498 | -2.179932 | -2.35409 |
| H | -1.134753 | -2.322811 | -2.78223 |
| H | -2.544151 | -1.256120 | -2.76677 |
| H | -2.759306 | -3.011514 | -2.70577 |
| H | 4.457851 | 1.130569 | -3.16065 |
| H | 5.898054 | -1.212276 | -1.81764 |
| H | 2.180924 | 0.431653 | -3.45983 |
| H | 4.042709 | -2.188040 | -3.00144 |
| H | 2.712973 | 2.287729 | -2.01487 |
| H | 4.518899 | -2.867160 | -0.74240 |
| Si | 4.264151 | 0.516892 | 0.46367 |
| H | 4.766808 | -0.532229 | 1.39070 |
| H | 5.434338 | 1.305648 | -0.00779 |
| H | 3.364331 | 1.419905 | 1.21679 |
| H | 1.261297 | -1.889618 | -1.70235 |
| C | -0.346145 | 1.197644 | -0.00196 |
| C | -1.375351 | 1.731822 | -0.96136 |
| C | -2.352047 | 2.650412 | -0.53474 |
| C | -1.362222 | 1.365837 | -2.31913 |
| C | -3.287433 | 3.170139 | -1.42871 |
| H | -2.369427 | 2.972251 | 0.50158 |
| C | -2.297288 | 1.890479 | -3.21251 |
| H | -0.598818 | 0.681440 | -2.67080 |
| C | -3.267868 | 2.794158 | -2.77369 |
| H | -4.028987 | 3.880673 | -1.07221 |
| H | -2.255404 | 1.602186 | -4.26016 |
| H | -3.990569 | 3.208255 | -3.47152 |
| C | 0.159892 | 2.232560 | 0.98056 |
| C | 1.142035 | 3.151010 | 0.57876 |
| C | -0.405701 | 2.380742 | 2.25453 |
| C | 1.570033 | 4.163618 | 1.43775 |
| H | 1.567386 | 3.074256 | -0.41616 |
| C | 0.009194 | 3.402787 | 3.11030 |
| H | -1.170894 | 1.680985 | 2.57684 |

| | | | |
|---|-----------|----------|---------|
| C | 1.004753 | 4.294070 | 2.70772 |
| H | 2.341300 | 4.855899 | 1.11000 |
| H | -0.440212 | 3.494060 | 4.09571 |
| H | 1.335730 | 5.084230 | 3.37639 |

| | | | |
|---|-----------|----------|----------|
| C | 1.752653 | 3.984010 | 2.792754 |
| H | -0.043642 | 3.732716 | 3.957586 |
| H | 3.399786 | 4.039728 | 1.397047 |
| H | 2.191007 | 4.712962 | 3.469311 |

8g

SCF done: -1234.192989

| | | | |
|----|-----------|-----------|-----------|
| Ru | -1.343414 | -0.471518 | 0.509658 |
| Si | 2.025684 | -0.890210 | 0.872184 |
| H | 2.448873 | 0.018172 | 1.958846 |
| Si | 4.643570 | -2.490663 | 0.895363 |
| Si | 2.939388 | -2.438295 | -1.705233 |
| O | 0.791929 | -0.163258 | -0.088119 |
| O | -1.012232 | -0.551020 | 3.508053 |
| C | 3.512765 | -1.391054 | -0.204958 |
| C | -1.049095 | -0.448188 | 2.344635 |
| C | -3.166296 | -0.266123 | -0.989391 |
| C | -3.570371 | -0.409141 | 0.389141 |
| C | -3.198408 | -1.750167 | 0.816646 |
| C | -2.465502 | -2.360031 | -0.235604 |
| C | -2.448489 | -1.432921 | -1.356536 |
| C | -3.511407 | 0.893463 | -1.874358 |
| H | -4.512520 | 0.755654 | -2.307878 |
| H | -2.803503 | 1.008447 | -2.698406 |
| H | -3.520697 | 1.835474 | -1.319386 |
| C | -4.497438 | 0.517321 | 1.125851 |
| H | -4.314210 | 1.562630 | 0.859367 |
| H | -4.379778 | 0.427504 | 2.209735 |
| H | -5.548369 | 0.295220 | 0.888520 |
| C | -3.608065 | -2.395310 | 2.110887 |
| H | -2.897780 | -3.165963 | 2.423953 |
| H | -4.592414 | -2.871937 | 2.004128 |
| H | -3.681727 | -1.667498 | 2.923413 |
| C | -1.935726 | -3.765709 | -0.265425 |
| H | -2.648893 | -4.448964 | -0.749389 |
| H | -1.748292 | -4.145197 | 0.743140 |
| H | -0.994965 | -3.831885 | -0.821629 |
| C | -1.879322 | -1.749793 | -2.710287 |
| H | -0.948672 | -2.322064 | -2.632894 |
| H | -1.667181 | -0.844964 | -3.284477 |
| H | -2.584985 | -2.359463 | -3.292613 |
| H | 4.087846 | -3.203014 | -2.258639 |
| H | 5.962342 | -2.675959 | 0.239906 |
| H | 1.888878 | -3.406180 | -1.296307 |
| H | 4.028608 | -3.825522 | 1.110728 |
| H | 2.397281 | -1.581196 | -2.789128 |
| H | 4.859231 | -1.856500 | 2.221916 |
| Si | 4.535039 | 0.099938 | -0.835781 |
| H | 5.141340 | 0.839165 | 0.301678 |
| H | 5.631768 | -0.382375 | -1.715275 |
| H | 3.689871 | 1.033613 | -1.618986 |
| H | 1.448730 | -2.136871 | 1.425638 |
| C | 0.027610 | 1.091746 | 0.057066 |
| C | -0.156726 | 1.718521 | -1.296151 |
| C | -0.784921 | 2.976493 | -1.387497 |
| C | 0.277276 | 1.115924 | -2.489065 |
| C | -0.979410 | 3.598283 | -2.618688 |
| H | -1.113253 | 3.472910 | -0.478910 |
| C | 0.083587 | 1.742760 | -3.722828 |
| H | 0.780434 | 0.157765 | -2.446738 |
| C | -0.547279 | 2.985377 | -3.798231 |
| H | -1.465376 | 4.570187 | -2.655821 |
| H | 0.441045 | 1.257689 | -4.628251 |
| H | -0.692369 | 3.473266 | -4.758293 |
| C | 0.618784 | 2.077391 | 1.047086 |
| C | -0.056837 | 2.486021 | 2.202685 |
| C | 1.861353 | 2.675581 | 0.763689 |
| C | 0.502212 | 3.432204 | 3.067085 |
| H | -1.031298 | 2.063798 | 2.417848 |
| C | 2.432541 | 3.603010 | 1.632268 |
| H | 2.373084 | 2.420904 | -0.160307 |

