

Electronic Supplementary Information

“C–H \cdots π Interaction” Regulates Stereoselectivity in Olefin Polymerization

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COMPUTATIONAL DETAILS

All calculations were performed with the Gaussian 09 program.^{S1} The B3PW91 hybrid exchange-correlation functional was utilized for geometry optimization.^{S2-S4} Each optimized structure was subsequently analyzed by harmonic vibration frequencies for characterization of a minimum ($N_{\text{imag}} = 0$) or a transition state ($N_{\text{imag}} = 1$) and providing thermodynamic data. The transition state structures are shown to connect the reactant and product on either side via intrinsic reaction coordinate (IRC) following. The 6-31G* basis set was considered for C, H, O, N, F, and Cl atoms. The Sc and Si atoms were treated by the Stuttgart/Dresden effective core potential (ECP) and the associated basis sets.^{S5,S6} The basis sets of Si was augmented with one *d*-polarization function (exponent of 0.284). This basis set is denoted as “BSI”. Such a computational strategy has been widely used for the study of transition-metal containing systems.^{S7-S10} To obtain more reliable relative energies, the single-point calculations of optimized structures were carried out at the level of M06^{S11}/BSII, taking into account solvation effect of chlorobenzene with the SMD^{S12} solvation model. In the BSII, the 6-311+G(d,p) basis set was used for nonmetal atoms, while the basis sets together with associated pseudopotentials for Sc atoms are the same as that in geometry optimization. Therefore, unless otherwise mentioned, the free energy (ΔG , 298.15 K, 1 atm) in solution, which was used for description of energy profiles, was obtained from the solvation single-point calculation and the gas-phase Gibbs free energy correction. The 3D molecular structures displayed in this paper were drawn by using CYLview.^{S13}

In energy decomposition analysis (EDA), the energies of two fragments, viz., the monomer moiety (A) and the remaining metal complex (B), in the TS geometries were evaluated via single-point calculations. Such single-point energies of the fragments and the energy of TS were used to estimate the interaction energy ΔE_{int} . These energies, together with the energies of the respective fragments in their optimal geometry, allow for the estimation of the deformation energies of the two fragments, $\Delta E_{\text{def}}(\text{A})$ and $\Delta E_{\text{def}}(\text{B})$. As the energy of the TS, ΔE_{TS} , is evaluated with respect to the energy of the two separated fragments, the relation $\Delta E_{\text{TS}} = \Delta E_{\text{int}} + \Delta E_{\text{def}}(\text{A}) + \Delta E_{\text{def}}(\text{B})$ holds.

References

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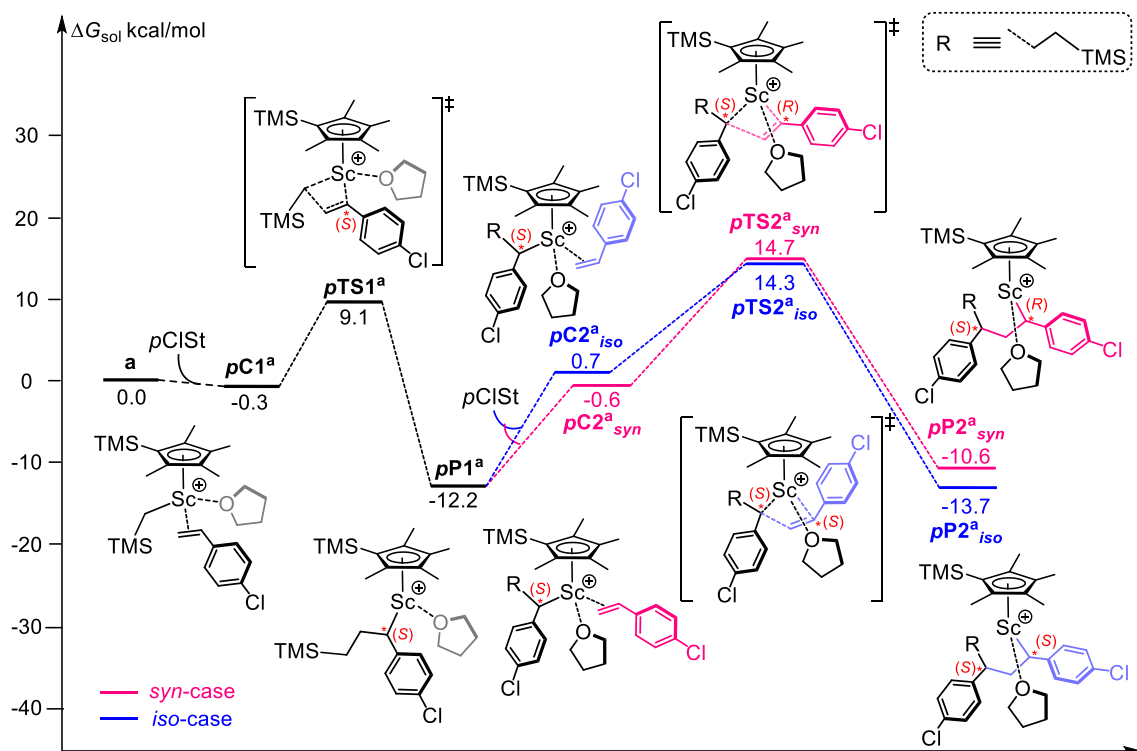


Fig. S1 Computed energy profiles (kcal mol^{-1}) for **a** mediated C=C insertion of the first and second *pClSt*. The syndiotactic pathway is in pink and the isospecific one is in blue.

