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***Electronic Supplementary Information for***

# Indenyl effect in dissociative reactions.

# Nucleophilic substitution in iron carbonyl complexes: a case study.

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# Complementary information on the mechanisms

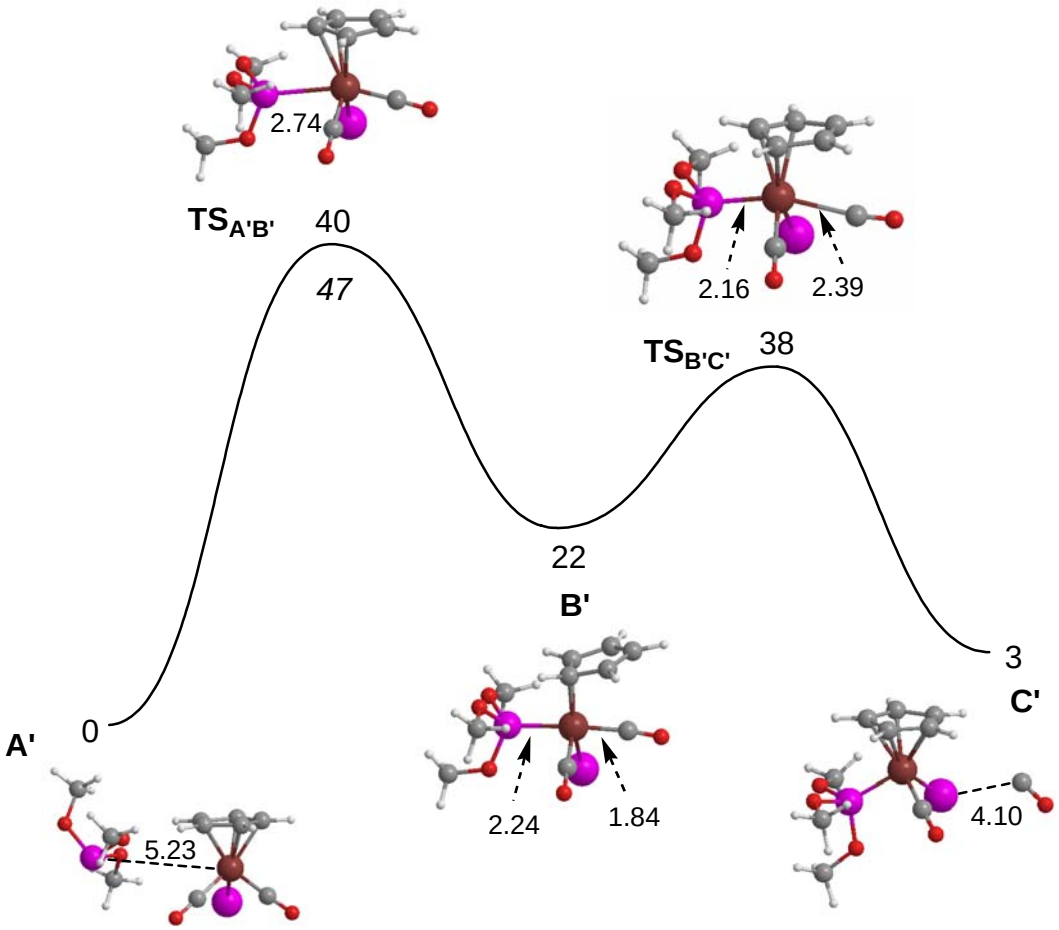


**Fig. S1**. Energy profile (PBE1PBE/b1) for carbonyl substitution by phosphite in [Fe(Cp)(CO)$_2$I], following an associative mechanism. The minima and the transition states were optimised and the corresponding structures are shown (distances in Å). The energy (kcal/mol) is referred to the pair of reagents, **A'**. The value in italics was obtained with the OPBE functional.

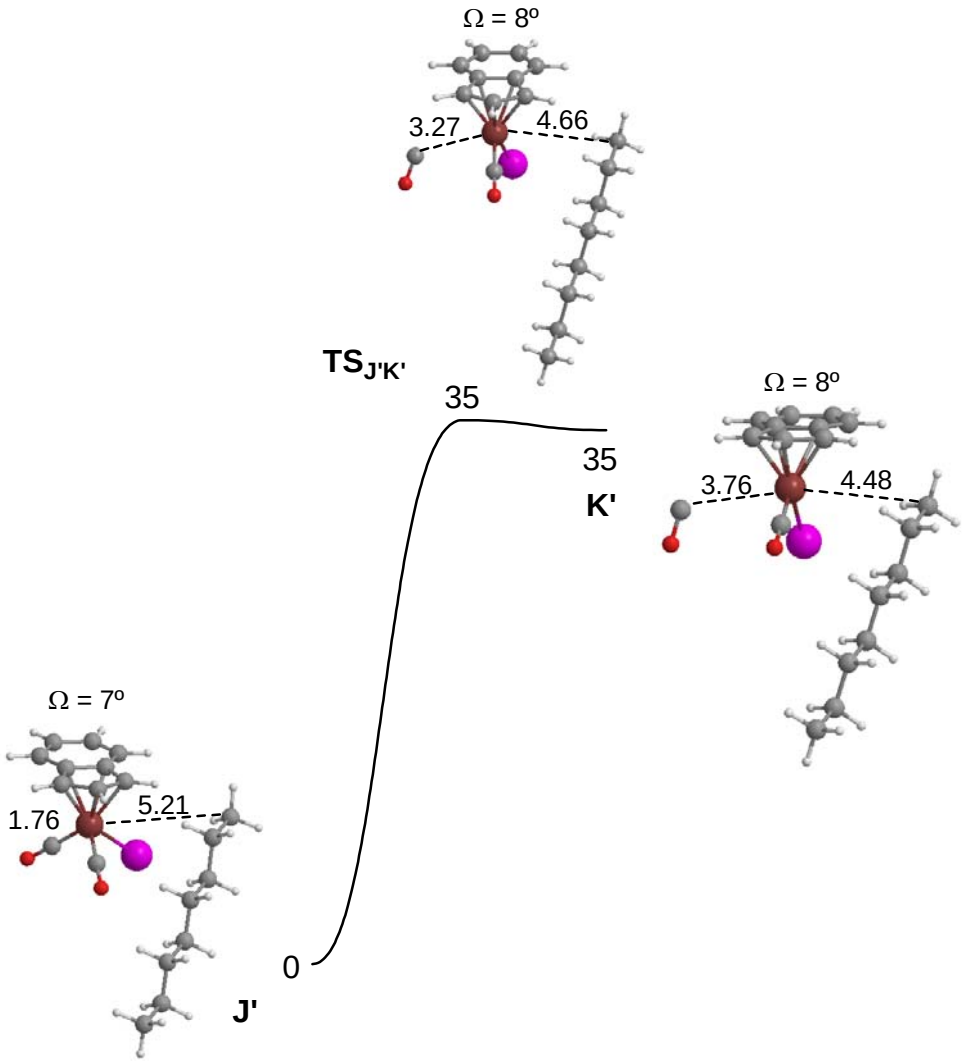


**Fig. S2.** Energy profile (PBE1PBE/b1) for carbonyl dissociation from[Fe(Ind)$(CO)_2$I], in the presence of one *n*-octane molecule. The minima and the transition state were optimised and the corresponding structures are shown (distances in Å). The energy (kcal/mol) is referred to the reagent, **J'**.

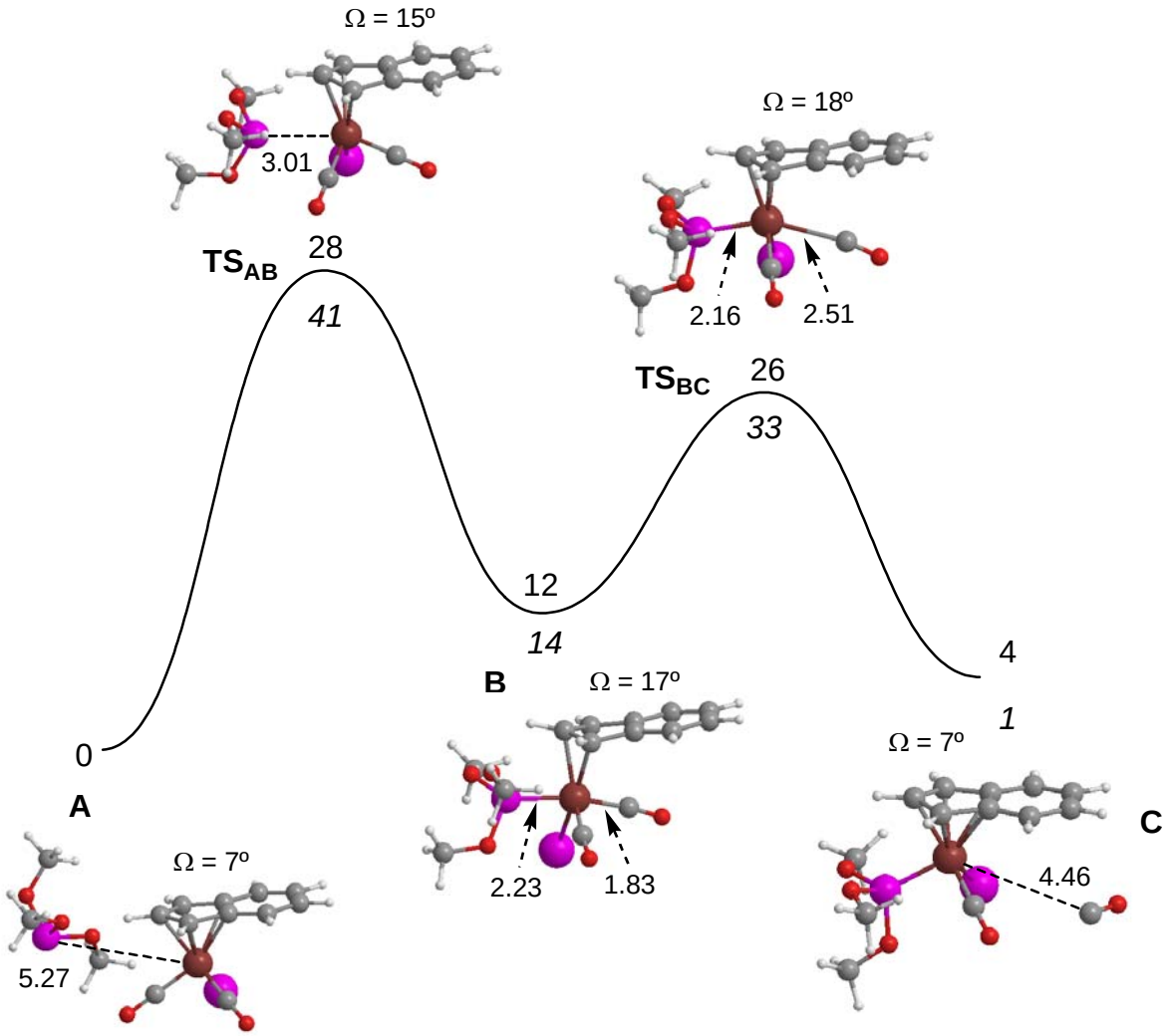


**Fig. S3**. Free energy profile (PBE1PBE/b1) for carbonyl substitution by phosphite in [Fe(Ind)(CO)$_2$I], following an associative mechanism. The free energy values (kcal/mol) are referred to the pair of reagents, **A**. The values in italics represent electronic energy obtained at the MP2/b2//PBE1PBE/b1 level.

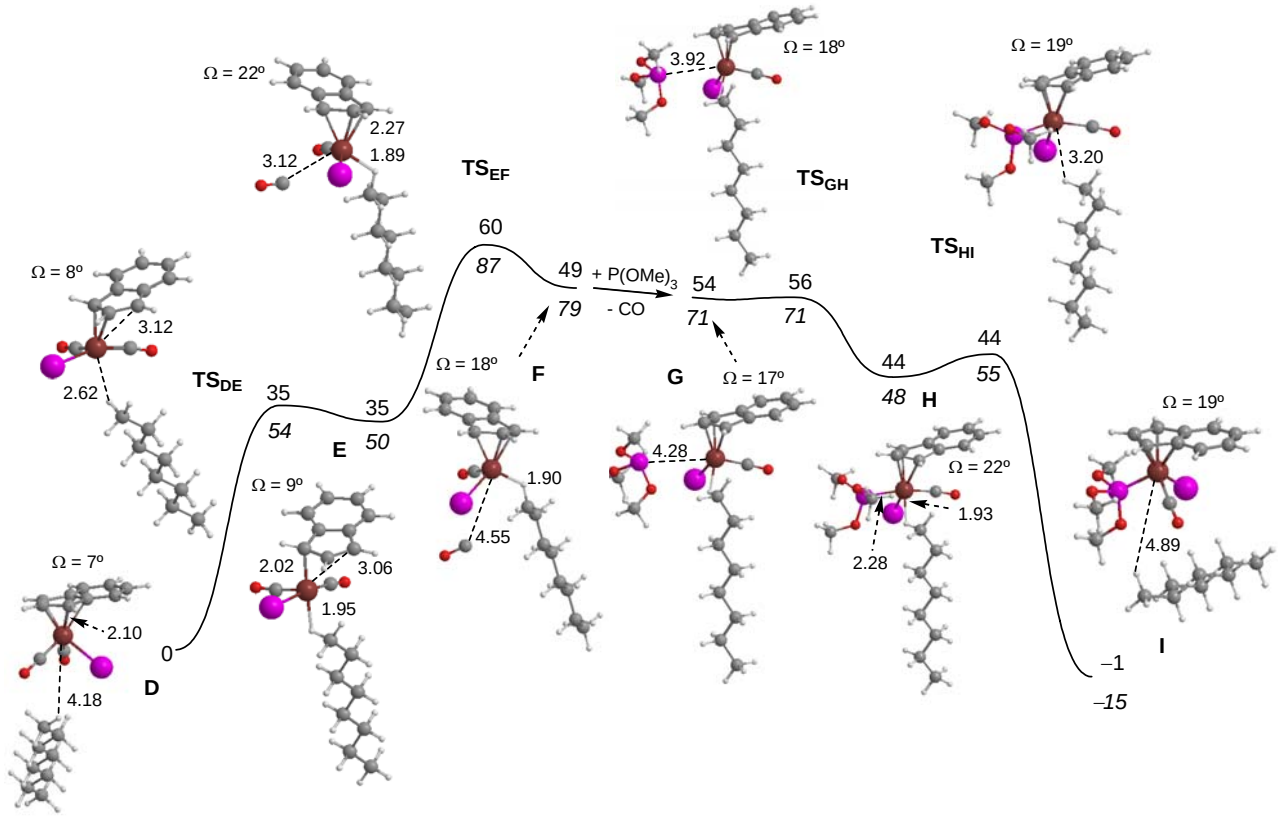


**Fig. S4**. Free energy profile (PBE1PBE/b1) for carbonyl substitution by phosphite in [Fe(Ind)(CO)$_2$I], with solvent (*n*-octane) participation. The free energy values (kcal/mol) are referred to the pair of reagents, **D**. The values in italics represent electronic energy obtained at the MP2/b2//PBE1PBE/b1 level.

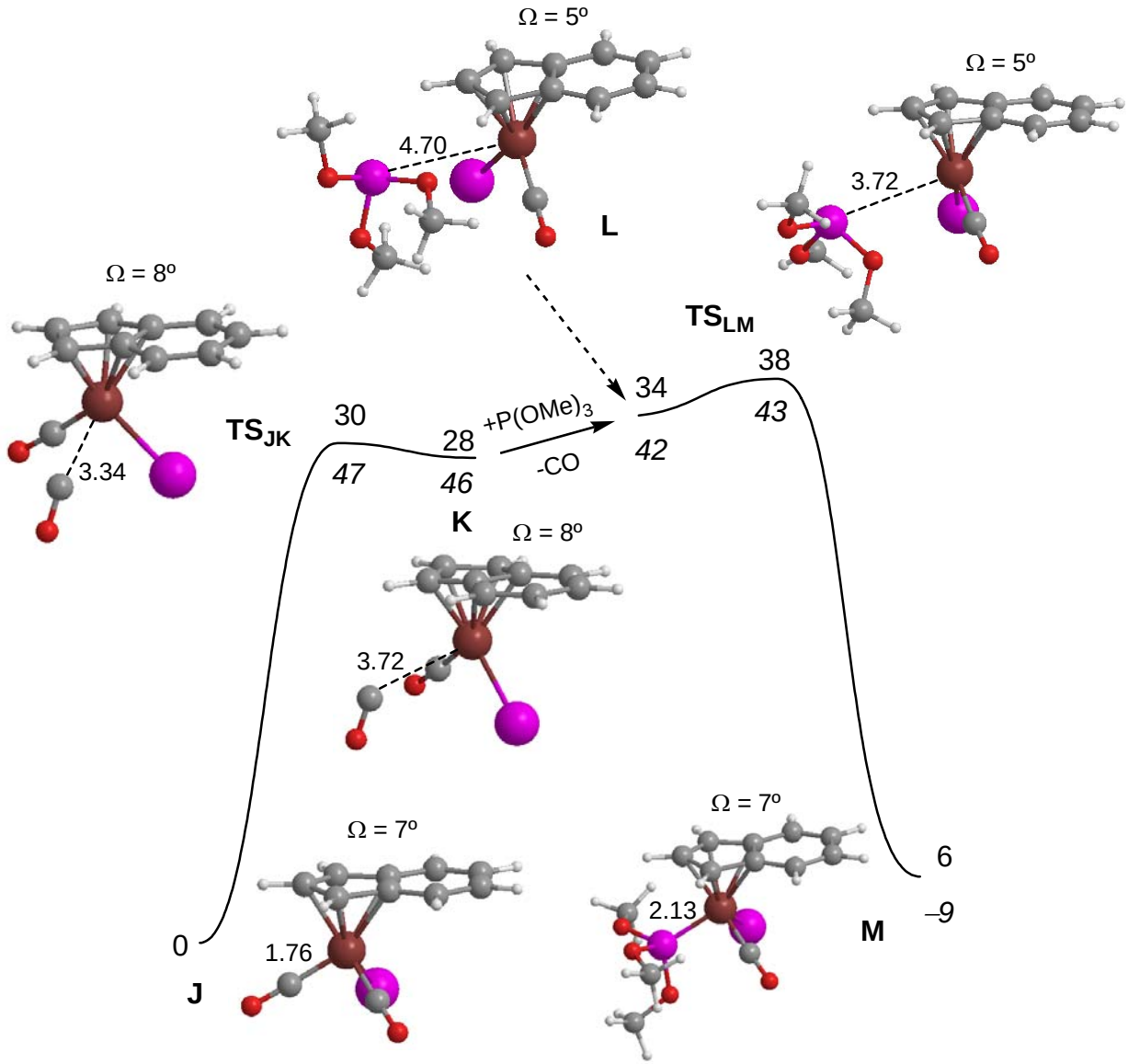


**Fig. S5**. Free energy profile (PBE1PBE/b1) for carbonyl substitution by phosphite in [Fe(Ind)(CO)$_2$I] (**J**), following a dissociative mechanism. The free energy values (kcal/mol) are referred to the reagent, **J**. The values in italics represent electronic energy obtained at the MP2/b2//PBE1PBE/b1 level.