2h

SCF done: -850.724881

| | | | |
|----|-----------|-----------|-----------|
| Ru | 0.937489 | -0.178349 | -0.455882 |
| Si | -1.207865 | 0.281837 | 0.329157 |
| H | -1.328311 | 0.962306 | 1.676630 |
| Si | -4.142316 | -0.058399 | 1.438961 |
| Si | -3.602250 | -0.688216 | -1.561585 |
| O | -2.061870 | 1.896219 | -0.632108 |
| O | -0.017435 | -1.942972 | -2.721155 |
| C | -2.848193 | -0.725978 | 0.202663 |
| C | 0.307668 | -1.250834 | -1.840982 |
| C | 3.020990 | 0.691189 | 0.139746 |
| C | 3.204750 | -0.623057 | -0.401319 |
| C | 2.553031 | -1.560807 | 0.488307 |
| C | 1.962923 | -0.822716 | 1.557262 |
| C | 2.237300 | 0.581502 | 1.334581 |
| C | 3.648474 | 1.948736 | -0.395329 |
| H | 4.652605 | 2.093402 | 0.028300 |
| H | 3.059060 | 2.836241 | -0.145035 |
| H | 3.750781 | 1.915979 | -1.483566 |
| C | 4.067658 | -0.982426 | -1.579338 |
| H | 4.064835 | -0.191490 | -2.335301 |
| H | 3.723095 | -1.899991 | -2.065439 |
| H | 5.111383 | -1.145175 | -1.273204 |
| C | 2.613590 | -3.059048 | 0.374834 |
| H | 1.745794 | -3.533349 | 0.842164 |
| H | 3.513373 | -3.454078 | 0.868038 |
| H | 2.643618 | -3.384774 | -0.669115 |
| C | 1.342048 | -1.396854 | 2.800478 |
| H | 2.101268 | -1.537367 | 3.584209 |
| H | 0.881067 | -2.370510 | 2.612716 |
| H | 0.570155 | -0.739449 | 3.212530 |
| C | 1.944711 | 1.680194 | 2.318028 |
| H | 0.951067 | 1.571578 | 2.766774 |
| H | 1.993151 | 2.667965 | 1.848531 |
| H | 2.673056 | 1.679450 | 3.142027 |
| H | -4.378836 | -1.933471 | -1.808216 |
| H | -5.471027 | -0.698146 | 1.231990 |
| H | -4.546018 | 0.452060 | -1.707923 |
| H | -4.319329 | 1.410173 | 1.284200 |
| H | -2.565548 | -0.569261 | -2.611950 |
| H | -3.725142 | -0.325075 | 2.841955 |
| Si | -2.448315 | -2.546693 | 0.657521 |
| H | -1.665046 | -2.620602 | 1.920248 |
| H | -3.718514 | -3.289845 | 0.880234 |
| H | -1.686817 | -3.234275 | -0.411569 |
| C | -1.664530 | 3.058897 | -0.750667 |
| H | 0.715988 | 1.051895 | -1.490843 |
| C | -0.498394 | 3.640919 | -0.030823 |
| H | 0.370765 | 3.055611 | -0.383440 |
| H | -0.587680 | 3.384264 | 1.033723 |
| H | -2.209215 | 3.690315 | -1.471348 |
| C | -0.315251 | 5.144242 | -0.252328 |
| H | -1.166888 | 5.715945 | 0.132632 |
| H | 0.581867 | 5.497849 | 0.263628 |
| H | -0.199839 | 5.380046 | -1.316090 |