As shown in Fig. S1, the chain initiation starts with the formation of a π -complex *pC1^a*, which surmounts an energy barrier of $9.4 \text{ kcal mol}^{-1}$ via the transition state (TS) *pTS1^a* to result in a more stable *pP1^a* complex.

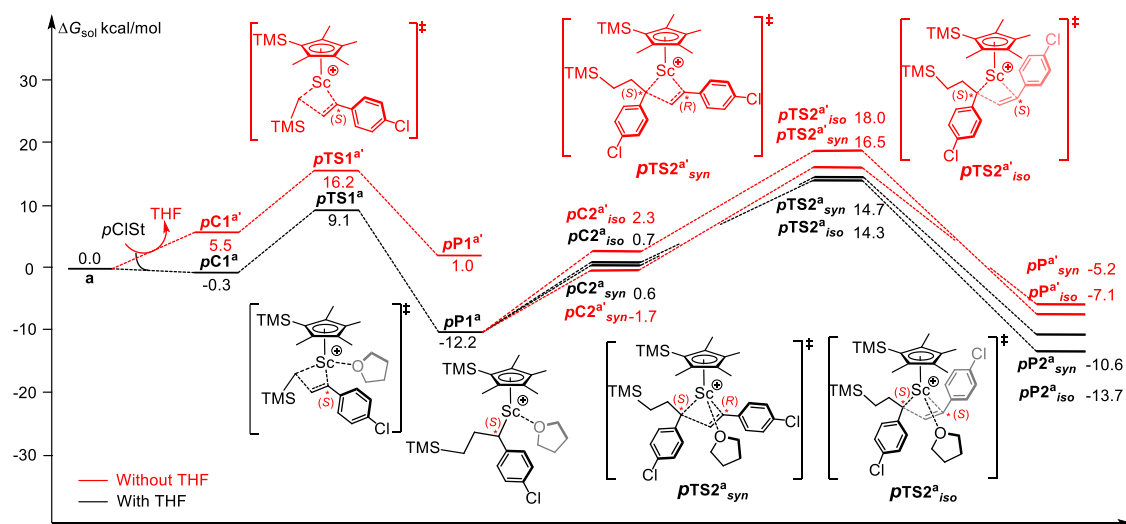


Fig. S2 Calculated energy profiles for olefin insertion into Sc species with THF (black curve) and without THF (red curve) of the first and second molecule of *pClSt*. The pathway with the superscript of **a'** represents the THF-free case.