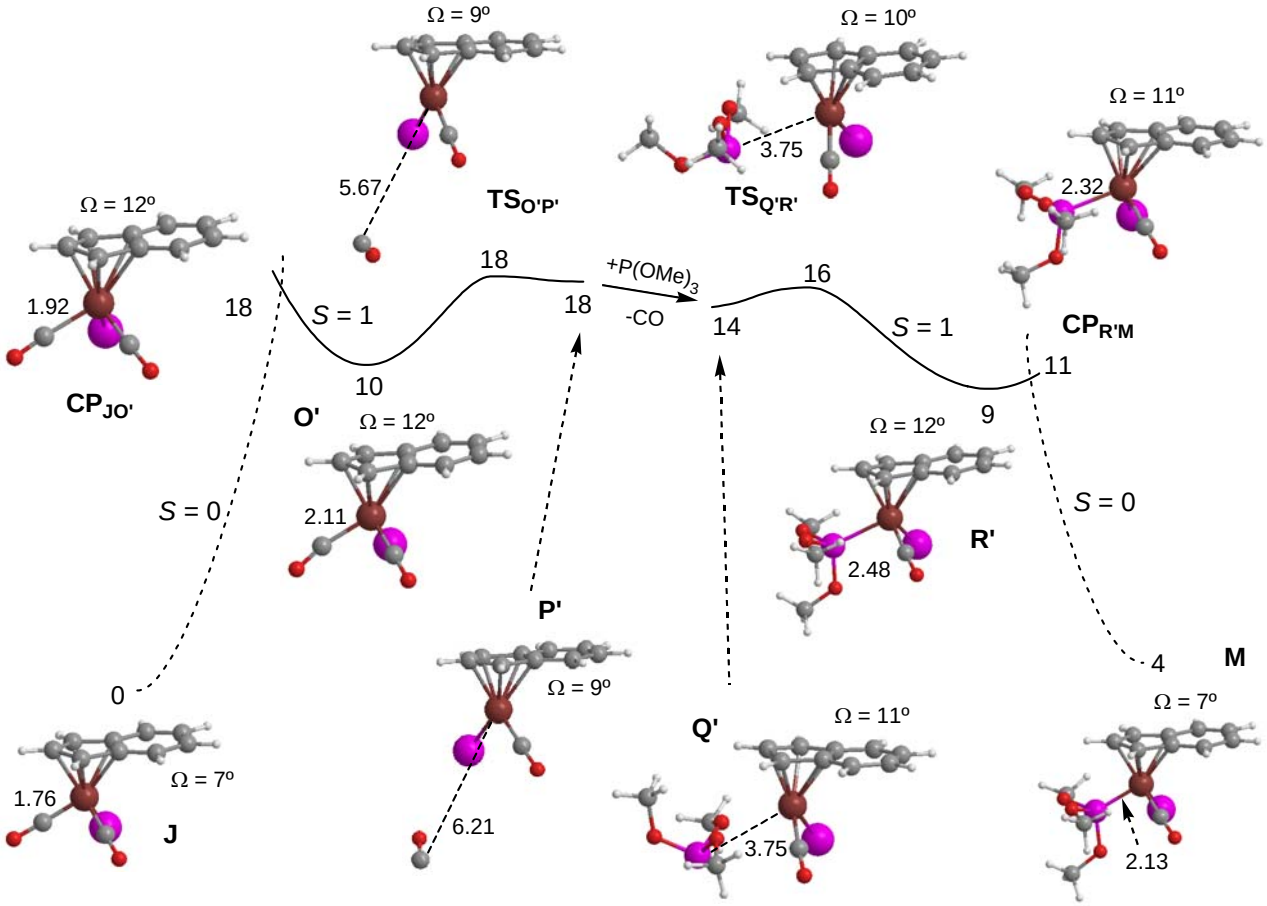


**Fig. S6**. Energy profile (PBE1PBE/b1) for dissociative carbonyl substitution by phosphite in [Fe(Ind)(CO)$_2$I] following a "spin forbidden" mechanism. The minima, the transition states, and the crossing points were optimised and the obtained structures are presented (distances in Å). The dashed curve corresponds to the spin singlet potential energy surface, PES, ($S$ = 0) and the plain curve to the spin triplet ($S$ = 1) PES. The energy values (kcal/mol) are referred to the reagent, **J**.

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# Atomic coordinates for all the optimized structures

## Optimizations with PBE1PBE

### CO

| | | | |
|---|---|---|---|
| C | -0.449794 | -0.042913 | 0.343504 |
| O | 0.449794 | 0.042913 | -0.343504 |

### $P(OMe)_3$

| | | | |
|---|---|---|---|
| P | 0.805520 | -0.159442 | -0.075869 |
| H | 1.370462 | -2.624326 | 2.433618 |
| H | -0.185389 | -2.425670 | 1.579588 |
| H | 0.414272 | -1.128109 | 2.635950 |
| H | -1.908368 | -1.654164 | -1.728901 |
| O | 1.447999 | -1.362500 | 0.839862 |
| H | -0.469220 | -2.592440 | -1.261110 |
| C | 0.713335 | -1.911048 | 1.932713 |
| O | -0.716378 | -0.717506 | -0.379111 |
| C | -0.844578 | -1.588003 | -1.491784 |
| O | 0.260859 | 0.903530 | 1.061236 |
| C | 1.215856 | 1.834875 | 1.544278 |
| H | -0.309241 | -1.209076 | -2.371887 |
| H | 0.664136 | 2.633573 | 2.044276 |
| H | 1.809804 | 2.271149 | 0.730840 |
| H | 1.899531 | 1.370158 | 2.264900 |

### A

| | | | |
|---|---|---|---|
| Fe | -0.897673 | 0.926712 | -0.321889 |
| I | -2.984962 | -0.441035 | -1.118048 |
| H | 3.283040 | -4.683068 | 2.086316 |
| H | 1.715749 | -3.924742 | 1.691790 |
| H | 3.156729 | -2.907813 | 1.935006 |
| C | -1.498369 | 2.349334 | -1.202354 |
| C | -0.037125 | 0.292574 | -1.715846 |
| P | 2.650864 | -2.917853 | -0.943800 |
| O | -1.868550 | 3.290202 | -1.741119 |
| O | 0.545681 | -0.109462 | -2.617992 |
| H | -0.853653 | -2.823901 | -1.131750 |
| O | 3.133666 | -4.019692 | 0.169958 |
| H | -0.006108 | -4.379993 | -0.896292 |
| C | 0.714609 | 0.408529 | 0.897150 |
| C | 2.798732 | -3.866813 | 1.547548 |
| H | 1.595490 | -0.082333 | 0.497171 |
| O | 1.082521 | -2.638534 | -0.527222 |
| C | -0.445813 | -0.265990 | 1.344297 |
| C | 0.091644 | -3.353665 | -1.267173 |
| H | -0.580547 | -1.338112 | 1.359435 |
| O | 3.155960 | -1.494406 | -0.247342 |
| C | 0.473120 | 1.812799 | 0.941592 |
| C | 4.538727 | -1.203812 | -0.397905 |
| H | 1.169449 | 2.589495 | 0.654534 |
| C | -1.374669 | 0.723656 | 1.833358 |
| C | -2.655192 | 0.618969 | 2.431509 |
| H | -3.099572 | -0.356894 | 2.595894 |
| C | -3.304802 | 1.769201 | 2.799698 |
| H | -4.281483 | 1.707352 | 3.269989 |
| C | -2.731685 | 3.049456 | 2.572340 |
| H | -3.281262 | 3.933526 | 2.881949 |
| C | -1.506315 | 3.188839 | 1.971903 |
| H | -1.068495 | 4.168867 | 1.806622 |
| H | 0.332193 | -3.380714 | -2.336054 |
| H | 5.155626 | -1.865292 | 0.221557 |
| C | -0.798849 | 2.016680 | 1.596593 |
| H | 4.689628 | -0.171762 | -0.074969 |
| H | 4.859891 | -1.298303 | -1.442756 |

### $TS_{AB}$

| | | | |
|---|---|---|---|
| Fe | -0.156016 | 0.300777 | -0.252941 |
| I | -1.638810 | -1.462908 | -1.481553 |
| H | 3.545841 | -4.232494 | -2.037693 |
| H | 2.477672 | -4.925939 | -0.790239 |
| H | 3.829330 | -3.865109 | -0.310561 |
| C | -1.151201 | 1.450716 | -1.126174 |
| C | 1.117085 | 0.559216 | -1.419191 |
| P | 1.716382 | -2.034784 | 0.034355 |
| O | -1.774845 | 2.208463 | -1.716336 |
| O | 1.953059 | 0.732475 | -2.188683 |
| H | 0.100378 | -4.766886 | 1.587140 |
| O | 2.220610 | -2.909938 | -1.243247 |
| H | 0.137234 | -4.390888 | -0.157799 |
| C | 0.470577 | 0.217037 | 1.850388 |
| C | 3.068330 | -4.050002 | -1.073800 |
| H | 1.334881 | -0.397786 | 2.065157 |
| O | 1.230602 | -3.150770 | 1.126938 |
| C | -0.865175 | -0.205067 | 1.856243 |
| C | 0.090867 | -3.962560 | 0.848868 |
| H | -1.219415 | -1.196409 | 2.104616 |
| O | 3.105259 | -1.740963 | 0.879249 |
| C | 0.509282 | 1.566772 | 1.390264 |
| C | 3.922278 | -0.674448 | 0.411624 |
| H | 1.403908 | 2.173966 | 1.318868 |
| C | -1.706057 | 0.976661 | 1.715056 |
| C | -3.092368 | 1.156312 | 1.771188 |
| H | -3.754734 | 0.307585 | 1.911901 |
| C | -3.597129 | 2.444153 | 1.657037 |
| H | -4.669088 | 2.606097 | 1.720326 |
| C | -2.746789 | 3.545759 | 1.467551 |
| H | -3.174747 | 4.541054 | 1.393104 |
| C | -1.371347 | 3.381830 | 1.368117 |
| H | -0.720117 | 4.235095 | 1.200307 |
| H | -0.836406 | -3.389915 | 0.935139 |
| H | 4.810509 | -0.658561 | 1.045540 |
| C | -0.842890 | 2.095310 | 1.498690 |
| H | 3.410864 | 0.292316 | 0.495826 |
| H | 4.229380 | -0.824167 | -0.629576 |

### B

| | | | |
|---|---|---|---|
| Fe | -0.027547 | -0.423206 | -0.305749 |
| I | -1.127685 | -2.239357 | -1.892454 |
| H | 3.777306 | -3.448348 | -2.229679 |
| H | 2.782539 | -4.412656 | -1.104619 |
| H | 4.023640 | -3.303365 | -0.463481 |
| C | -1.435910 | 0.572459 | -0.916006 |
| C | 1.021100 | 0.362443 | -1.457132 |
| P | 1.610393 | -1.891141 | 0.071023 |
| O | -2.266149 | 1.187781 | -1.403108 |
| O | 1.695236 | 0.941224 | -2.187198 |
| H | 0.221636 | -4.562064 | 1.934525 |
| O | 2.326724 | -2.393794 | -1.285078 |
| H | -0.001515 | -4.539296 | 0.156876 |
| C | -0.099880 | -0.418083 | 1.837948 |
| C | 3.285010 | -3.454223 | -1.256695 |
| H | 0.497277 | -1.229210 | 2.236169 |
| O | 1.375979 | -3.209968 | 0.975625 |
| C | -1.495898 | -0.387939 | 1.800259 |
| C | 0.143464 | -3.927499 | 1.049775 |
| H | -2.151701 | -1.223977 | 2.014208 |
| O | 2.866167 | -1.377107 | 0.984707 |
| C | 0.391170 | 0.847171 | 1.366703 |
| C | 3.745383 | -0.389736 | 0.455592 |
| H | 1.416715 | 1.172682 | 1.499171 |
| C | -1.914572 | 1.003632 | 1.696605 |
| C | -3.166509 | 1.604741 | 1.769167 |
| H | -4.060276 | 1.011784 | 1.943278 |
| C | -3.248865 | 2.988739 | 1.621989 |
| H | -4.214262 | 3.480854 | 1.692725 |
| C | -2.102438 | 3.750389 | 1.382870 |
| H | -2.191339 | 4.827342 | 1.271845 |
| C | -0.844651 | 3.151986 | 1.283869 |
| H | 0.037577 | 3.755106 | 1.085984 |
| H | -0.708610 | -3.250040 | 1.148100 |
| H | 4.517077 | -0.227489 | 1.209373 |
| C | -0.746401 | 1.775878 | 1.446819 |
| H | 3.226073 | 0.555638 | 0.267027 |
| H | 4.210944 | -0.729350 | -0.475337 |

### $TS_{BC}$

| | | | |
|---|---|---|---|
| Fe | 0.055992 | -0.268844 | 0.023542 |
| I | -1.412926 | -1.890084 | -1.480123 |
| H | 3.405873 | -3.427368 | -2.296722 |
| H | 2.457323 | -4.411259 | -1.151569 |
| H | 3.765131 | -3.358527 | -0.545256 |
| C | -1.544940 | 1.226000 | -1.201059 |
| C | 1.038635 | 0.421577 | -1.267534 |
| P | 1.528274 | -1.831151 | 0.207953 |
| O | -2.249595 | 1.734503 | -1.932725 |

| | | | |
|---|---|---|---|
| O | 1.688324 | 0.919424 | -2.075857 |
| H | 0.276852 | -4.739619 | 1.813409 |
| O | 2.045049 | -2.376230 | -1.221962 |
| H | 0.064640 | -4.436169 | 0.061773 |
| C | 0.217012 | -0.292705 | 2.128164 |
| C | 2.975189 | -3.459275 | -1.295259 |
| H | 0.886930 | -1.032820 | 2.547150 |
| O | 1.291423 | -3.132489 | 1.135583 |
| C | -1.162136 | -0.452806 | 1.910626 |
| C | 0.139712 | -3.972983 | 1.048802 |
| H | -1.739940 | -1.342249 | 2.125643 |
| O | 2.912917 | -1.439730 | 0.982318 |
| C | 0.589970 | 1.002622 | 1.661433 |
| C | 3.750867 | -0.431714 | 0.426887 |
| H | 1.577552 | 1.434963 | 1.767368 |
| C | -1.727030 | 0.872840 | 1.695404 |
| C | -3.043072 | 1.317260 | 1.569124 |
| H | -3.874120 | 0.623239 | 1.655538 |
| C | -3.264923 | 2.667376 | 1.321151 |
| H | -4.282268 | 3.036658 | 1.230308 |
| C | -2.194319 | 3.564532 | 1.190367 |
| H | -2.400352 | 4.614529 | 1.003589 |
| C | -0.877142 | 3.131756 | 1.304198 |
| H | -0.052849 | 3.831155 | 1.193245 |
| H | -0.776921 | -3.410963 | 1.238820 |
| H | 4.642863 | -0.392184 | 1.053737 |
| C | -0.639785 | 1.782174 | 1.561159 |
| H | 3.259254 | 0.545949 | 0.437568 |
| H | 4.039736 | -0.675387 | -0.601095 |

**C**

| | | | |
|---|---|---|---|
| Fe | 0.076122 | -0.241822 | 0.579303 |
| I | -1.633015 | -1.457325 | -1.004630 |
| H | 3.048418 | -3.142783 | -2.506013 |
| H | 2.288036 | -4.213008 | -1.299002 |
| H | 3.675673 | -3.195877 | -0.831336 |
| C | -2.166020 | 1.980734 | -2.576138 |
| C | 0.736822 | 0.642561 | -0.794953 |
| P | 1.522768 | -1.795704 | 0.369611 |
| O | -3.276369 | 1.979172 | -2.815752 |
| O | 1.184718 | 1.261223 | -1.653656 |
| H | 0.321626 | -4.873462 | 1.645024 |
| O | 1.877562 | -2.178445 | -1.161538 |
| H | 0.009211 | -4.301411 | -0.021452 |
| C | 0.324128 | -0.374156 | 2.647614 |
| C | 2.777870 | -3.247876 | -1.454706 |
| H | 0.965415 | -1.116667 | 3.106248 |
| O | 1.347478 | -3.204200 | 1.150627 |
| C | -1.045029 | -0.544303 | 2.340028 |
| C | 0.165165 | -3.994892 | 1.016707 |
| H | -1.644940 | -1.421839 | 2.536502 |
| O | 2.987739 | -1.516209 | 1.041476 |
| C | 0.750436 | 0.900321 | 2.169570 |
| C | 3.767035 | -0.443056 | 0.526023 |
| H | 1.740810 | 1.320819 | 2.280575 |
| C | -1.531295 | 0.699725 | 1.795616 |
| C | -2.816347 | 1.113582 | 1.365761 |
| H | -3.653390 | 0.425095 | 1.412798 |
| C | -2.974026 | 2.395475 | 0.903296 |
| H | -3.954622 | 2.734026 | 0.582440 |
| C | -1.875879 | 3.293135 | 0.822287 |
| H | -2.045268 | 4.299162 | 0.449474 |
| C | -0.612492 | 2.914283 | 1.199481 |
| H | 0.223369 | 3.605032 | 1.138412 |
| H | -0.719733 | -3.447103 | 1.349222 |
| H | 4.683141 | -0.412026 | 1.117835 |
| C | -0.421008 | 1.602991 | 1.706831 |
| H | 3.242623 | 0.513663 | 0.619149 |
| H | 4.020468 | -0.606835 | -0.527031 |

**D**

| | | | |
|---|---|---|---|
| Fe | -3.049151 | 2.601718 | -1.377465 |
| C | -1.239194 | 0.061513 | 2.349498 |
| C | -3.871541 | 1.841212 | -0.024748 |
| C | 0.243187 | -0.256131 | 2.200514 |
| O | -4.448972 | 1.342357 | 0.831036 |
| C | 0.568223 | -1.731187 | 2.414038 |
| I | -1.950386 | 4.210225 | 0.364078 |
| C | 2.051550 | -2.054408 | 2.268661 |
| C | 2.378139 | -3.530436 | 2.471218 |
| C | 3.862144 | -3.851035 | 2.326864 |
| C | -1.630477 | 1.533405 | -1.272474 |
| O | -0.719362 | 0.839976 | -1.249252 |
| C | 4.190085 | -5.327797 | 2.523537 |
| C | 5.674840 | -5.636067 | 2.376327 |
| H | -1.439121 | 1.126002 | 2.188824 |
| H | -1.602784 | -0.197820 | 3.350299 |
| H | -1.838652 | -0.508135 | 1.629149 |
| H | 0.820359 | 0.348401 | 2.912992 |
| H | 0.583046 | 0.047990 | 1.201630 |
| C | -4.847524 | 2.695876 | -2.421385 |
| H | -0.007654 | -2.336271 | 1.698566 |
| H | 0.224611 | -2.038810 | 3.412425 |
| H | 2.625971 | -1.453242 | 2.987955 |
| H | -5.767170 | 2.302279 | -2.006664 |
| H | 2.394888 | -1.739767 | 1.272636 |
| C | -3.883898 | 1.941058 | -3.149620 |
| H | 1.804950 | -4.131336 | 1.750492 |
| H | 2.033640 | -3.845950 | 3.466619 |
| H | -3.976712 | 0.904929 | -3.446088 |
| H | 4.435682 | -3.253149 | 3.049774 |
| H | 4.208111 | -3.532540 | 1.332792 |
| H | 3.616672 | -5.924066 | 1.800836 |
| C | -4.354780 | 4.008671 | -2.225922 |
| H | 3.845040 | -5.645378 | 3.516869 |
| H | -4.833873 | 4.795685 | -1.660288 |
| H | 5.882598 | -6.700928 | 2.521143 |
| C | -2.846081 | 2.855515 | -3.566873 |
| H | 6.268600 | -5.078937 | 3.109595 |
| C | -1.684603 | 2.683594 | -4.364633 |
| H | 6.039142 | -5.358651 | 1.380791 |
| H | -1.469255 | 1.720646 | -4.818011 |
| C | -0.867682 | 3.765865 | -4.570451 |
| H | 0.016938 | 3.659829 | -5.191332 |
| C | -1.150507 | 5.030626 | -3.987463 |
| H | -0.470925 | 5.857001 | -4.171907 |
| C | -2.253372 | 5.223930 | -3.196058 |
| H | -2.461099 | 6.187195 | -2.742889 |
| C | -3.133841 | 4.134152 | -2.983433 |