TS_{23h}
SCF done: -850.708385

| | | | |
|----|-----------|-----------|-----------|
| Ru | 0.952271 | -0.063414 | -0.422133 |
| Si | -1.222802 | 0.508087 | 0.444945 |
| H | -1.188061 | 0.755740 | 1.932698 |
| Si | -4.114562 | 0.057474 | 1.571527 |
| Si | -3.710690 | 0.224942 | -1.505821 |
| O | -1.772707 | 2.173590 | -0.135901 |
| O | -0.186997 | -0.993578 | -3.075036 |

| | | | | | | | |
|----|-----------|-----------|-----------|-------------------------|-----------|-----------|-----------|
| C | -2.916848 | -0.365008 | 0.139831 | H | 4.928832 | -1.816060 | -0.994658 |
| C | 0.202299 | -0.610519 | -2.048038 | C | 2.072351 | -3.085475 | 0.615696 |
| C | 3.178618 | -0.060298 | 0.226480 | H | 1.112420 | -3.365716 | 1.055489 |
| C | 2.909075 | -1.299768 | -0.424881 | H | 2.862938 | -3.576612 | 1.199862 |
| C | 1.914686 | -2.006441 | 0.358566 | H | 2.108212 | -3.499722 | -0.395784 |
| C | 1.608830 | -1.204981 | 1.508529 | C | 1.038673 | -1.011804 | 2.851233 |
| C | 2.360081 | 0.017333 | 1.414565 | H | 1.730977 | -1.052260 | 3.703882 |
| C | 4.221866 | 0.942115 | -0.182701 | H | 0.543253 | -1.982558 | 2.781204 |
| H | 5.187197 | 0.707650 | 0.287537 | H | 0.277210 | -0.262114 | 3.087400 |
| H | 3.949705 | 1.957471 | 0.120132 | C | 2.171624 | 1.851630 | 2.146521 |
| H | 4.374140 | 0.948811 | -1.265505 | H | 1.182082 | 1.893888 | 2.611204 |
| C | 3.618901 | -1.845012 | -1.632684 | H | 2.311011 | 2.770111 | 1.570131 |
| H | 3.985871 | -1.043972 | -2.280844 | H | 2.914622 | 1.851727 | 2.956370 |
| H | 2.963499 | -2.481399 | -2.234576 | H | -4.399321 | -1.978009 | -1.672152 |
| H | 4.484801 | -2.453554 | -1.335774 | H | -5.168296 | -1.187119 | 1.492129 |
| C | 1.465434 | -3.419805 | 0.113855 | H | -4.715404 | 0.373010 | -1.355359 |
| H | 0.477241 | -3.610017 | 0.540307 | H | -4.204619 | 1.009880 | 1.707831 |
| H | 2.166450 | -4.136009 | 0.566078 | H | -2.812839 | -0.440291 | -2.602501 |
| H | 1.411444 | -3.645547 | -0.955190 | H | -3.296425 | -0.840851 | 2.956000 |
| C | 0.795044 | -1.628082 | 2.698162 | Si | -2.119913 | -2.648653 | 0.422130 |
| H | 1.456118 | -2.009106 | 3.489553 | H | -1.232869 | -2.803344 | 1.606093 |
| H | 0.088299 | -2.423879 | 2.448717 | H | -3.295995 | -3.530260 | 0.647247 |
| H | 0.225415 | -0.796153 | 3.123723 | H | -1.389346 | -3.162426 | -0.762598 |
| C | 2.436806 | 1.077278 | 2.477793 | C | -1.823712 | 3.039555 | -0.690136 |
| H | 1.474316 | 1.211530 | 2.982504 | H | 1.430084 | 0.889323 | -1.844179 |
| H | 2.734857 | 2.046497 | 2.064879 | C | -0.957931 | 3.751973 | 0.043417 |
| H | 3.174920 | 0.815571 | 3.249859 | H | -0.430005 | 3.279213 | 0.869476 |
| H | -4.659469 | -0.813277 | -1.995720 | H | 0.383446 | 1.500565 | -0.724482 |
| H | -5.498017 | -0.396793 | 1.258122 | C | -0.693503 | 5.212708 | -0.194568 |
| H | -4.488942 | 1.475972 | -1.318938 | H | -0.939932 | 5.817999 | 0.689129 |
| H | -4.158133 | 1.520363 | 1.821695 | H | 0.363779 | 5.404727 | -0.424512 |
| H | -2.699135 | 0.450963 | -2.564990 | H | -1.287405 | 5.593335 | -1.033484 |
| H | -3.693427 | -0.618576 | 2.828541 | H | -2.382064 | 3.502422 | -1.503819 |
| Si | -2.699294 | -2.260121 | 0.060460 | | | | |
| H | -1.908558 | -2.761623 | 1.216779 | | | | |
| H | -4.028084 | -2.926755 | 0.117870 | TS_{24h} | | | |
| H | -2.021052 | -2.693327 | -1.185528 | SCF done: -850.691180 | | | |
| C | -1.017769 | 3.194213 | -0.378825 | Ru | 1.154512 | 0.234356 | -0.496189 |
| H | 1.212644 | 1.421762 | -1.159629 | Si | -1.112214 | 0.118247 | -0.031167 |
| C | 0.277422 | 3.359680 | 0.111279 | H | -1.605340 | 1.131201 | 1.147415 |
| H | 0.480625 | 2.932648 | 1.094216 | Si | -3.222645 | -1.291252 | 1.899849 |
| H | 0.742115 | 2.192682 | -0.540424 | Si | -3.755325 | -1.278183 | -1.187528 |
| C | 1.088730 | 4.585598 | -0.255992 | O | -2.268401 | 1.309134 | -1.041792 |
| H | 1.032291 | 5.357405 | 0.521221 | O | 0.786681 | -1.078217 | -3.206403 |
| H | 2.146898 | 4.331120 | -0.388371 | C | -2.399309 | -1.313602 | 0.174283 |
| H | 0.739585 | 5.027192 | -1.196223 | C | 0.886209 | -0.578617 | -2.158841 |
| H | -1.397937 | 3.857871 | -1.162960 | C | 3.052767 | 1.314721 | 0.250991 |