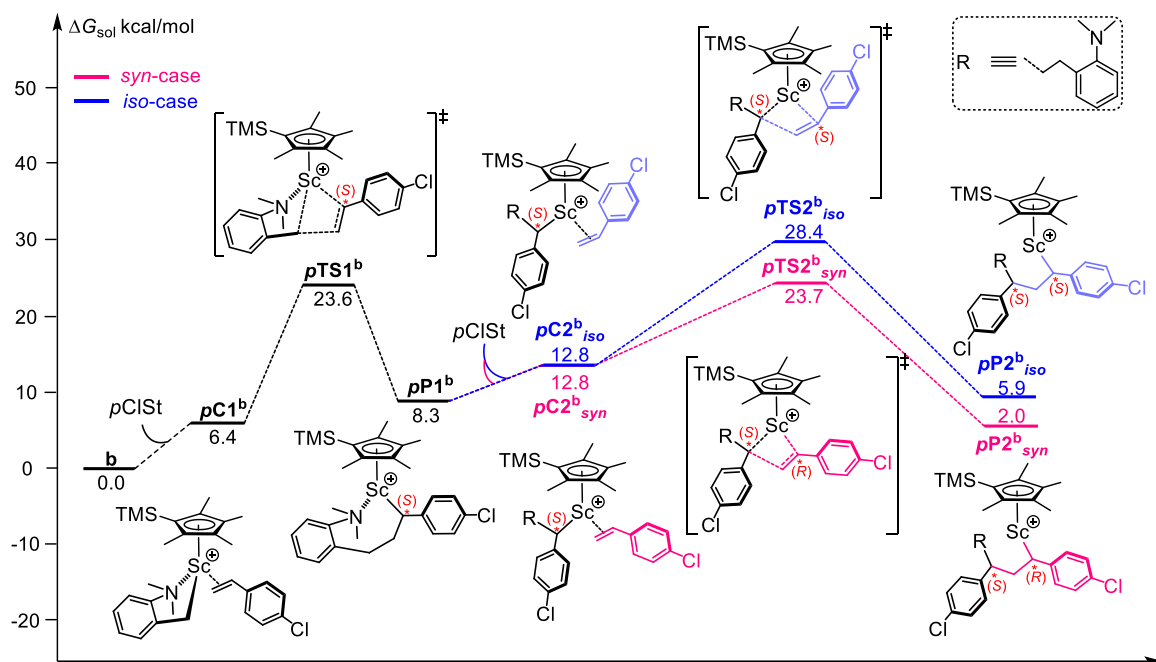


Fig. S3 Computed energy profiles (kcal mol^{-1}) for **b** mediated C=C insertion of the first and second *pClSt*. The syndiotactic pathway is in pink while the isospecific one is in blue.

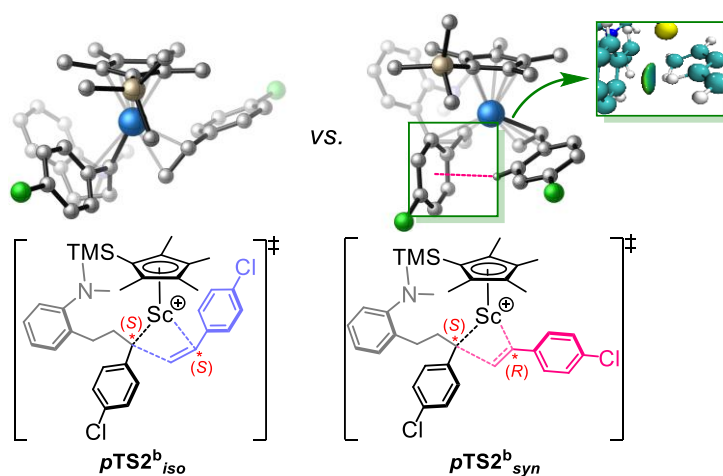


Fig. S4 Interaction analyses for $pTS2^b_{iso}$ and $pTS2^b_{syn}$. The green cloud represents the existence of weak interaction.

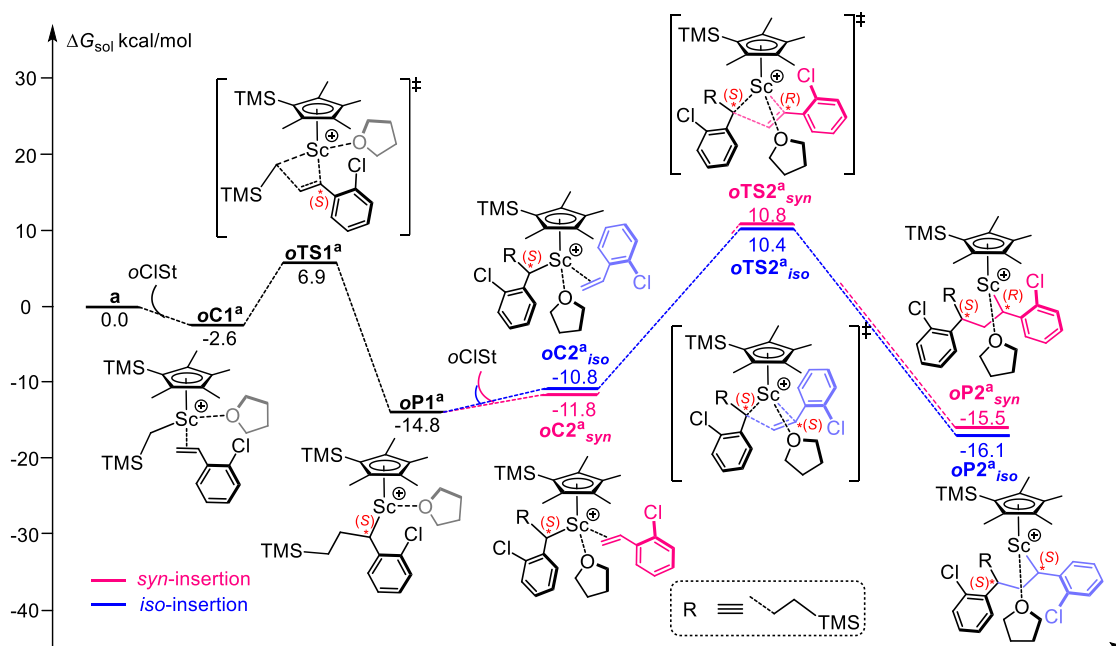


Fig. S5 Computed energy profiles (kcal mol^{-1}) for **a** mediated C=C insertion of the first and second molecules of *o*ClSt. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