**$TS_{DE}$**

| | | | |
|---|---|---|---|
| Fe | -3.250082 | 1.333589 | -0.668385 |
| C | -1.534777 | 0.463345 | 2.156701 |
| C | -3.443502 | -0.174306 | -1.518278 |
| C | -0.042106 | 0.184270 | 2.271644 |
| O | -3.587991 | -1.121566 | -2.148846 |
| C | 0.296710 | -1.301015 | 2.199347 |
| I | -5.343733 | 0.885766 | 0.697725 |
| C | 1.788453 | -1.591491 | 2.329073 |
| C | 2.128956 | -3.075277 | 2.238942 |
| C | 3.620079 | -3.366722 | 2.373861 |
| C | -1.505257 | 1.465925 | -1.078719 |
| O | -0.375335 | 1.456585 | -1.261781 |
| C | 3.962138 | -4.849972 | 2.276021 |
| C | 5.453285 | -5.130621 | 2.413891 |
| H | -1.756981 | 1.535089 | 2.197123 |
| H | -2.106194 | -0.017962 | 2.957761 |
| H | -1.941400 | 0.061074 | 1.215520 |
| H | 0.331297 | 0.596999 | 3.218536 |
| H | 0.497478 | 0.716652 | 1.476658 |
| C | -3.776871 | 3.553633 | -1.083907 |
| H | -0.071895 | -1.709873 | 1.247019 |
| H | -0.249851 | -1.837135 | 2.988159 |
| H | 2.153974 | -1.192097 | 3.285979 |
| H | -4.486644 | 3.706125 | -0.279696 |
| H | 2.334201 | -1.045470 | 1.546242 |
| C | -3.894215 | 2.533465 | -2.127794 |
| H | 1.766352 | -3.472861 | 1.280161 |
| H | 1.579747 | -3.622262 | 3.018557 |
| H | -4.871862 | 2.186329 | -2.457587 |
| H | 3.982563 | -2.974001 | 3.334858 |
| H | 4.170510 | -2.816068 | 1.597404 |
| H | 3.601318 | -5.240792 | 1.314985 |
| C | -2.660913 | 4.324948 | -1.321589 |
| H | 3.410732 | -5.399445 | 3.050904 |
| H | -2.295895 | 5.122321 | -0.682385 |
| H | 5.670952 | -6.200535 | 2.337919 |
| C | -2.849278 | 2.874427 | -3.113446 |
| H | 5.833813 | -4.782229 | 3.380581 |
| C | -2.517561 | 2.312760 | -4.340959 |
| H | 6.025824 | -4.618865 | 1.632257 |
| H | -3.099951 | 1.494544 | -4.756386 |
| C | -1.419633 | 2.822367 | -5.035668 |
| H | -1.156551 | 2.400175 | -6.001361 |
| C | -0.651896 | 3.867855 | -4.512943 |
| H | 0.198386 | 4.241208 | -5.075612 |
| C | -0.972101 | 4.437059 | -3.283582 |
| H | -0.379654 | 5.253784 | -2.880116 |

| | | | |
|---|---|---|---|
| C | -2.079836 | 3.947874 | -2.591585 |

**E**

| | | | |
|---|---|---|---|
| Fe | -2.817263 | 1.095188 | -0.575935 |
| C | -1.579861 | 0.483928 | 1.602614 |
| C | -3.236448 | -0.289041 | -1.549351 |
| C | -0.093847 | 0.205653 | 1.782844 |
| O | -3.515906 | -1.141915 | -2.264879 |
| C | 0.227444 | -1.281836 | 1.885880 |
| I | -5.029363 | 0.544317 | 0.724826 |
| C | 1.711167 | -1.564403 | 2.097094 |
| C | 2.035847 | -3.050682 | 2.204558 |
| C | 3.519531 | -3.333084 | 2.416923 |
| C | -1.196223 | 1.259616 | -1.336299 |
| O | -0.142783 | 1.245815 | -1.784420 |
| C | 3.846420 | -4.818976 | 2.527319 |
| C | 5.330742 | -5.089688 | 2.738993 |
| H | -1.791932 | 1.558804 | 1.534148 |
| H | -2.194667 | 0.096221 | 2.420373 |
| H | -1.960111 | -0.082709 | 0.712542 |
| H | 0.247694 | 0.717710 | 2.692087 |
| H | 0.476278 | 0.646694 | 0.955253 |
| C | -3.406462 | 3.315305 | -0.633315 |
| H | -0.114024 | -1.791598 | 0.972953 |
| H | -0.350233 | -1.721261 | 2.711026 |
| H | 2.051870 | -1.051581 | 3.007868 |
| H | -3.985458 | 3.368193 | 0.280878 |
| H | 2.286102 | -1.124873 | 1.269525 |
| C | -3.715358 | 2.454645 | -1.771082 |
| H | 1.694364 | -3.563944 | 1.294363 |
| H | 1.460223 | -3.489358 | 3.032015 |
| H | -4.738559 | 2.154704 | -1.982697 |
| H | 3.861849 | -2.818521 | 3.326323 |
| H | 4.095609 | -2.895617 | 1.588842 |
| H | 3.503848 | -5.332181 | 1.618716 |
| C | -2.303713 | 4.089998 | -0.929873 |
| H | 3.270689 | -5.254781 | 3.354950 |
| H | -1.812700 | 4.778390 | -0.249366 |
| H | 5.538330 | -6.161558 | 2.814316 |
| C | -2.825283 | 2.920580 | -2.854235 |
| H | 5.691750 | -4.615889 | 3.658668 |
| C | -2.709930 | 2.538884 | -4.186014 |
| H | 5.926902 | -4.693065 | 1.909629 |
| H | -3.379711 | 1.797302 | -4.613349 |
| C | -1.715692 | 3.127895 | -4.968287 |
| H | -1.622150 | 2.845876 | -6.013221 |
| C | -0.837126 | 4.075945 | -4.433628 |
| H | -0.072270 | 4.514839 | -5.067191 |
| C | -0.939791 | 4.465106 | -3.101379 |
| H | -0.261562 | 5.206167 | -2.686767 |
| C | -1.943431 | 3.896389 | -2.317040 |

**$TS_{EF}$**

| | | | |
|---|---|---|---|
| Fe | -2.996327 | 1.565334 | -0.419598 |
| C | -1.671007 | 0.258592 | 1.326358 |
| C | -3.874425 | -1.054643 | -1.869234 |
| C | -0.161620 | 0.057659 | 1.375477 |
| O | -4.764306 | -1.511450 | -2.403803 |
| C | 0.222150 | -1.358804 | 1.794409 |
| I | -5.134101 | 0.917957 | 0.889481 |
| C | 1.730115 | -1.576539 | 1.865122 |
| C | 2.117882 | -2.991145 | 2.283621 |
| C | 3.625358 | -3.210608 | 2.357456 |
| C | -1.690260 | 1.077730 | -1.569091 |
| O | -0.879176 | 0.627546 | -2.238734 |
| C | 4.013592 | -4.624486 | 2.778981 |
| C | 5.520847 | -4.834074 | 2.852169 |
| H | -1.891587 | 1.333256 | 1.092506 |
| H | -2.162027 | 0.096776 | 2.290343 |
| H | -2.149247 | -0.438287 | 0.625383 |
| H | 0.278880 | 0.778038 | 2.076929 |
| H | 0.277836 | 0.276886 | 0.394151 |
| C | -3.528172 | 3.494519 | -0.613388 |
| H | -0.217617 | -2.077131 | 1.087867 |
| H | -0.225692 | -1.582663 | 2.772625 |
| H | 2.168246 | -0.855896 | 2.570337 |
| H | -4.174027 | 3.690437 | 0.233122 |
| H | 2.176018 | -1.351173 | 0.885959 |
| C | -3.912503 | 2.896772 | -1.847554 |
| H | 1.679875 | -3.711670 | 1.578253 |
| H | 1.669564 | -3.216258 | 3.261767 |
| H | -4.936006 | 2.675386 | -2.126363 |
| H | 4.064309 | -2.489142 | 3.061601 |
| H | 4.074474 | -2.987484 | 1.379033 |
| H | 3.575240 | -5.344205 | 2.074507 |
| C | -2.127195 | 3.654003 | -0.637944 |
| H | 3.562850 | -4.846027 | 3.755777 |
| H | -1.535126 | 4.052966 | 0.178039 |
| H | 5.771324 | -5.855173 | 3.156027 |
| C | -2.829796 | 3.184338 | -2.802233 |
| H | 5.980430 | -4.150293 | 3.574523 |
| C | -2.732364 | 3.039184 | -4.179179 |
| H | 5.993182 | -4.651198 | 1.880594 |
| H | -3.572991 | 2.672999 | -4.762355 |
| C | -1.530225 | 3.382651 | -4.804923 |
| H | -1.443235 | 3.288347 | -5.883487 |
| C | -0.442708 | 3.848329 | -4.066455 |
| H | 0.478534 | 4.112767 | -4.577107 |
| C | -0.524305 | 3.980753 | -2.677236 |
| H | 0.329050 | 4.335801 | -2.105524 |
| C | -1.718907 | 3.656923 | -2.051005 |

**F**

| | | | |
|---|---|---|---|
| Fe | -3.032854 | 1.777566 | -0.542989 |
| C | -1.487791 | 0.479611 | 1.249469 |
| C | -1.700195 | -2.514877 | -1.226679 |
| C | -0.047580 | 0.024813 | 1.046392 |
| O | -2.118491 | -3.309926 | -1.919354 |
| C | 0.275654 | -1.233730 | 1.845771 |
| I | -4.738412 | -0.081892 | -0.641100 |
| C | 1.710397 | -1.715990 | 1.656394 |
| C | 2.035286 | -2.971328 | 2.459434 |
| C | 3.465897 | -3.464082 | 2.266585 |
| C | -2.080517 | 1.147575 | -1.884569 |
| O | -1.482698 | 0.681305 | -2.741866 |
| C | 3.789872 | -4.718949 | 3.071226 |
| C | 5.219683 | -5.205367 | 2.870310 |
| H | -1.632608 | 1.449482 | 0.705463 |
| H | -1.709792 | 0.712464 | 2.296678 |
| H | -2.200300 | -0.278926 | 0.916539 |
| H | 0.643177 | 0.829060 | 1.332190 |
| H | 0.124661 | -0.170965 | -0.019279 |
| C | -3.467152 | 3.749995 | -0.353482 |
| H | -0.419309 | -2.031268 | 1.550048 |
| H | 0.091285 | -1.045712 | 2.913138 |
| H | 2.406401 | -0.913074 | 1.938677 |
| H | -3.985831 | 3.776848 | 0.604069 |
| H | 1.888833 | -1.909980 | 0.589230 |
| C | -4.048078 | 3.357479 | -1.592501 |
| H | 1.334932 | -3.771504 | 2.180795 |
| H | 1.859242 | -2.775447 | 3.526818 |
| H | -5.107114 | 3.220748 | -1.771344 |
| H | 4.167642 | -2.664260 | 2.543808 |
| H | 3.642029 | -3.662173 | 1.199532 |
| H | 3.087071 | -5.516267 | 2.794314 |
| C | -2.073220 | 3.847294 | -0.529929 |
| H | 3.614814 | -4.519673 | 4.137093 |
| H | -1.358127 | 4.102380 | 0.243510 |
| H | 5.425638 | -6.105864 | 3.457253 |
| C | -3.051394 | 3.635861 | -2.626818 |
| H | 5.943715 | -4.439913 | 3.171136 |
| C | -3.116595 | 3.613677 | -4.017006 |
| H | 5.411901 | -5.443422 | 1.818205 |
| H | -4.047097 | 3.377674 | -4.525490 |
| C | -1.963101 | 3.904917 | -4.742730 |
| H | -1.999526 | 3.905614 | -5.828167 |
| C | -0.757937 | 4.196889 | -4.095689 |
| H | 0.125061 | 4.420882 | -4.686982 |
| C | -0.674091 | 4.205193 | -2.704536 |
| H | 0.266873 | 4.427079 | -2.208354 |
| C | -1.823453 | 3.932782 | -1.968010 |

**G**

| | | | |
|---|---|---|---|
| Fe | -1.755070 | 1.872252 | -0.428880 |
| C | -0.257398 | 1.638261 | 1.612370 |
| I | -2.085404 | -0.564971 | -1.104996 |
| H | -1.919646 | 0.029549 | 5.167612 |
| C | 1.172078 | 1.114837 | 1.696926 |
| C | 1.248028 | -0.363520 | 2.063932 |
| C | 2.677379 | -0.887423 | 2.150729 |
| H | -3.470848 | -0.789199 | 4.828567 |
| C | 2.760323 | -2.365446 | 2.517616 |
| C | 4.189636 | -2.891172 | 2.598328 |
| H | -3.463052 | 0.783508 | 5.660785 |
| C | -0.351691 | 2.055487 | -1.477284 |
| P | -4.398637 | 1.123347 | 2.848761 |
| O | 0.573597 | 2.122409 | -2.147416 |
| C | 4.275512 | -4.369560 | 2.964248 |

| | | | |
|---|---|---|---|
| C | 5.707411 | -4.884289 | 3.040648 |
| H | -5.818694 | -1.929368 | 1.909819 |
| H | -0.285894 | 2.696727 | 1.339258 |
| H | -0.821556 | 1.507801 | 2.540785 |
| H | -0.791343 | 0.972648 | 0.880483 |
| O | -2.979039 | 0.846416 | 3.633600 |
| H | 1.720660 | 1.710409 | 2.438894 |
| H | -4.045719 | -1.820375 | 2.069187 |
| H | 1.680705 | 1.279767 | 0.738110 |
| C | -3.268761 | 3.239292 | -0.374266 |
| H | 0.686832 | -0.947626 | 1.321152 |
| H | 0.739224 | -0.524468 | 3.025415 |
| C | -2.966274 | 0.178599 | 4.896292 |
| H | 3.238978 | -0.297140 | 2.889304 |
| H | -3.919067 | 2.786314 | 0.373752 |
| H | 3.180934 | -0.724506 | 1.187174 |
| O | -5.176657 | -0.312246 | 2.960844 |
| C | -3.189690 | 2.850182 | -1.738580 |
| C | -4.965455 | -1.248365 | 1.907271 |
| H | 2.197086 | -2.953640 | 1.779479 |
| H | 2.257694 | -2.529698 | 3.481729 |
| H | -3.892210 | 2.202616 | -2.247689 |
| H | 4.754009 | -2.302039 | 3.335663 |
| O | -5.319088 | 1.810757 | 4.029556 |
| H | 4.692118 | -2.727135 | 1.634181 |
| H | 3.711689 | -4.956785 | 2.227056 |
| C | -2.182143 | 4.091756 | -0.094254 |
| C | -5.111050 | 3.195525 | 4.253472 |
| H | 3.773635 | -4.533208 | 3.927590 |
| H | -1.963940 | 4.532540 | 0.871720 |
| H | 5.740843 | -5.946127 | 3.303759 |
| C | -2.290126 | 3.796319 | -2.395132 |
| H | 6.284788 | -4.336868 | 3.794100 |
| C | -1.967195 | 4.006869 | -3.733668 |
| H | 6.222353 | -4.763434 | 2.081050 |
| H | -2.439940 | 3.421118 | -4.517064 |
| C | -1.028086 | 4.986258 | -4.047395 |
| H | -0.774602 | 5.172182 | -5.086992 |
| C | -0.404018 | 5.735422 | -3.043238 |
| H | 0.324349 | 6.493121 | -3.317246 |
| C | -0.705232 | 5.525580 | -1.699684 |
| H | -0.214715 | 6.109643 | -0.925414 |
| H | -4.898434 | -0.756826 | 0.930041 |
| H | -5.940290 | 3.550620 | 4.868376 |
| C | -1.656032 | 4.561145 | -1.372384 |
| H | -5.100937 | 3.764562 | 3.314211 |
| H | -4.169522 | 3.379494 | 4.785436 |

**$TS_{GH}$**

| | | | |
|---|---|---|---|
| Fe | -1.880047 | 1.873534 | -0.357824 |
| C | -0.360090 | 1.677296 | 1.688990 |
| I | -2.159027 | -0.580037 | -1.020222 |
| H | -2.147224 | -0.494527 | 5.316186 |
| C | 1.075707 | 1.166446 | 1.719432 |
| C | 1.176929 | -0.306271 | 2.102331 |
| C | 2.613795 | -0.813641 | 2.158317 |
| H | -3.757805 | -1.058310 | 4.786986 |
| C | 2.722587 | -2.285511 | 2.542256 |
| C | 4.159793 | -2.792280 | 2.602821 |
| H | -3.597729 | 0.505417 | 5.620376 |
| C | -0.452967 | 2.033640 | -1.381825 |
| P | -4.109265 | 1.014986 | 2.751279 |
| O | 0.490322 | 2.080236 | -2.027816 |
| C | 4.271536 | -4.264331 | 2.986511 |
| C | 5.711315 | -4.758915 | 3.046604 |
| H | -6.121017 | -1.689931 | 1.776158 |
| H | -0.413276 | 2.732625 | 1.407171 |
| H | -0.876854 | 1.546601 | 2.644180 |
| H | -0.929090 | 1.001103 | 0.994487 |
| O | -2.866354 | 0.455273 | 3.667142 |
| H | 1.648427 | 1.775216 | 2.431994 |
| H | -4.354334 | -1.891087 | 1.916895 |
| H | 1.545558 | 1.323106 | 0.739756 |
| C | -3.370414 | 3.258767 | -0.422927 |
| H | 0.602212 | -0.905142 | 1.382086 |
| H | 0.694490 | -0.459684 | 3.078314 |
| C | -3.115472 | -0.183662 | 4.920388 |
| H | 3.187281 | -0.207828 | 2.874959 |
| H | -4.063943 | 2.836141 | 0.300643 |
| H | 3.091372 | -0.657927 | 1.180417 |
| O | -5.199853 | -0.202440 | 2.806092 |
| C | -3.237055 | 2.837972 | -1.771823 |
| C | -5.162105 | -1.168719 | 1.758245 |
| H | 2.152793 | -2.890393 | 1.822926 |
| H | 2.240448 | -2.443067 | 3.517909 |
| H | -3.922968 | 2.184529 | -2.295835 |
| H | 4.729987 | -2.186275 | 3.321813 |
| O | -4.952200 | 1.930594 | 3.833667 |
| H | 4.642490 | -2.634781 | 1.627514 |
| H | 3.703966 | -4.868835 | 2.266363 |
| C | -2.285629 | 4.103619 | -0.111689 |
| C | -4.405519 | 3.205027 | 4.127820 |
| H | 3.787413 | -4.421741 | 3.959959 |
| H | -2.110249 | 4.569890 | 0.851107 |
| H | 5.763445 | -5.816490 | 3.323593 |
| C | -2.305602 | 3.766655 | -2.410608 |
| H | 6.293205 | -4.193413 | 3.783051 |
| C | -1.931200 | 3.950445 | -3.738926 |
| H | 6.209312 | -4.644534 | 2.077293 |
| H | -2.377531 | 3.352956 | -4.528960 |
| C | -0.974171 | 4.918686 | -4.034775 |
| H | -0.680162 | 5.083908 | -5.067157 |
| C | -0.384260 | 5.681726 | -3.021359 |
| H | 0.358994 | 6.430159 | -3.280523 |
| C | -0.738121 | 5.498158 | -1.686182 |
| H | -0.273507 | 6.093699 | -0.904691 |
| H | -5.020212 | -0.701632 | 0.777773 |
| H | -5.165601 | 3.762202 | 4.678775 |
| C | -1.706769 | 4.546142 | -1.378195 |
| H | -4.154146 | 3.763522 | 3.215701 |
| H | -3.504203 | 3.123027 | 4.747754 |