3h

SCF done: -850.730777

| | | | |
|----|-----------|-----------|-----------|
| Ru | 1.040869 | 0.025205 | -0.549465 |
| Si | -1.279328 | 0.467969 | 0.248238 |
| H | -1.142510 | 0.894199 | 1.683360 |
| Si | -3.891542 | -0.438494 | 1.652177 |
| Si | -3.686010 | -0.691539 | -1.433114 |
| O | -2.152212 | 1.729788 | -0.555409 |
| O | -0.156570 | -1.570825 | -2.841446 |
| C | -2.691503 | -0.844971 | 0.208783 |
| C | 0.242569 | -0.963733 | -1.940572 |
| C | 3.172128 | 0.500724 | 0.136841 |
| C | 3.121760 | -0.870775 | -0.302009 |
| C | 2.271622 | -1.595840 | 0.612359 |
| C | 1.792369 | -0.674673 | 1.597959 |
| C | 2.326386 | 0.628116 | 1.288007 |
| C | 4.057693 | 1.577295 | -0.426179 |
| H | 5.022130 | 1.590673 | 0.100104 |
| H | 3.607555 | 2.567769 | -0.318565 |
| H | 4.261063 | 1.418849 | -1.488393 |
| C | 3.961158 | -1.478715 | -1.391206 |
| H | 4.163098 | -0.761034 | -2.191127 |
| H | 3.471336 | -2.346057 | -1.842906 |

TS_{24h}

SCF done: -850.691180

| | | | |
|----|-----------|-----------|-----------|
| Ru | 1.154512 | 0.234356 | -0.496189 |
| Si | -1.112214 | 0.118247 | -0.031167 |
| H | -1.605340 | 1.131201 | 1.147415 |
| Si | -3.222645 | -1.291252 | 1.899849 |
| Si | -3.755325 | -1.278183 | -1.187528 |
| O | -2.268401 | 1.309134 | -1.041792 |
| O | 0.786681 | -1.078217 | -3.206403 |
| C | -2.399309 | -1.313602 | 0.174283 |
| C | 0.886209 | -0.578617 | -2.158841 |
| C | 3.052767 | 1.314721 | 0.250991 |
| C | 3.446279 | 0.055475 | -0.306508 |
| C | 2.888952 | -0.996882 | 0.519709 |
| C | 2.138504 | -0.380499 | 1.561163 |
| C | 2.213997 | 1.055310 | 1.387453 |
| C | 3.526521 | 2.666510 | -0.205542 |
| H | 4.461637 | 2.942022 | 0.302921 |
| H | 2.790315 | 3.445579 | 0.011110 |
| H | 3.716803 | 2.684254 | -1.282075 |
| C | 4.415411 | -0.147347 | -1.438080 |
| H | 4.393761 | 0.689732 | -2.141739 |
| H | 4.193124 | -1.057666 | -2.003082 |
| H | 5.444380 | -0.237470 | -1.061473 |
| C | 3.176099 | -2.465027 | 0.371244 |
| H | 2.374244 | -3.077884 | 0.793304 |
| H | 4.108122 | -2.740310 | 0.886219 |
| H | 3.288675 | -2.749183 | -0.679567 |
| C | 1.522815 | -1.076937 | 2.742578 |
| H | 2.241859 | -1.134485 | 3.572691 |
| H | 1.220555 | -2.099119 | 2.500065 |
| H | 0.640915 | -0.547216 | 3.115343 |
| C | 1.703785 | 2.082111 | 2.360754 |
| H | 0.766432 | 1.766773 | 2.830297 |
| H | 1.519336 | 3.042363 | 1.869618 |
| H | 2.428714 | 2.261282 | 3.168576 |
| H | -4.411404 | -2.614426 | -1.221611 |