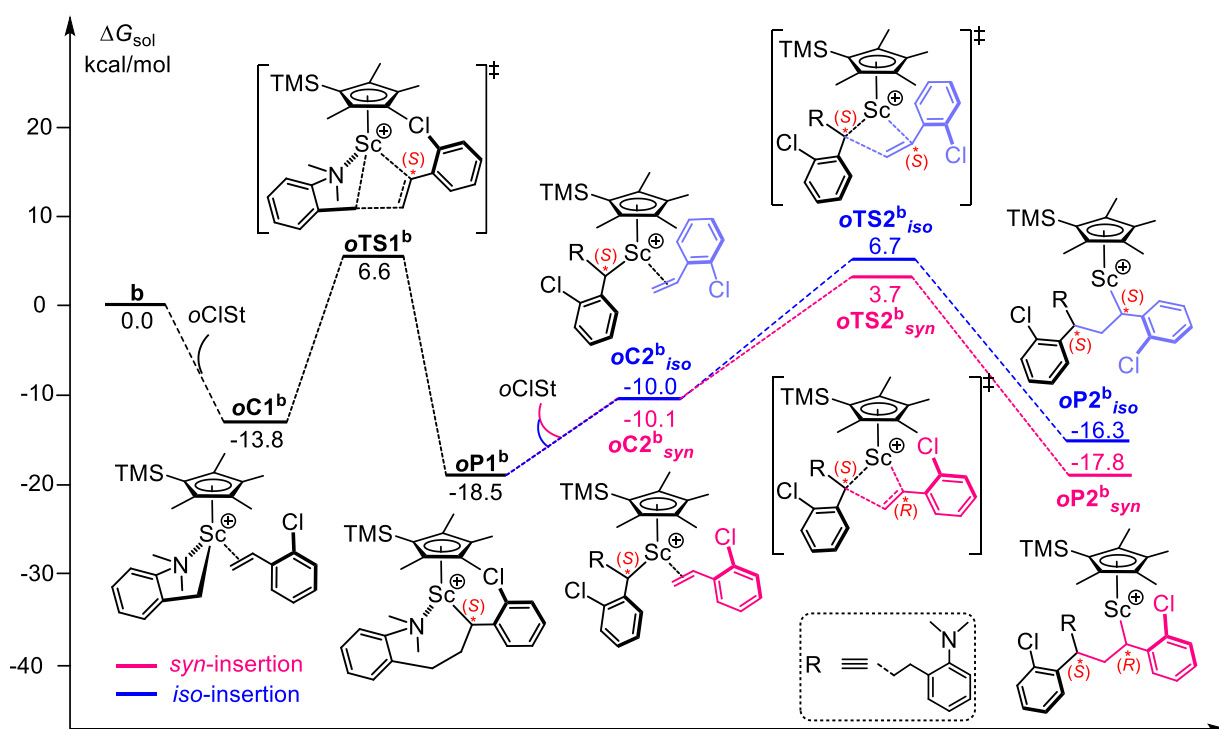


Fig. S6 Computed energy profiles (kcal mol^{-1}) for **b** mediated C=C insertion of the first and second molecules of *o*ClSt. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

The computational results also show that *iso* and *syndio*-enchainment are kinetically competitive

in **a** system ($\Delta G^\ddagger = 25.2$ vs. 25.6 kcal mol⁻¹, Fig. S5). However, in the **b** mediated polymerization of *o*ClSt, the *syndio*-fashion is more favorable than the *iso*-fashion by 3.0 kcal mol⁻¹ ($\Delta G^\ddagger = 22.2$ vs. 25.2 kcal mol⁻¹, Fig. S6). These results are in good agreement with the experimentally observed various stereoselectivities (ref. 10).