**H**

| | | | |
|---|---|---|---|
| Fe | -2.099896 | 1.844762 | 0.383204 |
| C | -0.044539 | 1.978015 | 2.111377 |
| I | -1.747085 | -0.682847 | -0.324623 |
| H | -2.985471 | -1.183025 | 4.620419 |
| C | 1.298160 | 1.307630 | 1.854037 |
| C | 1.416666 | -0.061113 | 2.516922 |
| C | 2.750185 | -0.745389 | 2.237821 |
| H | -4.451903 | -1.257337 | 3.607697 |
| C | 2.876868 | -2.115699 | 2.895989 |
| C | 4.204208 | -2.807495 | 2.604179 |
| H | -4.148241 | 0.177797 | 4.620690 |
| C | -0.750454 | 2.093875 | -0.845050 |
| P | -3.525516 | 1.125189 | 2.004210 |
| O | 0.155201 | 2.180261 | -1.536725 |
| C | 4.333008 | -4.179979 | 3.257993 |
| C | 5.661025 | -4.863260 | 2.956956 |
| H | -6.343041 | -0.550950 | 0.660601 |
| H | -0.114277 | 2.971310 | 1.660405 |
| H | -0.255541 | 2.072049 | 3.181681 |
| H | -0.846362 | 1.289112 | 1.736776 |
| O | -2.904142 | -0.029694 | 2.953664 |
| H | 2.096764 | 1.968807 | 2.216847 |
| H | -4.771902 | -1.339807 | 0.999126 |
| H | 1.453951 | 1.202472 | 0.773580 |
| C | -3.621969 | 3.228889 | 0.140669 |
| H | 0.596931 | -0.700396 | 2.162112 |
| H | 1.279768 | 0.047006 | 3.603019 |
| C | -3.677568 | -0.599782 | 4.012160 |
| H | 3.573265 | -0.100152 | 2.578097 |
| H | -4.414102 | 3.116999 | 0.869993 |
| H | 2.877172 | -0.853071 | 1.151540 |
| O | -5.020311 | 0.640075 | 1.616629 |
| C | -3.547986 | 2.588858 | -1.124602 |
| C | -5.260532 | -0.414313 | 0.682056 |
| H | 2.050531 | -2.756370 | 2.557179 |
| H | 2.752685 | -2.010832 | 3.983613 |
| H | -4.280420 | 1.887013 | -1.505481 |
| H | 5.031736 | -2.166307 | 2.940876 |
| O | -4.089739 | 2.225701 | 3.081124 |
| H | 4.327508 | -2.911791 | 1.516756 |
| H | 3.505436 | -4.818579 | 2.920893 |
| C | -2.516740 | 4.104199 | 0.247084 |
| C | -3.137784 | 3.020614 | 3.776676 |
| H | 4.210225 | -4.075691 | 4.344647 |
| H | -2.324932 | 4.755127 | 1.093018 |
| H | 5.727563 | -5.845076 | 3.436168 |
| C | -2.713180 | 3.444721 | -1.974558 |
| H | 6.504826 | -4.261589 | 3.312916 |
| C | -2.456337 | 3.443427 | -3.339642 |
| H | 5.794127 | -5.009787 | 1.879319 |
| H | -2.932716 | 2.718871 | -3.994513 |
| C | -1.573706 | 4.394546 | -3.855913 |
| H | -1.374752 | 4.416889 | -4.923482 |
| C | -0.944427 | 5.318105 | -3.019659 |
| H | -0.264330 | 6.050154 | -3.445786 |

| | | | |
|---|---|---|---|
| C | -1.178880 | 5.315151 | -1.642638 |
| H | -0.678694 | 6.032517 | -0.996849 |
| H | -4.894141 | -0.153673 | -0.313248 |
| H | -3.696780 | 3.806018 | 4.287839 |
| C | -2.069650 | 4.385913 | -1.121658 |
| H | -2.417936 | 3.478930 | 3.089224 |
| H | -2.594427 | 2.424900 | 4.519346 |

**$TS_{HI}$**

| | | | |
|---|---|---|---|
| Fe | -2.365276 | 2.120014 | 0.244406 |
| C | 0.463275 | 2.193086 | 2.996607 |
| I | -1.425488 | -0.223082 | -0.364234 |
| H | -2.737104 | -0.835768 | 4.483342 |
| C | 1.635408 | 1.398474 | 2.434310 |
| C | 1.724906 | -0.011807 | 3.006962 |
| C | 2.896139 | -0.814818 | 2.451267 |
| H | -4.248737 | -1.087614 | 3.568236 |
| C | 2.998487 | -2.222369 | 3.029324 |
| C | 4.171690 | -3.023939 | 2.475071 |
| H | -4.020124 | 0.411837 | 4.502104 |
| C | -0.628542 | 2.768789 | -0.416720 |
| P | -3.651129 | 1.256999 | 1.787090 |
| O | 0.423454 | 3.094712 | -0.710393 |
| C | 4.279258 | -4.429925 | 3.056918 |
| C | 5.455234 | -5.221169 | 2.497867 |
| H | -6.127138 | -0.908222 | 0.497133 |
| H | 0.409486 | 3.197485 | 2.561653 |
| H | 0.546624 | 2.308502 | 4.084045 |
| H | -0.483227 | 1.676882 | 2.793478 |
| O | -2.859288 | 0.242289 | 2.771004 |
| H | 2.573593 | 1.935313 | 2.630487 |
| H | -4.490424 | -1.430176 | 0.994530 |
| H | 1.541782 | 1.331527 | 1.342890 |
| C | -4.036700 | 3.230395 | -0.137659 |
| H | 0.786065 | -0.541624 | 2.792554 |
| H | 1.806833 | 0.043481 | 4.102757 |
| C | -3.514939 | -0.346130 | 3.896566 |
| H | 3.833712 | -0.273711 | 2.645469 |
| H | -4.875350 | 3.085274 | 0.531931 |
| H | 2.802338 | -0.877226 | 1.358002 |
| O | -5.059278 | 0.529605 | 1.439756 |
| C | -3.734082 | 2.463425 | -1.304865 |
| C | -5.080744 | -0.609533 | 0.575906 |
| H | 2.062637 | -2.764135 | 2.831277 |
| H | 3.086373 | -2.160390 | 4.123866 |
| H | -4.316243 | 1.625368 | -1.666905 |
| H | 5.107704 | -2.479742 | 2.667590 |
| O | -4.348337 | 2.310432 | 2.828258 |
| H | 4.082112 | -3.090416 | 1.381360 |
| H | 3.344494 | -4.973102 | 2.862785 |
| C | -3.073748 | 4.259186 | -0.042689 |
| C | -3.484241 | 3.208708 | 3.519488 |
| H | 4.367277 | -4.362440 | 4.149859 |
| H | -3.047653 | 5.016909 | 0.731343 |
| H | 5.509390 | -6.225003 | 2.930969 |
| C | -2.873700 | 3.281679 | -2.144403 |
| H | 6.405532 | -4.717222 | 2.706942 |
| C | -2.386454 | 3.106396 | -3.439739 |
| H | 5.375378 | -5.332153 | 1.410710 |
| H | -2.664086 | 2.231749 | -4.020943 |
| C | -1.541643 | 4.075981 | -3.970891 |
| H | -1.163012 | 3.963470 | -4.982462 |
| C | -1.175821 | 5.200340 | -3.219919 |
| H | -0.523363 | 5.947193 | -3.663184 |
| C | -1.632871 | 5.376221 | -1.915466 |
| H | -1.327205 | 6.242320 | -1.334728 |
| H | -4.684576 | -0.368734 | -0.413616 |
| H | -4.125914 | 3.879598 | 4.092598 |
| C | -2.481249 | 4.414926 | -1.374007 |
| H | -2.873903 | 3.794578 | 2.822958 |
| H | -2.820192 | 2.669203 | 4.203863 |

**I**

| | | | |
|---|---|---|---|
| Fe | -2.344562 | 1.949996 | -0.090242 |
| C | 0.808284 | 2.619401 | 4.781546 |
| I | -0.800105 | -0.173242 | -0.229709 |
| H | -1.643096 | 0.515305 | 4.838334 |
| C | 1.896460 | 1.899885 | 3.994347 |
| C | 1.547108 | 0.447871 | 3.682717 |
| C | 2.623599 | -0.276589 | 2.881552 |
| H | -2.893722 | -0.534495 | 4.117100 |
| C | 2.266520 | -1.723796 | 2.559597 |
| C | 3.329253 | -2.441849 | 1.734783 |
| H | -3.311107 | 1.125754 | 4.615593 |
| C | -1.028239 | 2.827579 | 0.682726 |
| P | -3.181787 | 1.363085 | 1.781681 |
| O | -0.175855 | 3.442175 | 1.150369 |
| C | 2.967314 | -3.884763 | 1.397209 |
| C | 4.033275 | -4.591969 | 0.569498 |
| H | -5.015385 | -1.644612 | 1.448379 |
| H | 1.081431 | 3.657606 | 4.996844 |
| H | 0.617363 | 2.122011 | 5.740317 |
| H | -0.130275 | 2.630649 | 4.215978 |
| O | -2.099001 | 0.969357 | 2.917716 |
| H | 2.842229 | 1.937285 | 4.552307 |
| H | -3.257337 | -1.582997 | 1.775776 |
| H | 2.074845 | 2.434818 | 3.052447 |
| C | -4.286255 | 2.264458 | -0.786959 |
| H | 0.602523 | 0.415728 | 3.122198 |
| H | 1.369979 | -0.092592 | 4.625473 |
| C | -2.524255 | 0.491428 | 4.196484 |
| H | 3.575711 | -0.245812 | 3.431793 |
| H | -5.159489 | 2.037082 | -0.188072 |
| H | 2.795174 | 0.266957 | 1.941933 |
| O | -4.321938 | 0.212683 | 1.845046 |
| C | -3.627013 | 1.367028 | -1.657981 |
| C | -4.095301 | -1.081516 | 1.283282 |
| H | 1.312160 | -1.740326 | 2.015027 |
| H | 2.097797 | -2.276075 | 3.496034 |
| H | -3.910837 | 0.344336 | -1.863802 |
| H | 4.287285 | -2.424885 | 2.275104 |
| O | -4.132697 | 2.464447 | 2.526344 |
| H | 3.498292 | -1.885224 | 0.801849 |
| H | 2.012004 | -3.897261 | 0.855291 |
| C | -3.559264 | 3.491229 | -0.750200 |
| C | -3.535490 | 3.684114 | 2.953191 |
| H | 2.794358 | -4.441974 | 2.328211 |
| H | -3.833209 | 4.374301 | -0.188934 |
| H | 3.748824 | -5.623851 | 0.339660 |
| C | -2.551901 | 2.085069 | -2.297647 |
| H | 4.991387 | -4.621762 | 1.100728 |
| C | -1.606484 | 1.704726 | -3.282100 |
| H | 4.201545 | -4.074213 | -0.381447 |
| H | -1.618924 | 0.698475 | -3.687098 |
| C | -0.691990 | 2.633229 | -3.709085 |
| H | 0.032565 | 2.362921 | -4.471214 |
| C | -0.661853 | 3.946007 | -3.166527 |
| H | 0.080311 | 4.649248 | -3.533054 |
| C | -1.545122 | 4.338929 | -2.193409 |
| H | -1.522352 | 5.345571 | -1.786275 |
| H | -3.878149 | -1.018496 | 0.214220 |
| H | -4.329526 | 4.274605 | 3.412677 |
| C | -2.519725 | 3.408641 | -1.746519 |
| H | -3.112531 | 4.239586 | 2.109417 |
| H | -2.745420 | 3.502621 | 3.690209 |

**J**

| | | | |
|---|---|---|---|
| Fe | -0.144614 | -0.780767 | 1.177433 |
| I | 0.530143 | -2.882889 | -0.220105 |
| C | -0.235086 | -1.846566 | 2.569806 |
| C | 1.576404 | -0.410656 | 1.434485 |
| O | 2.675456 | -0.134654 | 1.598671 |
| C | -2.010981 | 0.012223 | 1.651038 |
| H | -2.571022 | -0.325918 | 2.513953 |
| C | -2.064900 | -0.565262 | 0.360238 |
| H | -2.679632 | -1.401310 | 0.056986 |
| C | -1.014676 | 1.030787 | 1.663630 |
| H | -0.742417 | 1.646042 | 2.510608 |
| C | -1.205426 | 0.209285 | -0.501549 |
| C | -0.915727 | 0.120713 | -1.885901 |
| H | -1.387581 | -0.644859 | -2.492361 |
| C | -0.039831 | 1.023768 | -2.431269 |
| H | 0.185195 | 0.979655 | -3.492471 |
| C | 0.591957 | 2.017857 | -1.636127 |
| H | 1.278359 | 2.712325 | -2.111444 |
| C | 0.354393 | 2.115639 | -0.288896 |
| H | 0.833876 | 2.880978 | 0.314035 |
| C | -0.563637 | 1.208964 | 0.303080 |
| O | -0.327852 | -2.519454 | 3.493662 |

**$TS_{JK}$**

| | | | |
|---|---|---|---|
| Fe | -0.326314 | -0.887271 | 0.951766 |
| I | 1.310479 | -2.241451 | -0.382338 |
| C | -0.381099 | -2.034549 | 2.273089 |
| C | 2.453464 | 0.254298 | 2.409088 |
| O | 3.241019 | -0.379248 | 2.924240 |
| C | -1.991372 | 0.069987 | 1.682014 |
| H | -2.477663 | -0.247673 | 2.595801 |

| | | | |
|---|---|---|---|
| C | -2.242538 | -0.461536 | 0.386171 |
| H | -2.980691 | -1.212371 | 0.137717 |
| C | -0.904809 | 0.977640 | 1.599024 |
| H | -0.443110 | 1.498946 | 2.426426 |
| C | -1.435268 | 0.281190 | -0.554538 |
| C | -1.297989 | 0.198830 | -1.957297 |
| H | -1.931263 | -0.470340 | -2.531071 |
| C | -0.347596 | 0.980413 | -2.571118 |
| H | -0.231504 | 0.937008 | -3.649745 |
| C | 0.497485 | 1.836667 | -1.823854 |
| H | 1.242445 | 2.428159 | -2.347588 |
| C | 0.395374 | 1.929952 | -0.455130 |
| H | 1.046442 | 2.585082 | 0.114904 |
| C | -0.593289 | 1.161566 | 0.200764 |
| O | -0.479801 | -2.759400 | 3.159174 |

**K**

| | | | |
|---|---|---|---|
| Fe | -0.390410 | -0.948528 | 0.894012 |
| I | 1.429107 | -2.140575 | -0.336662 |
| C | -0.448023 | -2.103393 | 2.207810 |
| C | 2.605895 | 0.442404 | 2.600436 |
| O | 3.315038 | -0.315148 | 3.058244 |
| C | -1.973756 | 0.087651 | 1.696415 |
| H | -2.448392 | -0.219159 | 2.619954 |
| C | -2.299311 | -0.398739 | 0.400920 |
| H | -3.088722 | -1.099512 | 0.163592 |
| C | -0.834104 | 0.927754 | 1.594193 |
| H | -0.312564 | 1.401529 | 2.414585 |
| C | -1.474633 | 0.308224 | -0.551908 |
| C | -1.378774 | 0.236197 | -1.959078 |
| H | -2.064475 | -0.387444 | -2.524055 |
| C | -0.405381 | 0.975992 | -2.589179 |
| H | -0.321294 | 0.941432 | -3.671137 |
| C | 0.501656 | 1.779375 | -1.856020 |
| H | 1.259968 | 2.340500 | -2.393688 |
| C | 0.443767 | 1.856660 | -0.483864 |
| H | 1.145304 | 2.465978 | 0.076912 |
| C | -0.561168 | 1.126689 | 0.189669 |
| O | -0.541326 | -2.825989 | 3.096348 |

**L**

| | | | |
|---|---|---|---|
| Fe | -1.958162 | -0.223004 | 0.825638 |
| I | -2.998858 | -2.425819 | 1.428209 |
| H | 2.404124 | -0.451659 | -2.403110 |
| H | 2.647360 | -2.204148 | -2.158330 |
| H | 3.896675 | -1.052327 | -1.627727 |
| C | -1.759332 | -0.586662 | -0.901530 |
| P | 2.270834 | -2.266018 | 0.659329 |
| O | -1.546949 | -0.787033 | -2.011827 |
| H | 0.550580 | -5.029645 | -0.625124 |
| O | 2.160180 | -1.071076 | -0.477000 |
| H | 0.116907 | -3.389459 | -1.168096 |
| C | -0.545874 | 0.146675 | 2.290377 |
| C | 2.819331 | -1.210013 | -1.736628 |
| H | -0.026408 | -0.679087 | 2.759677 |
| O | 1.954576 | -3.619731 | -0.208824 |
| C | -1.791134 | 0.678313 | 2.700505 |
| C | 0.582433 | -3.970199 | -0.364032 |
| H | -2.365212 | 0.369187 | 3.563067 |
| O | 3.890370 | -2.565956 | 0.681627 |
| C | -0.163556 | 0.737664 | 1.055385 |
| C | 4.670154 | -1.693599 | 1.482780 |
| H | 0.723726 | 0.493827 | 0.483915 |
| C | -2.156209 | 1.705081 | 1.760063 |
| C | -3.304670 | 2.531716 | 1.648541 |
| H | -4.087092 | 2.480967 | 2.399510 |
| C | -3.383561 | 3.412355 | 0.598478 |
| H | -4.247133 | 4.065213 | 0.511083 |
| C | -2.356330 | 3.498979 | -0.379780 |
| H | -2.456178 | 4.220023 | -1.185462 |
| C | -1.252186 | 2.687496 | -0.324866 |
| H | -0.466090 | 2.755694 | -1.071156 |
| H | 0.009505 | -3.811899 | 0.557289 |
| H | 5.654609 | -2.152209 | 1.594803 |
| C | -1.135871 | 1.763283 | 0.747619 |
| H | 4.232046 | -1.551113 | 2.479283 |
| H | 4.788193 | -0.711109 | 1.009009 |

**$TS_{LM}$**

| | | | |
|---|---|---|---|
| Fe | -1.005926 | 0.080214 | 0.485491 |
| I | -2.569476 | -1.792271 | -0.190157 |
| H | 2.079637 | -1.612173 | -2.934291 |
| H | 2.019459 | -3.248670 | -2.219069 |
| H | 3.436415 | -2.209518 | -1.932650 |
| C | -0.409120 | 0.429020 | -1.164092 |
| P | 1.873394 | -2.267305 | 0.566022 |
| O | -0.026817 | 0.741224 | -2.198188 |
| H | 0.593951 | -5.534478 | 0.590165 |
| O | 1.694354 | -1.637883 | -0.940129 |
| H | -0.176501 | -4.266449 | -0.404425 |
| C | -0.251975 | 0.343150 | 2.409989 |
| C | 2.350597 | -2.217639 | -2.067913 |
| H | 0.382649 | -0.419266 | 2.843893 |
| O | 1.741808 | -3.881398 | 0.323592 |
| C | -1.665035 | 0.345639 | 2.448341 |
| C | 0.448126 | -4.458761 | 0.474030 |
| H | -2.294407 | -0.363522 | 2.967174 |
| O | 3.516868 | -2.342722 | 0.710442 |
| C | 0.203501 | 1.375758 | 1.548408 |
| C | 4.169271 | -1.116951 | 0.990373 |
| H | 1.233760 | 1.605065 | 1.312357 |
| C | -2.116841 | 1.468838 | 1.668824 |
| C | -3.415071 | 1.946805 | 1.342863 |
| H | -4.291652 | 1.442407 | 1.736547 |
| C | -3.527756 | 3.057899 | 0.549858 |
| H | -4.512384 | 3.443516 | 0.302884 |
| C | -2.379839 | 3.724915 | 0.035726 |
| H | -2.518071 | 4.608107 | -0.580859 |
| C | -1.114321 | 3.273912 | 0.299947 |
| H | -0.240833 | 3.788762 | -0.089175 |
| H | -0.070859 | -4.068325 | 1.356992 |
| H | 5.194911 | -1.355088 | 1.279562 |
| C | -0.956958 | 2.124373 | 1.123794 |
| H | 3.689040 | -0.576430 | 1.817936 |
| H | 4.190899 | -0.462047 | 0.110434 |