| | | | | | | | |
|----|-----------|-----------|-----------|-----------------------|-----------|-----------|-----------|
| H | -4.116105 | -2.466786 | 2.078276 | C | -3.721548 | 3.484480 | 1.226209 |
| H | -4.815351 | -0.280707 | -0.894314 | H | -3.838112 | 4.056904 | 2.153337 |
| H | -4.040325 | -0.064583 | 2.086055 | H | -4.414600 | 3.903068 | 0.485666 |
| H | -3.183173 | -1.015394 | -2.527816 | H | -4.029757 | 2.453272 | 1.424422 |
| H | -2.196961 | -1.326509 | 2.975683 | H | -2.707562 | 3.150034 | -1.365890 |
| Si | -1.441630 | -2.977844 | -0.015019 | | | | |
| H | -0.349385 | -3.097196 | 0.980859 | 5i | | | |
| H | -2.397913 | -4.090600 | 0.230154 | SCF done: -850.736869 | | | |
| H | -0.882906 | -3.130694 | -1.378249 | Ru | -0.835196 | 0.071519 | 0.126597 |
| C | -2.323337 | 2.174298 | -0.083316 | Si | 1.289007 | -1.163684 | -0.216893 |
| H | 0.697734 | 1.603415 | -1.225961 | H | 1.295633 | -2.381976 | 0.661397 |
| C | -3.635086 | 2.650356 | 0.458114 | Si | 4.263638 | -1.911486 | -0.459852 |
| H | -4.331937 | 1.811434 | 0.525625 | Si | 3.429839 | 0.925657 | -1.368645 |
| H | -3.484979 | 3.068645 | 1.459140 | O | 0.133130 | 1.393311 | -1.276390 |
| C | -4.198727 | 3.735788 | -0.489893 | O | 0.101755 | 0.738889 | 2.917805 |
| H | -5.148080 | 4.109085 | -0.093450 | C | 3.084389 | -0.445106 | -0.074582 |
| H | -3.512729 | 4.584962 | -0.582104 | C | -0.180596 | 0.509668 | 1.813285 |
| H | -4.376027 | 3.325279 | -1.487971 | C | -3.123747 | 0.150013 | -0.469057 |
| H | -1.455234 | 2.835782 | 0.056513 | C | -2.966178 | -0.428162 | 0.821558 |

4h

SCF done: -850.773130

| | | | |
|----|-----------|-----------|-----------|
| Ru | 1.068675 | 0.435273 | -0.189529 |
| Si | -1.210464 | 0.131796 | -0.220164 |
| H | -1.003722 | 2.936709 | -0.914972 |
| Si | -2.467671 | -2.106716 | 1.618840 |
| Si | -4.271789 | -0.670922 | -0.464125 |
| O | -2.311071 | 1.385898 | -0.440366 |
| O | 0.936137 | 1.959649 | -2.808264 |
| C | -2.482566 | -1.299948 | -0.120115 |
| C | 0.937871 | 1.369023 | -1.805397 |
| C | 2.846705 | 0.450405 | 1.281667 |
| C | 3.363115 | 0.365288 | -0.049008 |
| C | 2.947340 | -0.907010 | -0.607782 |
| C | 2.181753 | -1.593061 | 0.379215 |
| C | 2.087025 | -0.741913 | 1.543434 |
| C | 3.147169 | 1.535063 | 2.278072 |
| H | 4.043965 | 1.283455 | 2.861980 |
| H | 2.322703 | 1.675582 | 2.982244 |
| H | 3.329810 | 2.494676 | 1.786952 |
| C | 4.312540 | 1.335494 | -0.695717 |
| H | 4.166953 | 2.352176 | -0.319854 |
| H | 4.186413 | 1.364363 | -1.782097 |
| H | 5.355555 | 1.053455 | -0.493483 |
| C | 3.394269 | -1.460858 | -1.932392 |
| H | 2.689749 | -2.203117 | -2.318197 |
| H | 4.373929 | -1.951363 | -1.840221 |
| H | 3.493126 | -0.675602 | -2.687778 |
| C | 1.740192 | -3.026501 | 0.309938 |
| H | 2.518154 | -3.684178 | 0.724530 |
| H | 1.554775 | -3.346081 | -0.718572 |
| H | 0.826258 | -3.202856 | 0.882552 |
| C | 1.535284 | -1.140812 | 2.884585 |
| H | 0.710038 | -1.850801 | 2.789089 |
| H | 1.166471 | -0.275828 | 3.443433 |
| H | 2.311763 | -1.621401 | 3.497811 |
| H | -5.155635 | -1.871520 | -0.492240 |
| H | -3.645459 | -2.999252 | 1.773106 |
| H | -4.772635 | 0.211927 | 0.615623 |
| H | -2.521949 | -1.074690 | 2.686994 |
| H | -4.393072 | -0.002776 | -1.780224 |
| H | -1.248459 | -2.926538 | 1.836874 |
| Si | -2.070811 | -2.632518 | -1.440461 |
| H | -0.679192 | -3.123943 | -1.322572 |
| H | -2.985373 | -3.793949 | -1.278666 |
| H | -2.260642 | -2.080658 | -2.806801 |
| C | -2.034073 | 2.786245 | -0.580060 |
| H | 0.575143 | 1.791885 | 0.530586 |
| C | -2.276142 | 3.543713 | 0.723985 |
| H | -1.590703 | 3.150926 | 1.486531 |
| H | -1.983457 | 4.589119 | 0.551092 |