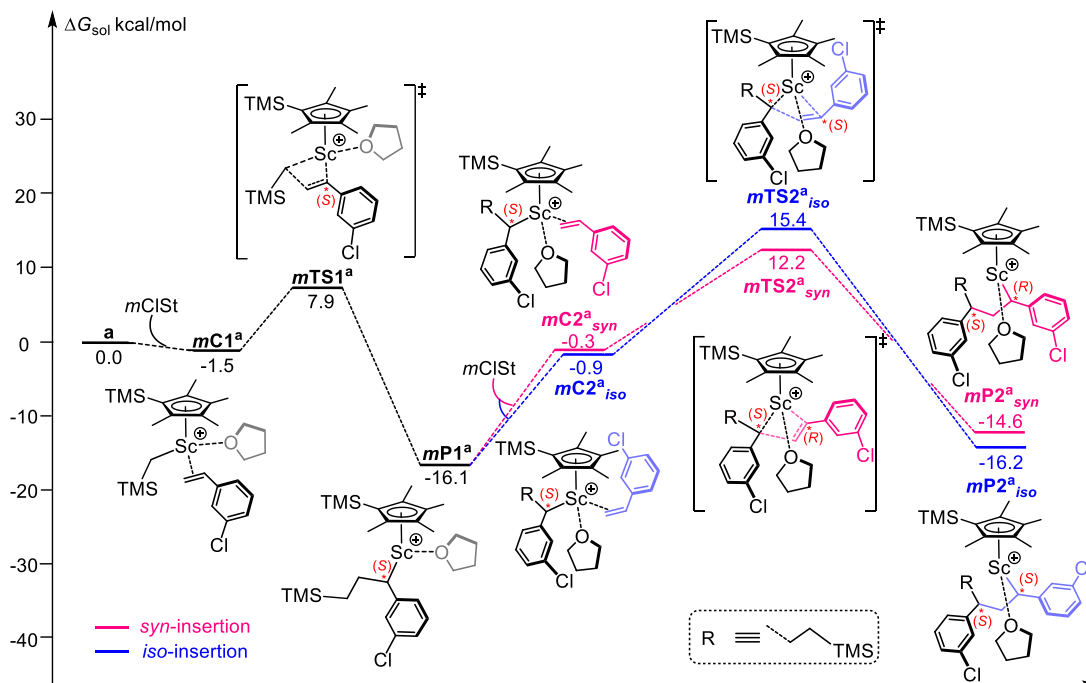


Fig. S7 Computed energy profiles (kcal mol⁻¹) for **a** mediated C=C insertion of the first and second molecules of *m*ClSt. The syndiotactic polymerization pathway is in pink and the isotactic one is in blue.

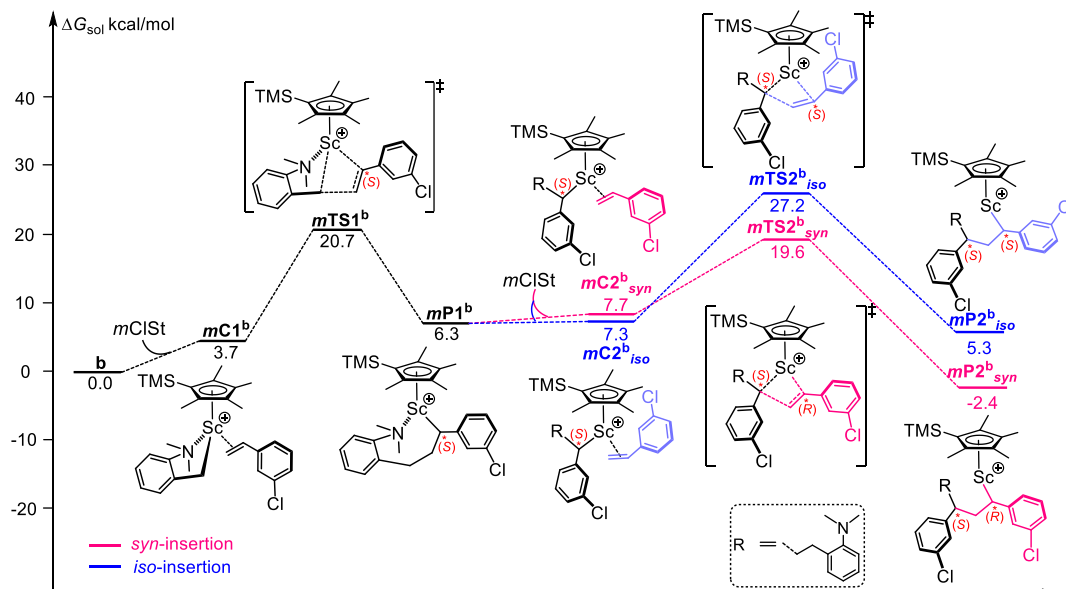


Fig. S8 Computed energy profiles (kcal mol⁻¹) for **b** mediated C=C insertion of the first and second molecules of *m*ClSt. The syndiotactic polymerization pathway is in pink and the isotactic one is in blue.