**M**

| | | | |
|---|---|---|---|
| Fe | -0.253299 | -0.032369 | 0.314418 |
| I | -1.969349 | -1.270011 | -1.245500 |
| H | 2.712407 | -2.933393 | -2.778968 |
| H | 1.989519 | -3.995365 | -1.541878 |
| H | 3.369320 | -2.950363 | -1.114924 |
| C | 0.355217 | 0.842421 | -1.086673 |
| P | 1.209370 | -1.569923 | 0.101769 |
| O | 0.748347 | 1.463058 | -1.971221 |
| H | 0.042162 | -4.633181 | 1.439567 |
| O | 1.550898 | -1.964939 | -1.429490 |
| H | -0.275407 | -4.106422 | -0.240651 |
| C | 0.009717 | -0.139378 | 2.383492 |
| C | 2.461711 | -3.025630 | -1.721549 |
| H | 0.654331 | -0.875623 | 2.847539 |
| O | 1.059177 | -2.972469 | 0.898829 |
| C | -1.360988 | -0.314253 | 2.086440 |
| C | -0.119743 | -3.772028 | 0.788931 |
| H | -1.958763 | -1.190022 | 2.296905 |
| O | 2.678771 | -1.266077 | 0.753187 |
| C | 0.432547 | 1.129219 | 1.886128 |
| C | 3.440639 | -0.191730 | 0.215016 |
| H | 1.423508 | 1.551237 | 1.985316 |
| C | -1.850559 | 0.920745 | 1.524402 |
| C | -3.136589 | 1.325326 | 1.087385 |
| H | -3.972839 | 0.637153 | 1.149313 |
| C | -3.294985 | 2.595904 | 0.596352 |
| H | -4.275373 | 2.926282 | 0.266782 |
| C | -2.197909 | 3.493206 | 0.497411 |
| H | -2.368503 | 4.490510 | 0.102441 |
| C | -0.934949 | 3.125250 | 0.885814 |
| H | -0.100325 | 3.816447 | 0.813210 |
| H | -1.006827 | -3.219726 | 1.107968 |
| H | 4.358465 | -0.136646 | 0.802450 |
| C | -0.741161 | 1.823615 | 1.417998 |
| H | 2.903420 | 0.759463 | 0.292234 |
| H | 3.692843 | -0.371590 | -0.835744 |

**J'**

| | | | |
|---|---|---|---|
| Fe | -0.714743 | -2.811620 | -1.009565 |
| C | -0.215241 | 5.129135 | -5.332279 |
| I | -1.877849 | -1.393292 | 0.853723 |
| C | -0.639829 | -1.337190 | -1.959199 |
| C | -2.314512 | -3.264754 | -1.642334 |
| O | -3.329879 | -3.591349 | -2.058752 |
| C | -0.401299 | 4.632664 | -3.903959 |
| C | 1.293493 | -3.190747 | -1.407938 |
| C | 0.715796 | 3.702435 | -3.441232 |
| C | 0.535548 | 3.200405 | -2.012637 |
| H | 1.889537 | -2.523985 | -2.018648 |
| C | 1.111317 | -3.077594 | -0.009178 |

| | | | |
|---|---|---|---|
| H | 1.554854 | -2.331802 | 0.635713 |
| C | 1.651344 | 2.270554 | -1.547447 |
| C | 0.474939 | -4.248205 | -1.900204 |
| C | 1.467330 | 1.774851 | -0.117078 |
| H | 0.399051 | -4.569526 | -2.930295 |
| C | 0.287592 | -4.183197 | 0.414823 |
| C | -0.171054 | -4.592269 | 1.691766 |
| H | 0.103788 | -4.025793 | 2.575002 |
| C | -0.955120 | -5.713619 | 1.778192 |
| C | 2.560370 | 0.815700 | 0.343018 |
| H | -1.306431 | -6.049657 | 2.748944 |
| C | 2.364800 | 0.335928 | 1.776311 |
| C | -1.329009 | -6.448357 | 0.620465 |
| H | -1.029309 | 5.794081 | -5.637640 |
| H | -1.950090 | -7.331515 | 0.737171 |
| C | -0.924975 | -6.065528 | -0.633032 |
| H | -0.185702 | 4.293470 | -6.040457 |
| H | 0.724115 | 5.683239 | -5.439146 |
| H | -1.207178 | -6.633745 | -1.514325 |
| C | -0.095615 | -4.919759 | -0.755411 |
| O | -0.560361 | -0.386624 | -2.596455 |
| H | -1.363510 | 4.110277 | -3.817663 |
| H | -0.462112 | 5.490707 | -3.220878 |
| H | 1.680289 | 4.223965 | -3.526873 |
| H | 0.776231 | 2.842303 | -4.123679 |
| H | -0.426314 | 2.675304 | -1.930875 |
| H | 0.470928 | 4.060132 | -1.330349 |
| H | 2.618506 | 2.786803 | -1.634673 |
| H | 1.705722 | 1.407997 | -2.227253 |
| H | 0.491370 | 1.278014 | -0.023299 |
| H | 1.433557 | 2.636320 | 0.565245 |
| H | 3.540766 | 1.301582 | 0.244831 |
| H | 2.587200 | -0.048806 | -0.336935 |
| H | 3.145040 | -0.371087 | 2.078990 |
| H | 1.390738 | -0.152890 | 1.896543 |
| H | 2.392912 | 1.176044 | 2.478849 |

**$TS_{J'K'}$**

| | | | |
|---|---|---|---|
| Fe | -0.286495 | -2.863690 | -1.159368 |
| C | -0.175262 | 5.404536 | -5.068818 |
| I | -2.026905 | -1.565665 | 0.104844 |
| C | -0.076508 | -1.626569 | -2.379523 |
| C | -2.871039 | -3.813885 | -2.926773 |
| O | -3.606676 | -3.156650 | -3.487119 |
| C | -0.452983 | 4.733201 | -3.729642 |
| C | 1.433834 | -3.801141 | -1.780330 |
| C | 0.685213 | 3.830470 | -3.263803 |
| C | 0.416636 | 3.154405 | -1.923548 |
| H | 2.013300 | -3.434742 | -2.618439 |
| C | 1.560567 | -3.358751 | -0.433559 |
| H | 2.276244 | -2.636986 | -0.063513 |
| C | 1.553012 | 2.248390 | -1.460524 |
| C | 0.334407 | -4.692593 | -1.865477 |
| C | 1.278798 | 1.569571 | -0.122776 |
| H | -0.048850 | -5.150191 | -2.767278 |
| C | 0.653647 | -4.144323 | 0.371066 |
| C | 0.376408 | -4.147391 | 1.755635 |
| H | 0.959314 | -3.529901 | 2.431659 |
| C | -0.644988 | -4.943480 | 2.218374 |
| C | 2.407397 | 0.652655 | 0.338312 |
| H | -0.869902 | -4.964979 | 3.280359 |
| C | 2.110338 | -0.035303 | 1.665589 |
| C | -1.423625 | -5.731585 | 1.336219 |
| H | -1.006912 | 6.044758 | -5.379664 |
| H | -2.228016 | -6.336920 | 1.743186 |
| C | -1.183032 | -5.742921 | -0.018194 |
| H | -0.015520 | 4.661115 | -5.857820 |
| H | 0.724104 | 6.028705 | -5.019373 |
| H | -1.782098 | -6.347941 | -0.691345 |
| C | -0.120122 | -4.957861 | -0.520366 |
| O | 0.125561 | -0.841430 | -3.194391 |
| H | -1.376099 | 4.142133 | -3.798234 |
| H | -0.641827 | 5.499471 | -2.965595 |
| H | 1.610903 | 4.420514 | -3.196349 |
| H | 0.872636 | 3.061706 | -4.027262 |
| H | -0.508346 | 2.564737 | -1.992710 |
| H | 0.229190 | 3.922447 | -1.159444 |
| H | 2.481519 | 2.833838 | -1.391267 |
| H | 1.734231 | 1.480548 | -2.226213 |
| H | 0.348816 | 0.987778 | -0.191592 |
| H | 1.099840 | 2.335329 | 0.645748 |
| H | 3.338418 | 1.230099 | 0.419985 |
| H | 2.591433 | -0.103998 | -0.438308 |
| H | 2.932681 | -0.689471 | 1.976960 |
| H | 1.197575 | -0.638552 | 1.597096 |
| H | 1.956183 | 0.699512 | 2.463484 |

**K'**

| | | | |
|---|---|---|---|
| Fe | -0.206123 | -2.792916 | -1.094025 |
| C | -0.150705 | 5.437951 | -5.052773 |
| I | -2.154516 | -1.665704 | -0.006822 |
| C | -0.015897 | -1.579383 | -2.340024 |
| C | -3.074524 | -4.152956 | -3.114773 |
| O | -3.767057 | -3.382714 | -3.576609 |
| C | -0.429141 | 4.771263 | -3.711416 |
| C | 1.435870 | -3.811437 | -1.794546 |
| C | 0.694626 | 3.844753 | -3.257445 |
| C | 0.423789 | 3.169773 | -1.917048 |
| H | 2.006476 | -3.460685 | -2.645297 |
| C | 1.636827 | -3.411247 | -0.446295 |
| H | 2.406448 | -2.740868 | -0.087587 |
| C | 1.546759 | 2.241029 | -1.466572 |
| C | 0.277861 | -4.631563 | -1.858983 |
| C | 1.270392 | 1.557649 | -0.131489 |
| H | -0.164892 | -5.044902 | -2.754852 |
| C | 0.707425 | -4.153484 | 0.373941 |
| C | 0.468967 | -4.158026 | 1.766283 |
| H | 1.103797 | -3.582126 | 2.432401 |
| C | -0.576498 | -4.909625 | 2.249973 |
| C | 2.385625 | 0.616021 | 0.312260 |
| H | -0.771084 | -4.933990 | 3.317910 |
| C | 2.086415 | -0.082004 | 1.633678 |
| C | -1.416182 | -5.650052 | 1.382600 |
| H | -0.970972 | 6.097282 | -5.353737 |
| H | -2.234768 | -6.223669 | 1.806768 |
| C | -1.218954 | -5.651915 | 0.021256 |
| H | -0.016575 | 4.692195 | -5.844324 |
| H | 0.763051 | 6.041535 | -5.012488 |
| H | -1.869356 | -6.213118 | -0.641946 |
| C | -0.138686 | -4.907607 | -0.503617 |
| O | 0.162213 | -0.821021 | -3.185316 |
| H | -1.364937 | 4.199535 | -3.771552 |
| H | -0.594704 | 5.540598 | -2.945027 |
| H | 1.632397 | 4.416065 | -3.196090 |
| H | 0.860447 | 3.074616 | -4.024509 |
| H | -0.512622 | 2.597799 | -1.981171 |
| H | 0.256640 | 3.938658 | -1.149074 |
| H | 2.485752 | 2.809660 | -1.399292 |
| H | 1.709944 | 1.475394 | -2.238372 |
| H | 0.328423 | 0.994710 | -0.196210 |
| H | 1.112464 | 2.320723 | 0.644256 |
| H | 3.326605 | 1.177038 | 0.393719 |
| H | 2.551095 | -0.135670 | -0.473256 |
| H | 2.903885 | -0.746935 | 1.935048 |
| H | 1.168730 | -0.677507 | 1.562579 |
| H | 1.942270 | 0.645875 | 2.439766 |

**$CP_{JO'}$**

| | | | |
|---|---|---|---|
| Fe | -0.2106 | -0.8838 | 1.1491 |
| I | 0.2809 | -3.0356 | -0.1953 |
| C | -0.3619 | -1.8448 | 2.8064 |
| C | 1.6409 | -0.4156 | 1.2968 |
| O | 2.7559 | -0.2188 | 1.4383 |
| C | -2.1347 | 0.1054 | 1.3813 |
| H | -2.7197 | -0.2327 | 2.2272 |
| C | -2.1408 | -0.4608 | 0.0957 |
| H | -2.7559 | -1.2890 | -0.2320 |
| C | -1.1171 | 1.0991 | 1.4151 |
| H | -0.8760 | 1.7168 | 2.2708 |
| C | -1.3125 | 0.3707 | -0.7790 |
| C | -1.0543 | 0.3247 | -2.1491 |
| H | -1.5094 | -0.4368 | -2.7757 |
| C | -0.1970 | 1.2754 | -2.6927 |
| H | 0.0088 | 1.2643 | -3.7591 |
| C | 0.4142 | 2.2447 | -1.8861 |
| H | 1.0816 | 2.9717 | -2.3394 |
| C | 0.1828 | 2.2905 | -0.5155 |
| H | 0.6704 | 3.0356 | 0.1063 |
| C | -0.6955 | 1.3586 | 0.0410 |
| O | -0.3767 | -2.4776 | 3.7591 |

**O'**

| | | | |
|---|---|---|---|
| Fe | -0.073614 | -0.892267 | 1.207501 |
| I | 0.374499 | -3.142823 | -0.009902 |
| C | -0.195318 | -1.935558 | 3.039841 |
| C | 1.713386 | -0.549262 | 1.487353 |
| O | 2.828976 | -0.340923 | 1.634359 |

| | | | |
|---|---|---|---|
| C | -2.012615 | -0.000683 | 1.559632 |
| H | -2.592903 | -0.351449 | 2.403533 |
| C | -2.017928 | -0.571057 | 0.265390 |
| H | -2.632761 | -1.399315 | -0.061747 |
| C | -1.008640 | 0.997564 | 1.599879 |
| H | -0.762161 | 1.621072 | 2.449945 |
| C | -1.206460 | 0.265199 | -0.600557 |
| C | -0.936460 | 0.217585 | -1.975053 |
| H | -1.394905 | -0.542078 | -2.600296 |
| C | -0.082177 | 1.165441 | -2.512572 |
| H | 0.123746 | 1.158643 | -3.578599 |
| C | 0.530089 | 2.138089 | -1.700488 |
| H | 1.192598 | 2.868041 | -2.156278 |
| C | 0.307297 | 2.178727 | -0.334298 |
| H | 0.790786 | 2.926417 | 0.287867 |
| C | -0.572483 | 1.240897 | 0.225794 |
| O | -0.250554 | -2.606358 | 3.956197 |

**$TS_{O'P'}$**

| | | | |
|---|---|---|---|
| Fe | -0.600019 | -0.212362 | 1.304741 |
| I | -0.397656 | -2.753117 | 1.518462 |
| C | 1.946165 | -4.397651 | 4.164675 |
| C | 0.978346 | 0.126861 | 2.147363 |
| O | 1.974314 | 0.328377 | 2.671720 |
| C | -2.539099 | 0.643981 | 1.099447 |
| H | -3.279612 | 0.460478 | 1.868042 |
| C | -2.292139 | -0.194504 | -0.016496 |
| H | -2.836233 | -1.096298 | -0.263449 |
| C | -1.554745 | 1.663040 | 1.121141 |
| H | -1.475030 | 2.462327 | 1.846605 |
| C | -1.272005 | 0.423926 | -0.832302 |
| C | -0.671640 | 0.047628 | -2.048958 |
| H | -1.004507 | -0.843298 | -2.572352 |
| C | 0.329479 | 0.846343 | -2.565151 |
| H | 0.788674 | 0.584700 | -3.513611 |
| C | 0.773451 | 1.998389 | -1.881361 |
| H | 1.560763 | 2.603245 | -2.321414 |
| C | 0.234828 | 2.363692 | -0.663700 |
| H | 0.588596 | 3.245548 | -0.137517 |
| C | -0.802060 | 1.577367 | -0.125528 |
| O | 1.672528 | -5.432774 | 3.787140 |

**P'**

| | | | |
|---|---|---|---|
| Fe | -0.526469 | -0.050269 | 1.357327 |
| I | -0.039432 | -2.523279 | 1.789237 |
| C | 1.584812 | -5.293725 | 3.936753 |
| C | 0.982714 | 0.539269 | 2.187147 |
| O | 1.936805 | 0.896827 | 2.706482 |
| C | -2.544687 | 0.559403 | 1.054163 |
| H | -3.275395 | 0.364323 | 1.829298 |
| C | -2.183126 | -0.343453 | 0.022948 |
| H | -2.617387 | -1.320014 | -0.144573 |
| C | -1.680820 | 1.680850 | 0.991669 |
| H | -1.705858 | 2.546568 | 1.640911 |
| C | -1.222629 | 0.310511 | -0.836632 |
| C | -0.560184 | -0.103747 | -2.007646 |
| H | -0.783548 | -1.068596 | -2.452249 |
| C | 0.358316 | 0.751390 | -2.583596 |
| H | 0.862686 | 0.458420 | -3.499383 |
| C | 0.659404 | 2.002015 | -2.003066 |
| H | 1.385211 | 2.648331 | -2.487657 |
| C | 0.057875 | 2.413340 | -0.830332 |
| H | 0.301853 | 3.372575 | -0.383095 |
| C | -0.897804 | 1.568284 | -0.233989 |
| O | 1.150061 | -6.013125 | 3.173780 |

**Q'**

| | | | |
|---|---|---|---|
| Fe | -0.904288 | -0.160506 | 0.067122 |
| I | -2.941146 | -0.990048 | -1.315163 |
| H | 4.021137 | -3.840883 | 0.869904 |
| H | 2.315989 | -3.515008 | 1.273301 |
| H | 3.439272 | -2.157113 | 0.998526 |
| C | -0.194074 | 0.712480 | -1.355410 |
| P | 1.909564 | -2.136307 | -1.428445 |
| O | 0.225080 | 1.296139 | -2.249064 |
| H | -0.958184 | -3.343322 | 0.252331 |
| O | 2.895664 | -3.226157 | -0.707607 |
| H | 0.482362 | -4.261873 | -0.278731 |
| C | -0.399089 | -0.704614 | 2.070615 |
| C | 3.177133 | -3.172979 | 0.689826 |
| H | 0.094421 | -1.657683 | 2.207487 |
| O | 0.580729 | -2.181622 | -0.410492 |
| C | -1.796486 | -0.500269 | 2.018435 |
| C | -0.164299 | -3.404006 | -0.492969 |
| H | -2.558926 | -1.251073 | 2.179847 |
| O | 2.425029 | -0.702019 | -0.798728 |
| C | 0.243782 | 0.508181 | 1.714628 |
| C | 3.313156 | 0.062755 | -1.609507 |
| H | 1.311882 | 0.666214 | 1.644519 |
| C | -2.039794 | 0.923528 | 1.880455 |
| C | -3.220777 | 1.681309 | 1.835206 |
| H | -4.187284 | 1.199591 | 1.945620 |
| C | -3.122357 | 3.048940 | 1.655664 |
| H | -4.024022 | 3.653771 | 1.637982 |
| C | -1.871365 | 3.674577 | 1.487596 |
| H | -1.831643 | 4.751296 | 1.350510 |
| C | -0.697862 | 2.942884 | 1.486497 |
| H | 0.263185 | 3.429755 | 1.346417 |
| H | -0.624851 | -3.517411 | -1.478841 |
| H | 3.284262 | 1.088396 | -1.237706 |
| C | -0.772589 | 1.554771 | 1.691062 |
| H | 3.004505 | 0.059507 | -2.660869 |
| H | 4.337683 | -0.317503 | -1.534318 |