5i

SCF done: -850.736869

| | | | |
|----|-----------|-----------|-----------|
| Ru | -0.835196 | 0.071519 | 0.126597 |
| Si | 1.289007 | -1.163684 | -0.216893 |
| H | 1.295633 | -2.381976 | 0.661397 |
| Si | 4.263638 | -1.911486 | -0.459852 |
| Si | 3.429839 | 0.925657 | -1.368645 |
| O | 0.133130 | 1.393311 | -1.276390 |
| O | 0.101755 | 0.738889 | 2.917805 |
| C | 3.084389 | -0.445106 | -0.074582 |
| C | -0.180596 | 0.509668 | 1.813285 |
| C | -3.123747 | 0.150013 | -0.469057 |
| C | -2.966178 | -0.428162 | 0.821558 |
| C | -2.173869 | -1.636064 | 0.672486 |
| C | -1.930197 | -1.830819 | -0.741851 |
| C | -2.454346 | -0.701635 | -1.429842 |
| C | -3.959978 | 1.347410 | -0.817044 |
| H | -4.981300 | 1.038748 | -1.080237 |
| H | -3.557831 | 1.887375 | -1.680310 |
| H | -4.034751 | 2.050882 | 0.017393 |
| C | -3.605151 | 0.045893 | 2.096940 |
| H | -3.781311 | 1.125422 | 2.084829 |
| H | -2.985577 | -0.179026 | 2.969448 |
| H | -4.575893 | -0.446382 | 2.246710 |
| C | -1.930311 | -2.660924 | 1.745526 |
| H | -1.001108 | -3.210749 | 1.572135 |
| H | -2.750526 | -3.391508 | 1.777468 |
| H | -1.860049 | -2.199439 | 2.734607 |
| C | -1.354956 | -3.069361 | -1.363759 |
| H | -2.157143 | -3.796017 | -1.553515 |
| H | -0.622724 | -3.553978 | -0.712060 |
| H | -0.862764 | -2.861277 | -2.316980 |
| C | -2.403225 | -0.446087 | -2.908734 |
| H | -1.697036 | -1.115878 | -3.405261 |
| H | -2.083815 | 0.579143 | -3.123453 |
| H | -3.389116 | -0.594319 | -3.369595 |
| H | 4.902610 | 1.025511 | -1.583576 |
| H | 5.684514 | -1.486248 | -0.343000 |
| H | 2.809934 | 0.608400 | -2.678399 |
| H | 4.048847 | -2.417888 | -1.841228 |
| H | 2.977994 | 2.262149 | -0.912894 |
| H | 4.043291 | -3.038339 | 0.484649 |
| Si | 3.506441 | 0.204486 | 1.669628 |
| H | 3.155328 | -0.794938 | 2.712867 |
| H | 4.965226 | 0.481780 | 1.777989 |
| H | 2.792622 | 1.471203 | 1.966823 |
| H | 1.228932 | -1.689754 | -1.617181 |
| C | 0.115418 | 3.212497 | 0.366534 |
| H | 1.036287 | 2.788838 | 0.777624 |
| H | -0.550498 | 3.451921 | 1.205341 |
| C | 0.433607 | 4.497797 | -0.420786 |
| H | 0.895905 | 5.244780 | 0.233845 |
| H | 1.126176 | 4.288526 | -1.242632 |
| H | -0.475114 | 4.941389 | -0.846219 |
| C | -0.554719 | 2.194640 | -0.534076 |
| H | -1.549017 | 2.499058 | -0.897109 |

TS₅₆₁

SCF done: -850.7049794

| | | | |
|----|-----------|-----------|-----------|
| Ru | -1.054122 | 0.083630 | 0.311856 |
| Si | 1.372853 | -0.874732 | -0.064754 |
| H | 1.415027 | -1.758802 | 1.146618 |
| Si | 4.157162 | -2.093045 | -0.528438 |
| Si | 3.567703 | 0.661487 | -1.802110 |
| O | 0.729033 | 0.878878 | -0.640650 |