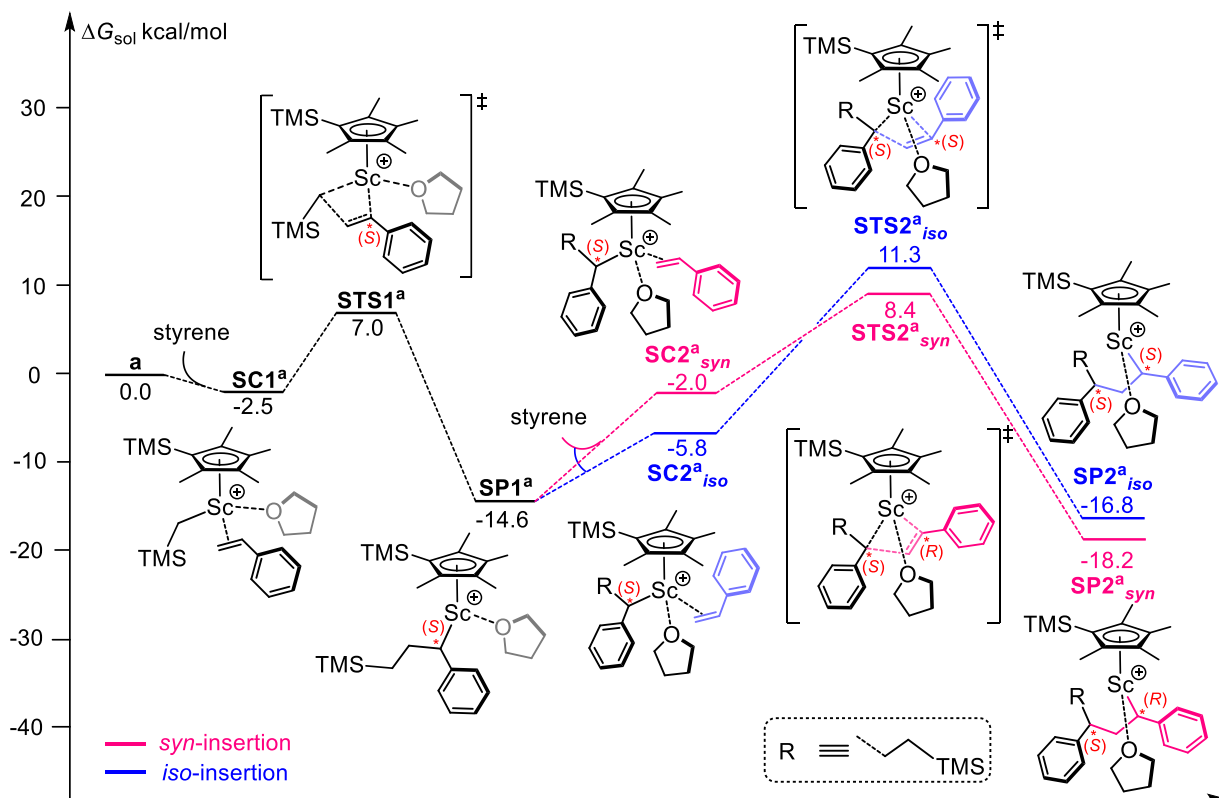


Fig. S9 Computed energy profiles (kcal mol^{-1}) for **a** mediated C=C insertion of the first and second molecules of styrene by cationic species. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

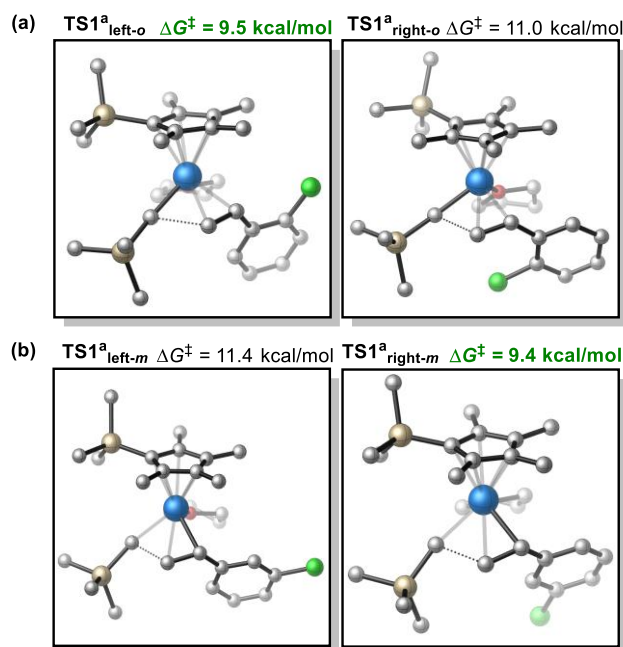


Fig. S10 (a) Transition states for the first insertion of isomer of *o*-ClSt in **a**-catalyzed systems. (b) Transition states for the first insertion of isomers of *m*-ClSt in **a**-catalyzed systems. Energies are given in kcal mol^{-1} .