**$TS_{Q'R'}$**

| | | | |
|---|---|---|---|
| Fe | -1.072932 | 0.232157 | -0.025658 |
| I | -2.853994 | -1.121163 | -1.294113 |
| H | 4.506952 | -4.274579 | -0.917362 |
| H | 3.102533 | -4.558505 | 0.145915 |
| H | 4.051534 | -3.062600 | 0.315169 |
| C | -0.405803 | 1.009822 | -1.525277 |
| P | 1.694374 | -2.104394 | -0.981101 |
| O | 0.006617 | 1.505666 | -2.471305 |
| H | -0.447167 | -4.205861 | 0.870122 |
| O | 2.861519 | -3.178495 | -1.396531 |
| H | 0.530856 | -4.730623 | -0.522137 |
| C | -0.400241 | -0.297350 | 1.921229 |
| C | 3.672118 | -3.799575 | -0.398923 |
| H | 0.159052 | -1.220537 | 2.008031 |
| O | 0.955508 | -2.854232 | 0.291692 |
| C | -1.809654 | -0.172431 | 1.953890 |
| C | 0.023092 | -3.876976 | -0.058208 |
| H | -2.513849 | -0.970077 | 2.149865 |
| O | 2.506066 | -1.069488 | 0.029635 |
| C | 0.146383 | 0.952347 | 1.532654 |
| C | 3.324257 | -0.109586 | -0.624761 |
| H | 1.198845 | 1.171403 | 1.412155 |
| C | -2.148690 | 1.227886 | 1.806129 |
| C | -3.378696 | 1.909004 | 1.798669 |
| H | -4.305443 | 1.369847 | 1.968680 |
| C | -3.376030 | 3.274276 | 1.585824 |
| H | -4.314296 | 3.820708 | 1.598154 |
| C | -2.175843 | 3.975065 | 1.346956 |
| H | -2.212992 | 5.048581 | 1.186813 |
| C | -0.959325 | 3.321213 | 1.303972 |
| H | -0.039474 | 3.865185 | 1.109087 |
| H | -0.753009 | -3.499183 | -0.733345 |
| H | 3.638298 | 0.615694 | 0.128962 |
| C | -0.933401 | 1.934301 | 1.539636 |
| H | 2.781422 | 0.416900 | -1.420607 |
| H | 4.216208 | -0.575701 | -1.059211 |

**R'**

| | | | |
|---|---|---|---|
| Fe | -0.369194 | 0.013720 | 0.110661 |
| I | -2.155581 | -1.204821 | -1.359809 |
| H | 3.063346 | -3.279028 | -2.708232 |
| H | 2.294600 | -4.277123 | -1.445000 |
| H | 3.620164 | -3.167397 | -1.011737 |
| C | 0.305671 | 0.866779 | -1.335454 |
| P | 1.382223 | -1.742294 | -0.007257 |
| O | 0.726828 | 1.413497 | -2.252466 |
| H | -0.016217 | -4.614027 | 1.491669 |
| O | 1.799776 | -2.255841 | -1.489737 |
| H | -0.067208 | -4.324660 | -0.268978 |
| C | -0.093139 | -0.065540 | 2.256633 |
| C | 2.752600 | -3.308437 | -1.663122 |
| H | 0.557694 | -0.830834 | 2.661553 |
| O | 1.178247 | -3.097678 | 0.873850 |
| C | -1.474343 | -0.212986 | 1.991464 |
| C | -0.028729 | -3.847354 | 0.715491 |
| H | -2.073287 | -1.088656 | 2.205131 |
| O | 2.814835 | -1.394673 | 0.711628 |
| C | 0.320324 | 1.196428 | 1.761795 |
| C | 3.547504 | -0.285442 | 0.201742 |
| H | 1.316158 | 1.614467 | 1.836008 |
| C | -1.996857 | 1.076173 | 1.581241 |
| C | -3.293196 | 1.518215 | 1.281359 |

| | | | |
|---|---|---|---|
| H | -4.138212 | 0.842528 | 1.367690 |
| C | -3.467127 | 2.830765 | 0.879161 |
| H | -4.465667 | 3.197109 | 0.660673 |
| C | -2.369557 | 3.701481 | 0.739754 |
| H | -2.542765 | 4.725994 | 0.423380 |
| C | -1.077608 | 3.275276 | 0.993508 |
| H | -0.234389 | 3.950058 | 0.875763 |
| H | -0.914938 | -3.215650 | 0.827624 |
| H | 4.403181 | -0.144774 | 0.863962 |
| C | -0.882260 | 1.953707 | 1.424522 |
| H | 2.945127 | 0.630363 | 0.194896 |
| H | 3.906796 | -0.480643 | -0.814668 |

**$CP_{R'M}$**

| | | | |
|---|---|---|---|
| Fe | -0.2837 | -0.0759 | 0.1278 |
| I | -2.0524 | -1.3131 | -1.3741 |
| H | 3.0303 | -3.2612 | -2.6888 |
| H | 2.2559 | -4.2539 | -1.4240 |
| H | 3.5751 | -3.1370 | -0.9886 |
| C | 0.3521 | 0.7805 | -1.3078 |
| P | 1.3397 | -1.7318 | 0.0086 |
| O | 0.7559 | 1.3597 | -2.2138 |
| H | 0.0098 | -4.6531 | 1.4862 |
| O | 1.7555 | -2.2341 | -1.4764 |
| H | -0.0378 | -4.3533 | -0.2773 |
| C | -0.0293 | -0.1305 | 2.2468 |
| C | 2.7128 | -3.2851 | -1.6459 |
| H | 0.6182 | -0.8765 | 2.6888 |
| O | 1.1446 | -3.0881 | 0.8845 |
| C | -1.4061 | -0.2970 | 1.9649 |
| C | -0.0304 | -3.8848 | 0.7117 |
| H | -2.0022 | -1.1729 | 2.1772 |
| O | 2.7707 | -1.3769 | 0.7221 |
| C | 0.3866 | 1.1296 | 1.7392 |
| C | 3.5503 | -0.3094 | 0.1936 |
| H | 1.3788 | 1.5522 | 1.8183 |
| C | -1.9232 | 0.9764 | 1.5081 |
| C | -3.2259 | 1.4223 | 1.2221 |
| H | -4.0696 | 0.7479 | 1.3296 |
| C | -3.4046 | 2.7385 | 0.8484 |
| H | -4.4095 | 3.1166 | 0.6781 |
| C | -2.3078 | 3.6154 | 0.7081 |
| H | -2.4904 | 4.6531 | 0.4384 |
| C | -1.0149 | 3.1915 | 0.9385 |
| H | -0.1767 | 3.8771 | 0.8497 |
| H | -0.9453 | -3.2942 | 0.8156 |
| H | 4.4095 | -0.1990 | 0.8589 |
| C | -0.8104 | 1.8620 | 1.3589 |
| H | 2.9954 | 0.6349 | 0.1673 |
| H | 3.9019 | -0.5397 | -0.8177 |

**A'**

| | | | |
|---|---|---|---|
| Fe | -1.808733 | 1.544864 | 0.364781 |
| I | -4.059553 | 0.323248 | -0.179923 |
| H | 2.987087 | -3.976484 | 1.665674 |
| H | 1.345384 | -3.275462 | 1.650777 |
| H | 2.767289 | -2.204015 | 1.646920 |
| C | -2.495965 | 3.031417 | -0.304632 |
| C | -1.188318 | 0.965966 | -1.188668 |
| P | 1.655802 | -2.107645 | -1.060742 |
| O | -2.915365 | 4.020859 | -0.704447 |
| O | -0.763960 | 0.600279 | -2.188707 |
| H | -1.817571 | -2.177858 | -0.565081 |
| O | 2.413817 | -3.227923 | -0.135849 |
| H | -0.896947 | -3.708709 | -0.597340 |
| C | 0.009464 | 1.078428 | 1.294581 |
| C | 2.370846 | -3.158924 | 1.287790 |
| H | 0.883439 | 0.746879 | 0.745274 |
| O | 0.192709 | -1.951939 | -0.318788 |
| C | -1.010125 | 0.215400 | 1.783262 |
| C | -0.899126 | -2.658542 | -0.909127 |
| H | -1.024337 | -0.858523 | 1.668821 |
| O | 2.221292 | -0.689596 | -0.399907 |
| C | -0.367215 | 2.417428 | 1.580813 |
| C | 3.530868 | -0.317488 | -0.809024 |
| H | 0.191143 | 3.307604 | 1.323853 |
| C | -2.001241 | 1.024450 | 2.409383 |
| H | -2.931148 | 0.669720 | 2.831666 |
| H | -2.172941 | 3.231569 | 2.649199 |
| H | -0.864346 | -2.609433 | -2.003201 |
| H | 4.290671 | -0.957667 | -0.345750 |
| C | -1.613659 | 2.376856 | 2.292466 |
| H | 3.690640 | 0.713656 | -0.487360 |
| H | 3.643599 | -0.368919 | -1.899215 |

**$TS_{A'B'}$**

| | | | |
|---|---|---|---|
| Fe | -0.893621 | 0.960285 | -0.233692 |
| I | -2.321128 | -0.777979 | -1.581882 |
| H | 2.545663 | -3.279431 | -2.067649 |
| H | 1.520585 | -4.031320 | -0.818079 |
| H | 2.880562 | -2.981821 | -0.335988 |
| C | -1.957784 | 2.115782 | -1.043815 |
| C | 0.355913 | 1.267522 | -1.417636 |
| P | 0.762744 | -1.183149 | 0.143170 |
| O | -2.610419 | 2.870953 | -1.606008 |
| O | 1.167350 | 1.482935 | -2.201455 |
| H | -0.796827 | -3.967588 | 1.659526 |
| O | 1.237689 | -2.001415 | -1.179528 |
| H | -0.812142 | -3.548486 | -0.077874 |
| C | -0.304778 | 0.957399 | 1.996768 |
| C | 2.097581 | -3.140530 | -1.082695 |
| H | 0.565906 | 0.380834 | 2.277689 |
| O | 0.298987 | -2.327436 | 1.207890 |
| C | -1.631314 | 0.517986 | 1.988993 |
| C | -0.837722 | -3.147404 | 0.940079 |
| H | -1.983408 | -0.463618 | 2.277234 |
| O | 2.172973 | -0.918848 | 0.954648 |
| C | -0.297194 | 2.289727 | 1.485780 |
| C | 3.000647 | 0.138071 | 0.483626 |
| H | 0.575872 | 2.926938 | 1.407306 |
| C | -2.476461 | 1.651159 | 1.680203 |
| H | -3.557435 | 1.624076 | 1.623337 |
| H | -1.983724 | 3.740625 | 1.153674 |
| H | -1.768640 | -2.588691 | 1.066677 |
| H | 3.903264 | 0.125534 | 1.096762 |
| C | -1.663140 | 2.749553 | 1.448853 |
| H | 2.510049 | 1.112480 | 0.595206 |
| H | 3.279450 | -0.003644 | -0.566620 |

**B'**

| | | | |
|---|---|---|---|
| Fe | -0.727921 | 0.200421 | -0.354603 |
| I | -1.734133 | -1.592286 | -2.006058 |
| H | 3.236907 | -2.709686 | -2.141349 |
| H | 2.276165 | -3.725023 | -1.033775 |
| H | 3.410334 | -2.517276 | -0.370807 |
| C | -2.221101 | 1.152808 | -0.836732 |
| C | 0.247770 | 1.010670 | -1.552404 |
| P | 0.972437 | -1.188052 | 0.074580 |
| O | -3.117952 | 1.727390 | -1.250083 |
| O | 0.885509 | 1.597131 | -2.307920 |
| H | -0.263558 | -4.050800 | 1.757000 |
| O | 1.680109 | -1.748237 | -1.264594 |
| H | -0.318893 | -3.887471 | -0.024951 |
| C | -1.168064 | 0.173893 | 1.832631 |
| C | 2.712973 | -2.734540 | -1.185216 |
| H | -0.817170 | -0.786639 | 2.190999 |
| O | 0.760612 | -2.459733 | 1.049996 |
| C | -2.476961 | 0.664716 | 1.997665 |
| C | -0.351843 | -3.349474 | 0.925759 |
| H | -3.345730 | 0.059617 | 2.233962 |
| O | 2.225984 | -0.610851 | 0.947175 |
| C | -0.340276 | 1.281325 | 1.433403 |
| C | 3.029940 | 0.420981 | 0.382236 |
| H | 0.726352 | 1.332219 | 1.618753 |
| C | -2.474585 | 2.073527 | 1.817216 |
| H | -3.348156 | 2.712917 | 1.840837 |
| H | -0.869078 | 3.455531 | 1.215268 |
| H | -1.300970 | -2.810654 | 0.989125 |
| H | 3.843235 | 0.598527 | 1.087098 |
| C | -1.191917 | 2.450918 | 1.466803 |
| H | 2.461876 | 1.348712 | 0.251495 |
| H | 3.445206 | 0.118618 | -0.584709 |

**$TS_{B'C'}$**

| | | | |
|---|---|---|---|
| Fe | -0.734056 | 0.521405 | -0.166829 |
| I | -2.114956 | -1.107396 | -1.762304 |
| H | 2.666324 | -2.638468 | -2.416901 |
| H | 1.699940 | -3.600463 | -1.267157 |
| H | 3.014571 | -2.555301 | -0.663811 |
| C | -2.384611 | 1.907042 | -1.201469 |
| C | 0.243828 | 1.210539 | -1.458783 |
| P | 0.748129 | -1.032841 | 0.056983 |
| O | -3.295166 | 2.477044 | -1.578884 |
| O | 0.886484 | 1.712393 | -2.268864 |
| H | -0.607912 | -3.854065 | 1.726489 |
| O | 1.310032 | -1.561860 | -1.362543 |
| H | -0.816057 | -3.625505 | -0.037110 |

| | | | |
|---|---|---|---|
| C | -0.607778 | 0.480073 | 1.978036 |
| C | 2.228568 | -2.655667 | -1.418212 |
| H | 0.038811 | -0.282340 | 2.391571 |
| O | 0.493540 | -2.345429 | 0.961746 |
| C | -2.000796 | 0.391182 | 1.802082 |
| C | -0.706546 | -3.119642 | 0.925276 |
| H | -2.614691 | -0.476973 | 2.004305 |
| O | 2.109277 | -0.635049 | 0.867065 |
| C | -0.211439 | 1.781935 | 1.551256 |
| C | 2.961775 | 0.367209 | 0.323359 |
| H | 0.786549 | 2.191888 | 1.644128 |
| C | -2.496849 | 1.721252 | 1.547734 |
| H | -3.539160 | 1.975444 | 1.400107 |
| H | -1.448375 | 3.612252 | 1.129883 |
| H | -1.587933 | -2.497068 | 1.093326 |
| H | 3.831048 | 0.422613 | 0.980135 |
| C | -1.416456 | 2.565130 | 1.406235 |
| H | 2.466045 | 1.342888 | 0.300160 |
| H | 3.287057 | 0.106975 | -0.689510 |

**C'**

| | | | |
|---|---|---|---|
| Fe | -0.691153 | 0.485512 | 0.301153 |
| I | -2.369330 | -0.790039 | -1.270421 |
| H | 2.377682 | -2.558954 | -2.561240 |
| H | 1.613068 | -3.575156 | -1.310990 |
| H | 2.969641 | -2.504338 | -0.873725 |
| C | -2.979161 | 2.990496 | -1.996951 |
| C | -0.061244 | 1.303633 | -1.115643 |
| P | 0.775290 | -1.075454 | 0.204115 |
| O | -3.362105 | 2.982958 | -3.064526 |
| O | 0.346549 | 1.896986 | -2.014003 |
| H | -0.450039 | -4.085283 | 1.605207 |
| O | 1.159804 | -1.544718 | -1.296857 |
| H | -0.683141 | -3.618916 | -0.105508 |
| C | -0.452635 | 0.529652 | 2.390140 |
| C | 2.086676 | -2.610084 | -1.511325 |
| H | 0.219339 | -0.121482 | 2.934780 |
| O | 0.593597 | -2.442610 | 1.057449 |
| C | -1.807643 | 0.255310 | 2.079072 |
| C | -0.578353 | -3.247238 | 0.918047 |
| H | -2.359478 | -0.635929 | 2.342249 |
| O | 2.226507 | -0.750482 | 0.886341 |
| C | -0.106352 | 1.786402 | 1.815840 |
| C | 2.998924 | 0.312686 | 0.341623 |
| H | 0.854265 | 2.277404 | 1.889668 |
| C | -2.314203 | 1.360652 | 1.330778 |
| H | -3.300790 | 1.429183 | 0.894987 |
| H | -1.352361 | 3.236385 | 0.632463 |
| H | -1.480744 | -2.686469 | 1.173536 |
| H | 3.903603 | 0.382115 | 0.947635 |
| C | -1.279100 | 2.306862 | 1.180658 |
| H | 2.459377 | 1.264725 | 0.386120 |
| H | 3.274708 | 0.110388 | -0.699169 |

## Optimizations with OPBE

**CO**

| | | | |
|---|---|---|---|
| C | -0.454356 | -0.043348 | 0.346988 |
| O | 0.454356 | 0.043348 | -0.346988 |

**$P(OMe)_3$**

| | | | |
|---|---|---|---|
| P | 0.838564 | -0.241890 | -0.014702 |
| H | 1.418358 | -2.706035 | 2.537609 |
| H | -0.153289 | -2.545761 | 1.697476 |
| H | 0.430229 | -1.228656 | 2.751585 |
| H | -1.926054 | -1.508983 | -1.798752 |
| O | 1.460451 | -1.447715 | 0.937654 |
| H | -0.533263 | -2.561496 | -1.426922 |
| C | 0.738808 | -2.004776 | 2.039402 |
| O | -0.705724 | -0.767748 | -0.353421 |
| C | -0.857265 | -1.516904 | -1.552922 |
| O | 0.273528 | 0.873387 | 1.087142 |
| C | 1.197276 | 1.882225 | 1.477016 |
| H | -0.299894 | -1.077812 | -2.395191 |
| H | 0.611093 | 2.689758 | 1.932069 |
| H | 1.755671 | 2.292776 | 0.621070 |
| H | 1.920111 | 1.510631 | 2.219485 |

**N**

| | | | |
|---|---|---|---|
| Fe | -0.127025 | -0.784619 | 1.189525 |
| I | 0.676967 | -2.811346 | -0.226238 |
| C | -0.278760 | -1.889186 | 2.485053 |
| C | 1.513099 | -0.423151 | 1.644522 |
| O | 2.589206 | -0.144590 | 1.986404 |
| C | -1.944253 | 0.007356 | 1.671905 |
| H | -2.504670 | -0.307991 | 2.547782 |
| C | -2.033541 | -0.575743 | 0.372010 |
| H | -2.671141 | -1.404884 | 0.084116 |
| C | -0.941629 | 1.029051 | 1.651785 |
| H | -0.641772 | 1.645527 | 2.493894 |
| C | -1.195809 | 0.200043 | -0.515932 |
| C | -0.965738 | 0.130624 | -1.913364 |
| H | -1.470541 | -0.622355 | -2.514924 |
| C | -0.103500 | 1.044671 | -2.486104 |
| H | 0.071637 | 1.015638 | -3.561294 |
| C | 0.566905 | 2.026464 | -1.706705 |
| H | 1.238475 | 2.727241 | -2.202198 |
| C | 0.380516 | 2.110817 | -0.341060 |
| H | 0.886123 | 2.871951 | 0.251975 |
| C | -0.517773 | 1.199973 | 0.276102 |
| O | -0.404378 | -2.599590 | 3.400246 |

**$CP_{NO}$**

| | | | |
|---|---|---|---|
| Fe | -0.1501 | -0.8184 | 1.0520 |
| I | 0.3049 | -3.0250 | -0.1806 |
| C | -0.3083 | -1.8466 | 2.8371 |
| C | 1.5836 | -0.4742 | 1.3151 |
| O | 2.7178 | -0.2440 | 1.4380 |
| C | -2.0761 | 0.0717 | 1.3877 |
| H | -2.6786 | -0.2625 | 2.2265 |
| C | -2.0809 | -0.5015 | 0.0857 |
| H | -2.7178 | -1.3178 | -0.2423 |
| C | -1.0673 | 1.0743 | 1.4249 |
| H | -0.8268 | 1.7051 | 2.2765 |
| C | -1.2796 | 0.3426 | -0.7854 |
| C | -1.0217 | 0.3044 | -2.1657 |
| H | -1.4827 | -0.4572 | -2.7938 |
| C | -0.1629 | 1.2591 | -2.7065 |
| H | 0.0449 | 1.2494 | -3.7767 |
| C | 0.4487 | 2.2332 | -1.8936 |
| H | 1.1149 | 2.9667 | -2.3500 |
| C | 0.2299 | 2.2728 | -0.5184 |
| H | 0.7115 | 3.0250 | 0.1049 |
| C | -0.6354 | 1.3186 | 0.0463 |
| O | -0.3267 | -2.5154 | 3.7767 |