| | | | | | | | |
|----|-----------|-----------|-----------|-----------------------|-----------|-----------|-----------|
| O | -0.341544 | 0.228611 | 3.247150 | H | 4.488887 | 0.927373 | -1.807295 |
| C | 3.237370 | -0.426768 | -0.263959 | H | 5.598620 | 0.552153 | -0.480817 |
| C | -0.551399 | 0.208460 | 2.101398 | C | 3.561529 | -1.854995 | -1.954734 |
| C | -3.033872 | 0.374943 | -0.918982 | H | 2.850371 | -2.596050 | -2.331922 |
| C | -3.305938 | 0.018787 | 0.441794 | H | 4.536291 | -2.354613 | -1.857487 |
| C | -2.789633 | -1.326937 | 0.656292 | H | 3.668218 | -1.081382 | -2.721223 |
| C | -2.198446 | -1.777088 | -0.563959 | C | 1.585015 | -3.209623 | 0.191691 |
| C | -2.316411 | -0.706878 | -1.522929 | H | 2.183991 | -4.003890 | 0.659473 |
| C | -3.472338 | 1.638856 | -1.602343 | H | 1.428296 | -3.486935 | -0.854743 |
| H | -4.443043 | 1.499461 | -2.098034 | H | 0.608657 | -3.208717 | 0.686617 |
| H | -2.760899 | 1.956584 | -2.371360 | C | 1.504827 | -1.362366 | 2.774193 |
| H | -3.583720 | 2.462826 | -0.891282 | H | 0.535297 | -1.836981 | 2.589613 |
| C | -4.156090 | 0.794630 | 1.408867 | H | 1.322828 | -0.470348 | 3.381725 |
| H | -4.046545 | 1.873938 | 1.265965 | H | 2.097792 | -2.057427 | 3.385950 |
| H | -3.890724 | 0.573022 | 2.446403 | H | -4.738735 | -1.002977 | 2.372212 |
| H | -5.219833 | 0.548831 | 1.280267 | H | -5.233022 | -2.792064 | -0.145662 |
| C | -3.011924 | -2.155483 | 1.891362 | H | -2.426120 | -1.602046 | 2.123019 |
| H | -2.223672 | -2.902059 | 2.024121 | H | -2.886707 | -3.108921 | -0.605092 |
| H | -3.970085 | -2.689875 | 1.830550 | H | -3.064907 | 0.720219 | 2.360481 |
| H | -3.036278 | -1.538371 | 2.793918 | H | -4.324430 | -2.145215 | -2.281410 |
| C | -1.660008 | -3.150644 | -0.841917 | Si | -5.169021 | 0.689420 | -0.507078 |
| H | -2.434201 | -3.791789 | -1.286729 | H | -5.313448 | 0.895237 | -1.971673 |
| H | -1.313972 | -3.641414 | 0.072776 | H | -6.427955 | 0.091390 | 0.006838 |
| H | -0.818428 | -3.123747 | -1.541133 | H | -4.980449 | 2.016608 | 0.133393 |
| C | -1.846594 | -0.769499 | -2.948790 | H | -1.610068 | -0.709274 | -1.988922 |
| H | -0.900774 | -1.312738 | -3.036483 | C | -0.400039 | 2.870650 | 0.243434 |
| H | -1.695697 | 0.228592 | -3.370174 | H | -0.526476 | 2.922894 | -0.844202 |
| H | -2.582492 | -1.285878 | -3.580819 | H | 0.475119 | 3.496259 | 0.465947 |
| H | 4.997840 | 0.534336 | -2.200928 | C | -1.628744 | 3.459674 | 0.957033 |
| H | 5.624212 | -1.895703 | -0.397270 | H | -1.801333 | 4.496416 | 0.645009 |
| H | 2.741919 | 0.219874 | -2.955312 | H | -2.543253 | 2.896478 | 0.739258 |
| H | 3.882447 | -2.636150 | -1.885291 | H | -1.491846 | 3.454511 | 2.045073 |
| H | 3.317247 | 2.101943 | -1.553172 | C | -0.009956 | 1.470425 | 0.667314 |
| H | 3.735501 | -3.111039 | 0.468636 | H | 0.023275 | 1.386609 | 1.760053 |
| Si | 3.962362 | 0.396318 | 1.300838 | | | | |
| H | 3.928313 | -0.544102 | 2.452376 | | | | |
| H | 5.377525 | 0.795364 | 1.075655 | acetone | | | |
| H | 3.202867 | 1.614418 | 1.678815 | SCF done: -193.151062 | | | |
| H | 1.035026 | -1.688720 | -1.260611 | O | 0.017670 | 1.393768 | 0.000296 |
| C | 0.457050 | 2.871919 | 0.850551 | C | -0.005743 | 0.178383 | -0.001693 |
| H | 1.042114 | 2.343994 | 1.611029 | C | 1.288976 | -0.628800 | -0.000560 |
| H | -0.401031 | 3.318408 | 1.370630 | H | 1.858509 | -0.390764 | 0.905143 |
| C | 1.302118 | 3.989245 | 0.216124 | H | 1.125180 | -1.709633 | -0.043122 |
| H | 1.640307 | 4.699603 | 0.979331 | H | 1.903168 | -0.323586 | -0.854829 |
| H | 2.186805 | 3.584328 | -0.284966 | C | -1.308271 | -0.600328 | -0.000509 |
| H | 0.721841 | 4.548990 | -0.527972 | H | -2.157073 | 0.086379 | -0.018944 |
| C | -0.093474 | 1.882586 | -0.153414 | H | -1.353571 | -1.272281 | -0.867252 |
| H | -0.615318 | 2.360394 | -0.991024 | H | -1.367342 | -1.235789 | 0.893211 |