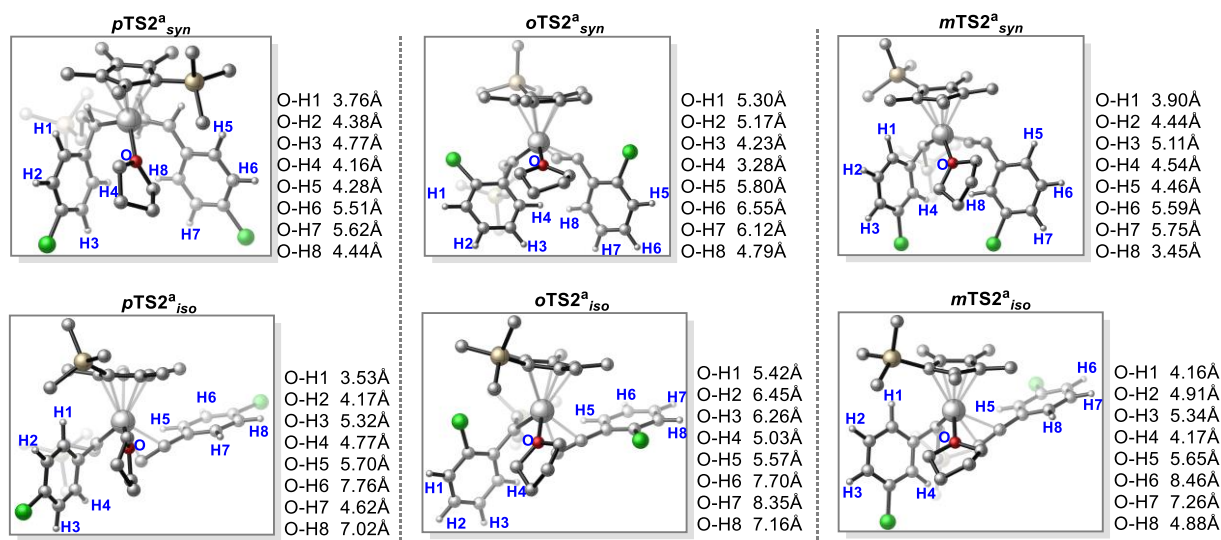


Fig. S11 Geometric structures of $pTS2^a_{syn}$, $pTS2^a_{iso}$, $oTS2^a_{syn}$, $oTS2^a_{iso}$, $mTS2^a_{syn}$, and $mTS2^a_{iso}$.

The results suggest that the related distances of $d_{(H\cdots O)}$ are too long to have noncovalent interactions ($d_{(H\cdots O)} > 3.2 \text{ \AA}$, being longer than the sum of the Van der Waals radius of the O and H atoms (2.70 \AA , see <https://www.webelements.com/>)) in all transition states. Besides, the NCI analysis also shows that there is no C–H \cdots O noncovalent interactions between the O atom of the THF and H atoms of the phenyl ring of monomer units. Therefore, it is the C–H \cdots π interactions that are the source of the stereoselectivity in these systems.

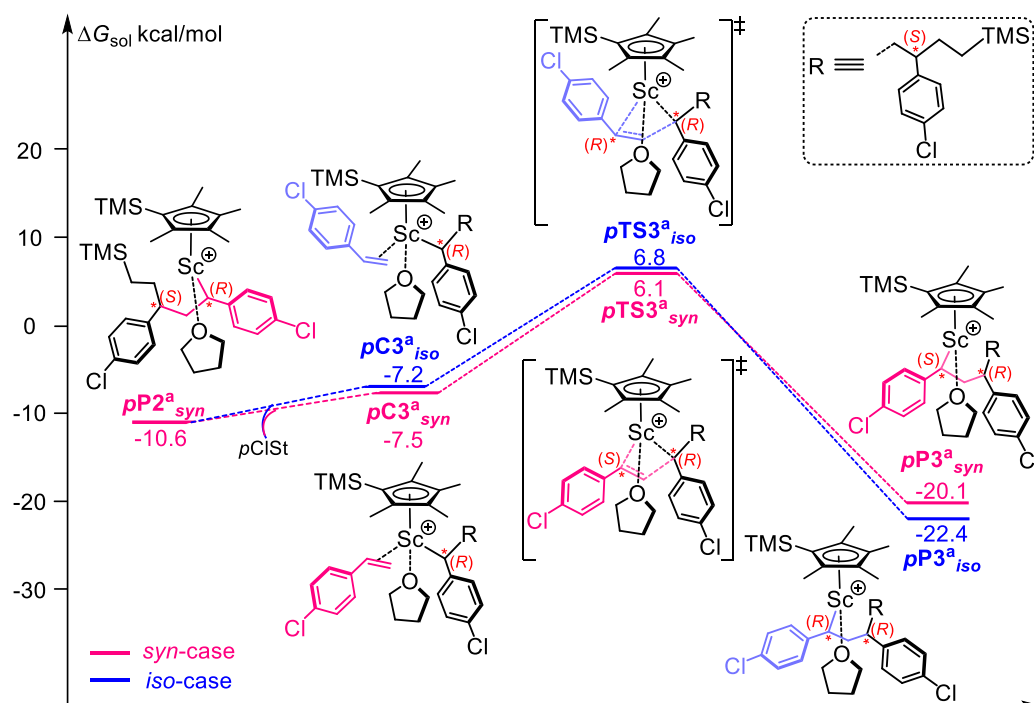


Fig. S12 Computed energy profiles (kcal mol^{-1}) for a mediated C=C insertion of the third molecules of $pClSt$ based on $pP2^a_{syn}$. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