**O**

| | | | |
|---|---|---|---|
| Fe | -0.107701 | -0.927942 | 1.248727 |
| I | 0.447647 | -3.045030 | -0.087233 |
| C | -0.215035 | -1.916706 | 2.917980 |
| C | 1.580891 | -0.563109 | 1.636301 |
| O | 2.684423 | -0.316262 | 1.910268 |
| C | -2.000142 | -0.011399 | 1.561319 |
| H | -2.596594 | -0.341834 | 2.406629 |
| C | -2.020686 | -0.582459 | 0.259939 |
| H | -2.663248 | -1.395732 | -0.063887 |
| C | -0.965936 | 0.967723 | 1.598486 |
| H | -0.702275 | 1.587086 | 2.451038 |
| C | -1.201218 | 0.241303 | -0.612233 |
| C | -0.976339 | 0.224062 | -1.998782 |
| H | -1.473229 | -0.509482 | -2.631543 |
| C | -0.115774 | 1.175171 | -2.542136 |
| H | 0.053472 | 1.193612 | -3.618433 |
| C | 0.541047 | 2.118679 | -1.724699 |
| H | 1.202316 | 2.852545 | -2.185378 |
| C | 0.357811 | 2.135040 | -0.344583 |
| H | 0.871760 | 2.864892 | 0.280029 |
| C | -0.524884 | 1.197134 | 0.222552 |
| O | -0.053904 | -2.501393 | 3.903139 |

**$TS_{OP}$**

| | | | |
|---|---|---|---|
| Fe | -0.514489 | -0.395056 | 1.087082 |
| I | -0.482213 | -2.934258 | 1.130802 |
| C | 1.602437 | -4.195546 | 5.106303 |
| C | 1.064019 | -0.188331 | 1.834426 |
| O | 2.106089 | -0.031677 | 2.330931 |
| C | -2.418071 | 0.509454 | 1.157151 |
| H | -3.101776 | 0.251559 | 1.962144 |
| C | -2.302686 | -0.191390 | -0.076841 |
| H | -2.913193 | -1.033518 | -0.386745 |
| C | -1.384738 | 1.489591 | 1.221664 |
| H | -1.208687 | 2.189761 | 2.033131 |
| C | -1.317600 | 0.485200 | -0.893140 |
| C | -0.839253 | 0.251483 | -2.200802 |
| H | -1.261121 | -0.549138 | -2.806851 |

| | | | |
|---|---|---|---|
| C | 0.155146 | 1.081297 | -2.701184 |
| H | 0.517109 | 0.931678 | -3.718118 |
| C | 0.710936 | 2.120372 | -1.917597 |
| H | 1.486025 | 2.753616 | -2.348836 |
| C | 0.295658 | 2.342074 | -0.612722 |
| H | 0.735677 | 3.136424 | -0.010732 |
| C | -0.728724 | 1.523802 | -0.083182 |
| O | 1.921856 | -5.101499 | 4.480613 |

**P**

| | | | |
|---|---|---|---|
| Fe | -0.488027 | -0.008828 | 1.295981 |
| I | -0.042147 | -2.449938 | 1.830390 |
| C | 1.647675 | -5.866861 | 4.343980 |
| C | 0.947192 | 0.609789 | 2.102035 |
| O | 1.890143 | 1.038619 | 2.634920 |
| C | -2.510514 | 0.541223 | 1.053580 |
| H | -3.223393 | 0.319974 | 1.844089 |
| C | -2.158987 | -0.343566 | -0.004781 |
| H | -2.591494 | -1.323437 | -0.180377 |
| C | -1.659264 | 1.683067 | 0.993752 |
| H | -1.681828 | 2.540648 | 1.659898 |
| C | -1.215376 | 0.333766 | -0.868624 |
| C | -0.571046 | -0.049596 | -2.065261 |
| H | -0.793719 | -1.010094 | -2.527955 |
| C | 0.326971 | 0.834836 | -2.647589 |
| H | 0.813609 | 0.565338 | -3.584668 |
| C | 0.625270 | 2.082416 | -2.049891 |
| H | 1.331522 | 2.751142 | -2.541567 |
| C | 0.044513 | 2.465356 | -0.849894 |
| H | 0.287081 | 3.422145 | -0.388729 |
| C | -0.886842 | 1.591701 | -0.242889 |
| O | 1.151059 | -6.331801 | 3.421098 |

**Q**

| | | | |
|---|---|---|---|
| Fe | -1.840907 | -0.011552 | 0.515443 |
| I | -3.564519 | -1.867371 | 0.758536 |
| H | 2.230864 | -0.735138 | -2.293930 |
| H | 2.778901 | -2.431445 | -2.154118 |
| H | 3.892845 | -1.097853 | -1.737501 |
| C | -1.536157 | -0.271286 | -1.195632 |
| P | 2.635933 | -2.647146 | 0.701005 |
| O | -1.312840 | -0.428712 | -2.328730 |
| H | 0.917789 | -5.492246 | -0.467750 |
| O | 2.342514 | -1.409747 | -0.370716 |
| H | 0.291703 | -3.858610 | -0.823336 |
| C | -0.733612 | 0.503654 | 2.233377 |
| C | 2.846436 | -1.430222 | -1.711467 |
| H | -0.171175 | -0.269563 | 2.750658 |
| O | 2.280037 | -4.012977 | -0.174406 |
| C | -2.099048 | 0.826595 | 2.471683 |
| C | 0.922517 | -4.446001 | -0.140440 |
| H | -2.731800 | 0.383125 | 3.233940 |
| O | 4.272567 | -2.912278 | 0.549861 |
| C | -0.284045 | 1.235987 | 1.095723 |
| C | 5.105985 | -2.190453 | 1.447267 |
| H | 0.708980 | 1.194394 | 0.658757 |
| C | -2.463228 | 1.927979 | 1.605336 |
| C | -3.660767 | 2.658057 | 1.445495 |
| H | -4.521862 | 2.448759 | 2.078732 |
| C | -3.703434 | 3.659811 | 0.484904 |
| H | -4.610960 | 4.251306 | 0.366034 |
| C | -2.590324 | 3.930378 | -0.345890 |
| H | -2.660552 | 4.729385 | -1.083800 |
| C | -1.418419 | 3.194453 | -0.246113 |
| H | -0.569356 | 3.399956 | -0.897215 |
| H | 0.490909 | -4.391928 | 0.870866 |
| H | 6.085913 | -2.682444 | 1.434578 |
| C | -1.340031 | 2.179716 | 0.735451 |
| H | 4.721549 | -2.202013 | 2.479340 |
| H | 5.235393 | -1.142873 | 1.133764 |

**$TS_{QR}$**

| | | | |
|---|---|---|---|
| Fe | -0.897015 | 0.208783 | 0.259308 |
| I | -2.452293 | -1.358509 | -1.034264 |
| H | 3.092035 | -3.003719 | -3.142113 |
| H | 2.419785 | -4.330989 | -2.153321 |
| H | 3.829363 | -3.402965 | -1.559410 |
| C | -0.085930 | 0.804331 | -1.183524 |
| P | 1.864219 | -2.136154 | 0.080849 |
| O | 0.444011 | 1.243302 | -2.124109 |
| H | 0.651125 | -5.079932 | 1.596888 |
| O | 1.989058 | -2.383703 | -1.543968 |
| H | 0.271271 | -4.758171 | -0.119153 |
| C | -0.587895 | 0.114622 | 2.341424 |
| C | 2.887916 | -3.338583 | -2.118553 |
| H | -0.014654 | -0.710165 | 2.754886 |
| O | 1.824060 | -3.653395 | 0.750553 |
| C | -1.989544 | 0.110698 | 2.109138 |
| C | 0.554307 | -4.295371 | 0.837162 |
| H | -2.673101 | -0.695365 | 2.356325 |
| O | 3.444032 | -1.923769 | 0.571534 |
| C | -0.045283 | 1.318734 | 1.798197 |
| C | 4.007142 | -0.635993 | 0.356845 |
| H | 0.995568 | 1.626307 | 1.827593 |
| C | -2.374613 | 1.423861 | 1.625521 |
| C | -3.624301 | 1.989409 | 1.300315 |
| H | -4.539741 | 1.413554 | 1.427168 |
| C | -3.659557 | 3.297531 | 0.834043 |
| H | -4.619164 | 3.758472 | 0.600909 |
| C | -2.473429 | 4.044469 | 0.651403 |
| H | -2.540967 | 5.069133 | 0.286169 |
| C | -1.226766 | 3.496327 | 0.922518 |
| H | -0.315582 | 4.074214 | 0.770583 |
| H | -0.246592 | -3.604336 | 1.136664 |
| H | 4.996369 | -0.645725 | 0.829332 |
| C | -1.165363 | 2.177219 | 1.421015 |
| H | 3.407481 | 0.163290 | 0.819542 |
| H | 4.128851 | -0.408715 | -0.712768 |

**R**

| | | | |
|---|---|---|---|
| Fe | -0.295373 | 0.003669 | 0.149847 |
| I | -2.061282 | -1.124771 | -1.372044 |
| H | 3.323261 | -2.887705 | -2.558303 |
| H | 2.065855 | -4.105060 | -2.202143 |
| H | 3.197590 | -3.586954 | -0.913679 |
| C | 0.428189 | 0.827316 | -1.210122 |
| P | 1.368394 | -1.731661 | 0.038811 |
| O | 0.910824 | 1.414620 | -2.097677 |
| H | 0.056756 | -4.614253 | 1.644471 |
| O | 1.713223 | -2.198594 | -1.491115 |
| H | -0.020904 | -4.440372 | -0.133188 |
| C | -0.078054 | -0.005754 | 2.262635 |
| C | 2.630997 | -3.258442 | -1.792831 |
| H | 0.582649 | -0.732168 | 2.726440 |
| O | 1.213927 | -3.116738 | 0.920113 |
| C | -1.462167 | -0.191988 | 1.996282 |
| C | 0.018386 | -3.894758 | 0.818960 |
| H | -2.042867 | -1.074369 | 2.246859 |
| O | 2.836566 | -1.417348 | 0.736867 |
| C | 0.308842 | 1.260048 | 1.731290 |
| C | 3.631984 | -0.348945 | 0.226960 |
| H | 1.292660 | 1.712633 | 1.807419 |
| C | -2.015593 | 1.074989 | 1.554740 |
| C | -3.328784 | 1.495789 | 1.282739 |
| H | -4.166362 | 0.812003 | 1.410229 |
| C | -3.532139 | 2.806109 | 0.859120 |
| H | -4.545478 | 3.156985 | 0.664899 |
| C | -2.448483 | 3.690468 | 0.672162 |
| H | -2.644787 | 4.710747 | 0.342298 |
| C | -1.137375 | 3.287040 | 0.904081 |
| H | -0.305536 | 3.974884 | 0.754565 |
| H | -0.885521 | -3.280477 | 0.907533 |
| H | 4.524500 | -0.307350 | 0.861090 |
| C | -0.910882 | 1.972955 | 1.358041 |
| H | 3.111769 | 0.616015 | 0.279131 |
| H | 3.940012 | -0.529862 | -0.811782 |

**$CP_{RS}$**

| | | | |
|---|---|---|---|
| Fe | -0.3180 | -0.0482 | 0.1621 |
| I | -2.1119 | -1.1698 | -1.3256 |
| H | 3.0684 | -3.2891 | -2.6861 |
| H | 2.3135 | -4.3261 | -1.4366 |
| H | 3.6429 | -3.2202 | -0.9870 |
| C | 0.3501 | 0.7864 | -1.2266 |
| P | 1.3924 | -1.7820 | 0.0527 |
| O | 0.7744 | 1.3668 | -2.1467 |
| H | 0.0307 | -4.6802 | 1.5695 |
| O | 1.8064 | -2.2997 | -1.4450 |
| H | -0.0309 | -4.3897 | -0.1925 |
| C | -0.0514 | -0.1344 | 2.2749 |
| C | 2.7668 | -3.3472 | -1.6353 |
| H | 0.6036 | -0.8966 | 2.6861 |
| O | 1.2054 | -3.1460 | 0.9607 |
| C | -1.4432 | -0.2773 | 2.0252 |
| C | 0.0043 | -3.9082 | 0.7937 |
| H | -2.0393 | -1.1534 | 2.2657 |
| O | 2.8312 | -1.4177 | 0.7872 |

| | | | |
|---|---|---|---|
| C | 0.3576 | 1.1398 | 1.7835 |
| C | 3.5842 | -0.3242 | 0.2591 |
| H | 1.3527 | 1.5644 | 1.8625 |
| C | -1.9731 | 1.0168 | 1.6330 |
| C | -3.2728 | 1.4651 | 1.3414 |
| H | -4.1217 | 0.7880 | 1.4141 |
| C | -3.4436 | 2.7854 | 0.9307 |
| H | -4.4437 | 3.1457 | 0.6869 |
| C | -2.3443 | 3.6551 | 0.7884 |
| H | -2.5148 | 4.6802 | 0.4563 |
| C | -1.0459 | 3.2235 | 1.0346 |
| H | -0.1951 | 3.8911 | 0.8916 |
| H | -0.8971 | -3.2941 | 0.9120 |
| H | 4.4437 | -0.1969 | 0.9256 |
| C | -0.8502 | 1.8955 | 1.4584 |
| H | 3.0041 | 0.6075 | 0.2400 |
| H | 3.9480 | -0.5352 | -0.7557 |

**S**

| | | | |
|---|---|---|---|
| Fe | -0.221244 | -0.019799 | 0.311137 |
| I | -1.930632 | -1.196871 | -1.274693 |
| H | 2.931916 | -2.725596 | -2.691837 |
| H | 1.829461 | -3.930434 | -1.970320 |
| H | 3.145785 | -3.222082 | -0.983760 |
| C | 0.455067 | 0.805278 | -1.042165 |
| P | 1.190037 | -1.552321 | 0.108630 |
| O | 0.913798 | 1.427356 | -1.918945 |
| H | 0.034236 | -4.624169 | 1.500486 |
| O | 1.528070 | -1.946459 | -1.440279 |
| H | -0.233270 | -4.180081 | -0.214036 |
| C | 0.066296 | -0.077220 | 2.338380 |
| C | 2.411846 | -3.021481 | -1.773423 |
| H | 0.735842 | -0.773519 | 2.834659 |
| O | 1.035202 | -2.964978 | 0.929675 |
| C | -1.316533 | -0.293573 | 2.073633 |
| C | -0.123211 | -3.791314 | 0.805504 |
| H | -1.891276 | -1.175890 | 2.331454 |
| O | 2.681004 | -1.298907 | 0.783102 |
| C | 0.438868 | 1.202260 | 1.810186 |
| C | 3.514535 | -0.265455 | 0.268965 |
| H | 1.420619 | 1.658375 | 1.882460 |
| C | -1.855487 | 0.925252 | 1.508835 |
| C | -3.169564 | 1.306553 | 1.136420 |
| H | -3.995035 | 0.606604 | 1.247731 |
| C | -3.375823 | 2.581281 | 0.646919 |
| H | -4.382688 | 2.894182 | 0.371143 |
| C | -2.302087 | 3.499248 | 0.488895 |
| H | -2.510160 | 4.495596 | 0.098947 |
| C | -1.007615 | 3.154834 | 0.823334 |
| H | -0.188883 | 3.865034 | 0.712821 |
| H | -1.039245 | -3.252821 | 1.070948 |
| H | 4.405737 | -0.249358 | 0.906462 |
| C | -0.765409 | 1.858062 | 1.351838 |
| H | 3.026371 | 0.716218 | 0.309181 |
| H | 3.818271 | -0.465102 | -0.767584 |

**T**

| | | | |
|---|---|---|---|
| Fe | -0.207399 | -0.264693 | 0.602689 |
| I | 1.064847 | -1.784374 | -1.079895 |
| C | -0.404393 | -1.642447 | 1.632065 |
| C | 1.318535 | 0.155440 | 1.305352 |
| O | 2.316350 | 0.479544 | 1.808177 |
| C | -2.002399 | 0.534984 | 1.183676 |
| H | -2.518029 | 0.284154 | 2.106201 |
| C | -2.175175 | -0.113459 | -0.087576 |
| H | -2.830200 | -0.952380 | -0.298788 |
| C | -1.026670 | 1.565127 | 1.026121 |
| H | -0.673871 | 2.231875 | 1.807562 |
| C | -1.303685 | 0.525020 | -1.016794 |
| H | -1.163078 | 0.232788 | -2.052045 |
| H | 0.157053 | 2.209288 | -0.785004 |
| C | -0.593410 | 1.560516 | -0.345155 |
| O | -0.574376 | -2.536584 | 2.356816 |

**$CP_{TU}$**

| | | | |
|---|---|---|---|
| Fe | -0.0607 | -0.2380 | -0.0204 |
| I | 0.4243 | -2.4643 | -1.1819 |
| C | -0.2713 | -1.1613 | 1.8441 |
| C | 1.6257 | 0.0871 | 0.3105 |
| O | 2.7461 | 0.3369 | 0.5115 |
| C | -2.1145 | 0.6548 | 0.5005 |
| H | -2.7133 | 0.3177 | 1.3399 |
| C | -2.1183 | 0.0739 | -0.8162 |
| H | -2.7461 | -0.7476 | -1.1462 |
| C | -1.1224 | 1.6489 | 0.5254 |
| H | -0.8433 | 2.2713 | 1.3696 |
| C | -1.2390 | 0.8268 | -1.6424 |
| H | -1.0269 | 0.6297 | -2.6878 |
| H | 0.1955 | 2.4643 | -1.1182 |
| C | -0.5523 | 1.7382 | -0.8065 |
| O | -0.2976 | -1.9454 | 2.6878 |

**U**

| | | | |
|---|---|---|---|
| Fe | -0.215700 | -0.374460 | 0.213113 |
| I | 0.306174 | -2.590772 | -1.231986 |
| C | -0.197748 | -1.290086 | 1.737114 |
| C | 1.501775 | -0.062821 | 0.502827 |
| O | 2.622357 | 0.155671 | 0.719001 |
| C | -2.149834 | 0.502773 | 0.616868 |
| H | -2.781275 | 0.205210 | 1.449656 |
| C | -2.214389 | -0.050311 | -0.717086 |
| H | -2.855608 | -0.866843 | -1.032506 |
| C | -1.193134 | 1.551491 | 0.628604 |
| H | -0.912353 | 2.161151 | 1.481228 |
| C | -1.255265 | 0.605956 | -1.502763 |
| H | -1.008712 | 0.385220 | -2.535775 |
| H | 0.225608 | 2.218626 | -0.975856 |
| C | -0.570775 | 1.552031 | -0.656037 |
| O | -0.172825 | -1.863637 | 2.746599 |

**$TS_{UV}$**

| | | | |
|---|---|---|---|
| Fe | -0.193109 | -0.264567 | -0.045415 |
| I | 0.301319 | -2.534346 | -1.082169 |
| C | -0.368615 | -1.742680 | 2.483361 |
| C | 1.436700 | 0.005249 | 0.499328 |
| O | 2.527423 | 0.240571 | 0.840184 |
| C | -2.141078 | 0.563523 | 0.523285 |
| H | -2.689223 | 0.211845 | 1.391551 |
| C | -2.232263 | 0.030113 | -0.790675 |
| H | -2.885430 | -0.776659 | -1.108788 |
| C | -1.104267 | 1.537867 | 0.526576 |
| H | -0.777593 | 2.132402 | 1.374845 |
| C | -1.325823 | 0.750979 | -1.636548 |
| H | -1.151142 | 0.548419 | -2.688828 |
| H | 0.160431 | 2.355218 | -1.163143 |
| C | -0.614952 | 1.670119 | -0.833968 |
| O | 0.185916 | -2.488852 | 3.153401 |