6i
SCF done: -850.728586

| | | | |
|----|-----------|-----------|-----------|
| Ru | 1.354277 | 0.228954 | -0.245269 |
| Si | -2.098206 | 0.233732 | -0.956522 |
| H | -2.352701 | 1.557783 | -1.573845 |
| Si | -4.046658 | -2.207330 | -0.823001 |
| Si | -3.445391 | -0.584305 | 1.768024 |
| O | -0.861653 | 0.359650 | 0.225662 |
| O | 1.493662 | 1.680144 | -2.902842 |
| C | -3.677703 | -0.455235 | -0.133982 |
| C | 1.345500 | 1.151459 | -1.871625 |
| C | 3.049939 | 0.109090 | 1.256299 |
| C | 3.550085 | 0.004225 | -0.094089 |
| C | 3.120257 | -1.278270 | -0.639144 |
| C | 2.270926 | -1.878696 | 0.315840 |
| C | 2.210324 | -1.021500 | 1.490992 |
| C | 3.410902 | 1.177859 | 2.247246 |
| H | 4.295230 | 0.884578 | 2.831241 |
| H | 2.600142 | 1.366305 | 2.958041 |
| H | 3.643473 | 2.124142 | 1.750517 |
| C | 4.583517 | 0.901404 | -0.717835 |
| H | 4.492307 | 1.929702 | -0.356590 |

acetophenone
SCF done: -384.888408

| | | | |
|---|-----------|-----------|-----------|
| O | 2.213317 | -1.311634 | -0.000907 |
| C | 1.698148 | -0.203619 | -0.000213 |
| C | 2.562453 | 1.047667 | 0.000856 |
| H | 2.364638 | 1.664973 | -0.883594 |
| H | 2.360461 | 1.665874 | 0.883927 |
| H | 3.611537 | 0.746779 | 0.003664 |
| C | 0.205114 | -0.053680 | -0.000068 |
| C | -0.432669 | 1.196281 | -0.000487 |
| C | -0.577083 | -1.219969 | 0.000279 |
| C | -1.825575 | 1.277755 | -0.000435 |
| H | 0.152933 | 2.110601 | -0.001165 |
| C | -1.966254 | -1.138753 | 0.000506 |
| H | -0.067346 | -2.177832 | 0.000435 |
| C | -2.593503 | 0.111545 | 0.000169 |
| H | -2.310657 | 2.250017 | -0.000848 |
| H | -2.563473 | -2.046549 | 0.000876 |
| H | -3.678415 | 0.175850 | 0.000315 |

benzophenone
SCF done: -576.6206082

| | | | |
|---|-----------|----------|-----------|
| O | -0.000149 | 2.307181 | -0.000356 |
|---|-----------|----------|-----------|

| | | | |
|---|-----------|-----------|-----------|
| C | -0.000019 | 1.080594 | -0.000245 |
| C | 1.303894 | 0.337335 | -0.023893 |
| C | 1.453978 | -0.926318 | -0.616524 |
| C | 2.434539 | 0.984226 | 0.501311 |
| C | 2.708840 | -1.535289 | -0.669274 |
| H | 0.596121 | -1.422105 | -1.059254 |
| C | 3.681518 | 0.367230 | 0.465853 |
| H | 2.310806 | 1.972994 | 0.931135 |
| C | 3.821214 | -0.895065 | -0.120335 |
| H | 2.817151 | -2.507682 | -1.141991 |
| H | 4.547480 | 0.870082 | 0.887801 |
| H | 4.796147 | -1.374159 | -0.154436 |
| C | -1.303706 | 0.337005 | 0.023785 |
| C | -1.453835 | -0.926658 | 0.616127 |
| C | -2.434620 | 0.984257 | -0.500799 |
| C | -2.708809 | -1.535501 | 0.669040 |
| H | -0.596000 | -1.422792 | 1.058624 |
| C | -3.681596 | 0.367446 | -0.465240 |
| H | -2.310710 | 1.973210 | -0.930128 |
| C | -3.821225 | -0.895153 | 0.120450 |
| H | -2.817004 | -2.508041 | 1.141487 |
| H | -4.547689 | 0.870613 | -0.886541 |
| H | -4.796157 | -1.374238 | 0.154617 |

propylaldehyde

SCF done: -193.139861

| | | | |
|---|-----------|-----------|-----------|
| O | 1.822334 | -0.037926 | -0.295132 |
| C | 0.786274 | -0.234806 | 0.299446 |
| H | 0.699876 | -1.079905 | 1.023521 |
| C | -0.473420 | 0.589586 | 0.150742 |
| H | -0.299136 | 1.353978 | -0.613040 |
| H | -0.643370 | 1.102856 | 1.109913 |
| C | -1.696668 | -0.282109 | -0.178894 |
| H | -1.842410 | -1.065618 | 0.574465 |
| H | -2.606547 | 0.325453 | -0.208130 |
| H | -1.584200 | -0.769390 | -1.153432 |