**V**

| | | | |
|---|---|---|---|
| Fe | -0.188647 | -0.219152 | -0.434997 |
| I | 0.001042 | -2.646135 | -1.118940 |
| C | -0.148973 | -1.765895 | 3.760364 |
| C | 1.437284 | -0.079752 | 0.171661 |
| O | 2.519130 | 0.046576 | 0.587656 |
| C | -2.139814 | 0.384844 | 0.318278 |
| H | -2.662701 | -0.173169 | 1.089706 |
| C | -2.235316 | 0.152622 | -1.088287 |
| H | -2.865200 | -0.590851 | -1.566739 |
| C | -1.151854 | 1.380876 | 0.529990 |
| H | -0.830473 | 1.782051 | 1.486524 |
| C | -1.368322 | 1.067514 | -1.758187 |
| H | -1.202557 | 1.112378 | -2.830879 |
| H | 0.077739 | 2.576778 | -0.945847 |
| C | -0.666249 | 1.805246 | -0.770512 |
| O | 0.505205 | -2.636728 | 4.115208 |

**W**

| | | | |
|---|---|---|---|
| Fe | -2.731604 | 0.887559 | 0.657300 |
| I | -4.572871 | -0.489223 | 1.711949 |
| H | 2.269832 | 0.040723 | -2.363910 |
| H | 1.845503 | -1.696715 | -2.380933 |
| H | 3.451110 | -1.177914 | -1.795182 |
| C | -2.593186 | -0.072178 | -0.786423 |
| P | 1.986058 | -1.890386 | 0.658945 |
| O | -2.474187 | -0.696253 | -1.764907 |
| H | 0.184452 | -4.767036 | -0.267781 |
| O | 1.843764 | -0.728469 | -0.524365 |
| H | -0.399470 | -3.163142 | -0.790240 |
| C | -1.266100 | 1.707045 | 2.048586 |
| C | 2.387080 | -0.912808 | -1.836135 |
| H | -0.775767 | 1.096242 | 2.801236 |
| O | 1.582704 | -3.298436 | -0.122290 |
| C | -2.505344 | 2.398013 | 2.214588 |
| C | 0.215291 | -3.693298 | -0.048281 |
| H | -3.099404 | 2.427242 | 3.122791 |

| | | | |
|---|---|---|---|
| O | 3.608134 | -2.264884 | 0.624855 |
| C | -0.860428 | 1.850798 | 0.696647 |
| C | 4.438804 | -1.500700 | 1.490247 |
| H | 0.029341 | 1.426874 | 0.241269 |
| C | -2.828850 | 3.047227 | 0.985141 |
| H | -3.727353 | 3.626778 | 0.792708 |
| H | -1.799229 | 3.006562 | -1.007066 |
| H | -0.216238 | -3.526707 | 0.950840 |
| H | 5.388182 | -2.042461 | 1.576981 |
| C | -1.841612 | 2.688457 | 0.030555 |
| H | 4.005246 | -1.389332 | 2.496580 |
| H | 4.641842 | -0.498181 | 1.083197 |

**$TS_{WX}$**

| | | | |
|---|---|---|---|
| Fe | -1.423055 | 1.084219 | 0.229018 |
| I | -2.986373 | -0.342413 | -1.184197 |
| H | 2.528791 | -2.414584 | -3.045531 |
| H | 1.756202 | -3.684917 | -2.055197 |
| H | 3.164446 | -2.787907 | -1.413253 |
| C | -0.529959 | 1.690021 | -1.132103 |
| P | 1.174910 | -1.387969 | 0.076247 |
| O | 0.065427 | 2.154085 | -2.022228 |
| H | -0.210480 | -4.240906 | 1.623124 |
| O | 1.363594 | -1.705390 | -1.530112 |
| H | -0.494340 | -3.953776 | -0.116994 |
| C | -0.980056 | 0.962219 | 2.373575 |
| C | 2.257510 | -2.708724 | -2.025042 |
| H | -0.331969 | 0.201577 | 2.797257 |
| O | 1.048700 | -2.874595 | 0.802454 |
| C | -2.383873 | 0.853994 | 2.185220 |
| C | -0.243930 | -3.474164 | 0.840187 |
| H | -3.003695 | 0.006677 | 2.461760 |
| O | 2.736038 | -1.211605 | 0.635121 |
| C | -0.558427 | 2.190562 | 1.789093 |
| C | 3.369415 | 0.034970 | 0.375005 |
| H | 0.454828 | 2.580034 | 1.764171 |
| C | -2.855315 | 2.065593 | 1.578955 |
| H | -3.881075 | 2.262674 | 1.283009 |
| H | -1.750002 | 3.868639 | 0.848899 |
| H | -1.035322 | -2.750571 | 1.081830 |
| H | 4.326541 | 0.015166 | 0.909202 |
| C | -1.739062 | 2.890136 | 1.319177 |
| H | 2.780312 | 0.888154 | 0.745281 |
| H | 3.565922 | 0.184204 | -0.697028 |

**X**

| | | | |
|---|---|---|---|
| Fe | -0.840020 | 0.644457 | 0.190227 |
| I | -2.646843 | -0.505559 | -1.408806 |
| H | 2.547518 | -2.204498 | -2.667041 |
| H | 1.405399 | -3.404580 | -1.999942 |
| H | 2.695539 | -2.724708 | -0.958931 |
| C | -0.117381 | 1.424880 | -1.165193 |
| P | 0.765641 | -0.993163 | 0.084883 |
| O | 0.364597 | 2.010622 | -2.055718 |
| H | -0.516053 | -3.930149 | 1.623306 |
| O | 1.104418 | -1.426644 | -1.452423 |
| H | -0.645881 | -3.677759 | -0.142974 |
| C | -0.582318 | 0.705315 | 2.411541 |
| C | 1.992619 | -2.506571 | -1.771567 |
| H | 0.084304 | 0.052748 | 2.966792 |
| O | 0.597969 | -2.385062 | 0.938974 |
| C | -1.964189 | 0.434870 | 2.110184 |
| C | -0.589209 | -3.176397 | 0.831658 |
| H | -2.514548 | -0.453627 | 2.403138 |
| O | 2.230228 | -0.691668 | 0.782614 |
| C | -0.248701 | 1.948292 | 1.835037 |
| C | 3.029423 | 0.382546 | 0.288648 |
| H | 0.711804 | 2.450865 | 1.879545 |
| C | -2.503246 | 1.550252 | 1.426887 |
| H | -3.509912 | 1.631220 | 1.031904 |
| H | -1.503973 | 3.397519 | 0.644197 |
| H | -1.497624 | -2.579573 | 0.971503 |
| H | 3.934746 | 0.391431 | 0.905332 |
| C | -1.430842 | 2.449930 | 1.170511 |
| H | 2.520718 | 1.349913 | 0.384329 |
| H | 3.311518 | 0.230494 | -0.761718 |

**$CP_{XY}$**

| | | | |
|---|---|---|---|
| Fe | -1.1574 | 0.9597 | 0.0744 |
| I | -2.9615 | -0.1513 | -1.4416 |
| H | 2.3197 | -2.3524 | -2.7459 |
| H | 1.5559 | -3.3829 | -1.5045 |
| H | 2.8779 | -2.2753 | -1.0470 |
| C | -0.4325 | 1.7534 | -1.2823 |
| P | 0.6294 | -0.8103 | -0.0159 |
| O | 0.0450 | 2.3316 | -2.1812 |
| H | -0.7037 | -3.7256 | 1.5143 |
| O | 1.0403 | -1.3539 | -1.5109 |
| H | -0.7655 | -3.4372 | -0.2503 |
| C | -0.7847 | 0.8125 | 2.3179 |
| C | 2.0046 | -2.4012 | -1.6978 |
| H | -0.1378 | 0.0553 | 2.7459 |
| O | 0.4244 | -2.1576 | 0.9110 |
| C | -2.1914 | 0.6768 | 2.0717 |
| C | -0.7501 | -2.9559 | 0.7362 |
| H | -2.7957 | -0.1918 | 2.3119 |
| O | 2.0705 | -0.4644 | 0.7204 |
| C | -0.3873 | 2.0654 | 1.8053 |
| C | 2.8436 | 0.6182 | 0.2019 |
| H | 0.6066 | 2.4979 | 1.8424 |
| C | -2.6825 | 1.8994 | 1.5352 |
| H | -3.6976 | 2.0826 | 1.1978 |
| H | -1.5944 | 3.7256 | 0.8537 |
| H | -1.6718 | -2.3727 | 0.8516 |
| H | 3.6976 | 0.7308 | 0.8790 |
| C | -1.5709 | 2.7332 | 1.2942 |
| H | 2.2806 | 1.5600 | 0.1773 |
| H | 3.2099 | 0.4052 | -0.8114 |

**Y**

| | | | |
|---|---|---|---|
| Fe | -0.793193 | 0.787507 | 0.324356 |
| I | -2.530029 | -0.147915 | -1.398602 |
| H | 2.246912 | -1.971358 | -2.764989 |
| H | 1.142677 | -3.171645 | -2.038718 |
| H | 2.485588 | -2.491276 | -1.067470 |
| C | -0.079840 | 1.657872 | -0.974281 |
| P | 0.556109 | -0.825708 | 0.083828 |
| O | 0.407062 | 2.317895 | -1.807488 |
| H | -0.909400 | -3.717554 | 1.520129 |
| O | 0.877626 | -1.189770 | -1.477152 |
| H | -0.863704 | -3.550453 | -0.260336 |
| C | -0.311731 | 0.935153 | 2.311597 |
| C | 1.739864 | -2.272403 | -1.841044 |
| H | 0.544899 | 0.472115 | 2.791631 |
| O | 0.325651 | -2.251675 | 0.863939 |
| C | -1.625340 | 0.368398 | 2.204631 |
| C | -0.877654 | -3.001994 | 0.690500 |
| H | -1.940193 | -0.597394 | 2.582495 |
| O | 2.059246 | -0.673138 | 0.762067 |
| C | -0.334168 | 2.226289 | 1.698371 |
| C | 2.887380 | 0.414242 | 0.362856 |
| H | 0.501999 | 2.915418 | 1.626835 |
| C | -2.444649 | 1.313321 | 1.518708 |
| H | -3.479569 | 1.161261 | 1.232096 |
| H | -2.007836 | 3.338805 | 0.669644 |
| H | -1.768907 | -2.364592 | 0.710704 |
| H | 3.828390 | 0.296854 | 0.912125 |
| C | -1.665314 | 2.462126 | 1.210121 |
| H | 2.440111 | 1.383212 | 0.620508 |
| H | 3.097112 | 0.396705 | -0.715359 |

**A**

| | | | |
|---|---|---|---|
| Fe | -1.147819 | 1.151331 | -0.299146 |
| I | -3.423506 | 0.330197 | -1.256665 |
| H | 3.704416 | -4.756311 | 2.263850 |
| H | 2.072892 | -4.191076 | 1.796848 |
| H | 3.399633 | -3.012139 | 2.005772 |
| C | -1.309049 | 2.663464 | -1.141729 |
| C | -0.418710 | 0.437424 | -1.671644 |
| P | 3.024120 | -3.255896 | -0.929649 |
| O | -1.363666 | 3.687589 | -1.691203 |
| O | 0.119230 | -0.025000 | -2.595790 |
| H | -0.455590 | -3.479464 | -1.407297 |
| O | 3.540031 | -4.230560 | 0.304550 |
| H | 0.451345 | -4.943088 | -0.926167 |
| C | 0.287898 | 0.302340 | 0.886279 |
| C | 3.150145 | -4.025271 | 1.664206 |
| H | 1.108857 | -0.284914 | 0.485510 |
| O | 1.391392 | -3.092120 | -0.642410 |
| C | -0.985630 | -0.212818 | 1.270603 |
| C | 0.534046 | -3.950275 | -1.393367 |
| H | -1.294756 | -1.250982 | 1.216712 |
| O | 3.336096 | -1.716294 | -0.353187 |
| C | 0.272927 | 1.725235 | 1.049670 |
| C | 4.616293 | -1.185539 | -0.681417 |
| H | 1.094811 | 2.400942 | 0.832350 |

| | | | |
|---|---|---|---|
| C | -1.753493 | 0.875251 | 1.835084 |
| C | -3.034769 | 0.927097 | 2.440470 |
| H | -3.632522 | 0.022845 | 2.534369 |
| C | -3.492817 | 2.140529 | 2.914504 |
| H | -4.468565 | 2.194259 | 3.396879 |
| C | -2.722930 | 3.328662 | 2.785351 |
| H | -3.124385 | 4.264170 | 3.174432 |
| C | -1.481180 | 3.318699 | 2.181133 |
| H | -0.889139 | 4.228923 | 2.092996 |
| H | 0.876671 | -4.075647 | -2.431401 |
| H | 5.406560 | -1.595201 | -0.034207 |
| C | -0.970207 | 2.081917 | 1.704203 |
| H | 4.561343 | -0.101510 | -0.525486 |
| H | 4.888219 | -1.374768 | -1.731306 |

**$TS_{AB}$**

| | | | |
|---|---|---|---|
| Fe | -0.127258 | 0.238305 | -0.205850 |
| I | -1.753584 | -1.448986 | -1.329943 |
| H | 3.807318 | -3.744438 | -2.143708 |
| H | 2.467272 | -4.831564 | -1.682285 |
| H | 3.561744 | -4.177742 | -0.423164 |
| C | -0.947114 | 1.333739 | -1.215417 |
| C | 1.166664 | 0.486523 | -1.279509 |
| P | 1.764424 | -2.131514 | 0.143441 |
| O | -1.440830 | 2.117851 | -1.922880 |
| O | 2.034922 | 0.699170 | -2.035344 |
| H | 0.187826 | -4.875774 | 1.788738 |
| O | 2.192155 | -2.820123 | -1.282413 |
| H | 0.154359 | -4.628610 | 0.019230 |
| C | 0.394107 | 0.365893 | 1.839744 |
| C | 3.058435 | -3.960736 | -1.372443 |
| H | 1.277369 | -0.209899 | 2.093143 |
| O | 1.394425 | -3.377416 | 1.163101 |
| C | -0.943446 | -0.080529 | 1.895439 |
| C | 0.187475 | -4.122315 | 0.992917 |
| H | -1.272965 | -1.060416 | 2.224968 |
| O | 3.197249 | -1.889618 | 0.955226 |
| C | 0.385867 | 1.690961 | 1.296884 |
| C | 4.084310 | -0.871791 | 0.498047 |
| H | 1.267797 | 2.312681 | 1.161548 |
| C | -1.813071 | 1.085527 | 1.736782 |
| C | -3.195280 | 1.250661 | 1.868241 |
| H | -3.841120 | 0.401432 | 2.087946 |
| C | -3.728605 | 2.537078 | 1.726347 |
| H | -4.801398 | 2.687793 | 1.847001 |
| C | -2.907121 | 3.638546 | 1.438685 |
| H | -3.351439 | 4.628971 | 1.342277 |
| C | -1.526004 | 3.481782 | 1.268911 |
| H | -0.894652 | 4.336812 | 1.027283 |
| H | -0.702846 | -3.490524 | 1.089018 |
| H | 4.976719 | -0.941238 | 1.130257 |
| C | -0.977500 | 2.206734 | 1.425625 |
| H | 3.652926 | 0.132630 | 0.608047 |
| H | 4.378068 | -1.017856 | -0.550187 |

**A’**

| | | | |
|---|---|---|---|
| Fe | -2.049234 | 1.883225 | 0.513632 |
| I | -4.614252 | 1.745002 | 0.096033 |
| H | 3.208920 | -4.017909 | 1.894520 |
| H | 1.581009 | -3.298409 | 1.715616 |
| H | 3.024869 | -2.245492 | 1.740456 |
| C | -2.048579 | 3.445100 | -0.231572 |
| C | -1.809348 | 1.071560 | -0.996869 |
| P | 2.042664 | -2.421064 | -1.108536 |
| O | -1.991749 | 4.502801 | -0.714436 |
| O | -1.604902 | 0.530729 | -2.006395 |
| H | -1.444812 | -2.819019 | -1.070945 |
| O | 2.786949 | -3.393974 | 0.004123 |
| H | -0.426329 | -4.228140 | -0.652801 |
| C | -0.419970 | 0.961022 | 1.356138 |
| C | 2.633719 | -3.218219 | 1.414188 |
| H | 0.375103 | 0.481227 | 0.793639 |
| O | 0.469623 | -2.337310 | -0.565307 |
| C | -1.614785 | 0.321138 | 1.831733 |
| C | -0.443391 | -3.254523 | -1.165088 |
| H | -1.886604 | -0.717939 | 1.680131 |
| O | 2.375114 | -0.877710 | -0.555048 |
| C | -0.474196 | 2.334790 | 1.742128 |
| C | 3.559346 | -0.281170 | -1.075718 |
| H | 0.278643 | 3.086882 | 1.524496 |
| C | -2.392859 | 1.305196 | 2.510087 |
| H | -3.377729 | 1.148031 | 2.936977 |
| H | -2.049973 | 3.488720 | 2.877869 |
| H | -0.231710 | -3.414817 | -2.233037 |
| H | 4.460771 | -0.651722 | -0.564643 |
| C | -1.700293 | 2.547541 | 2.465766 |
| H | 3.475716 | 0.798393 | -0.902633 |
| H | 3.671767 | -0.454438 | -2.157005 |

**$TS_{A'B'}$**

| | | | |
|---|---|---|---|
| Fe | -0.917654 | 0.932906 | -0.179573 |
| I | -2.483551 | -0.763810 | -1.386133 |
| H | 2.810479 | -2.927699 | -2.112114 |
| H | 1.533511 | -4.008318 | -1.485591 |
| H | 2.686750 | -3.235895 | -0.351761 |
| C | -1.815322 | 2.052916 | -1.093157 |
| C | 0.315255 | 1.205352 | -1.315083 |
| P | 0.792194 | -1.260066 | 0.186413 |
| O | -2.357566 | 2.849681 | -1.749429 |
| O | 1.132197 | 1.441878 | -2.118622 |
| H | -0.650013 | -4.105075 | 1.781147 |
| O | 1.234896 | -1.974350 | -1.220563 |
| H | -0.806980 | -3.707203 | 0.044542 |
| C | -0.413333 | 1.085290 | 1.934833 |
| C | 2.118743 | -3.103355 | -1.279956 |
| H | 0.466811 | 0.522427 | 2.223447 |
| O | 0.417801 | -2.478477 | 1.232846 |
| C | -1.751997 | 0.653213 | 1.984528 |
| C | -0.745694 | -3.288228 | 1.056493 |
| H | -2.101948 | -0.316823 | 2.321830 |
| O | 2.220834 | -0.998976 | 0.997048 |
| C | -0.428394 | 2.416026 | 1.406150 |
| C | 3.104078 | 0.019401 | 0.532484 |
| H | 0.447208 | 3.047017 | 1.271450 |
| C | -2.605404 | 1.807283 | 1.729453 |
| H | -3.691796 | 1.784584 | 1.721888 |
| H | -2.127924 | 3.886899 | 1.148032 |
| H | -1.664827 | -2.727114 | 1.259162 |
| H | 3.994552 | -0.039748 | 1.168332 |
| C | -1.800405 | 2.895586 | 1.446928 |
| H | 2.665590 | 1.021425 | 0.632679 |
| H | 3.401411 | -0.136248 | -0.513204 |