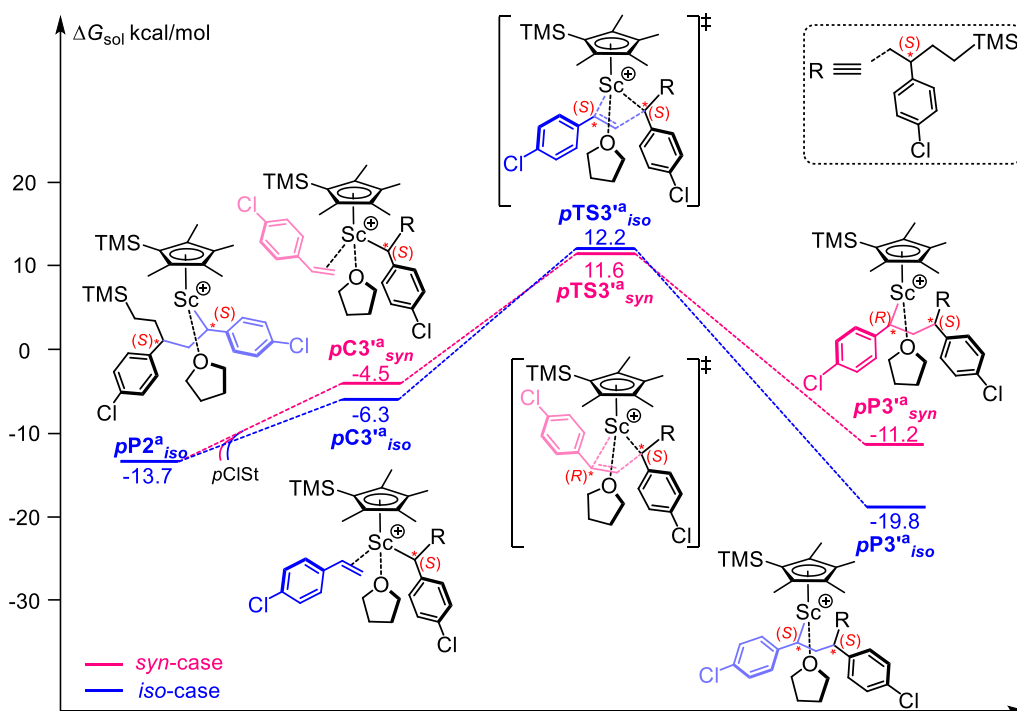


Fig. S13 Computed energy profiles (kcal mol⁻¹) for a mediated C=C insertion of the third molecule of *pClSt* based on *pP2*^a_{iso}. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

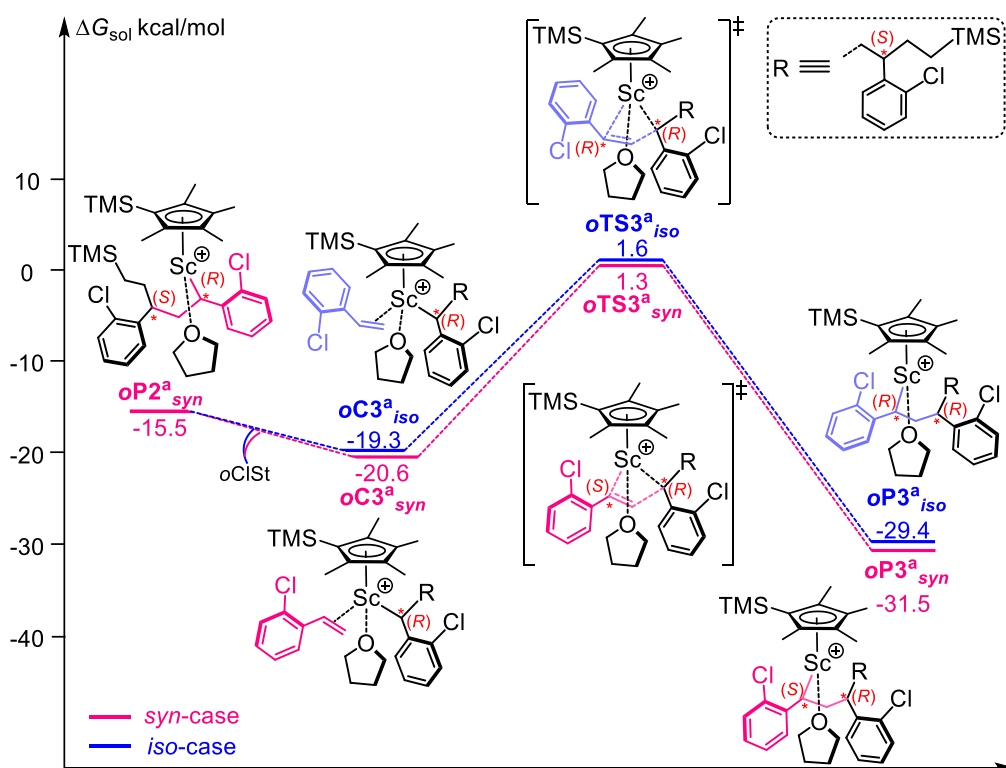


Fig. S14 Computed energy profiles (kcal mol⁻¹) for a mediated C=C insertion of the third molecule of *oClSt* based on *oP2*^a_{syn}. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

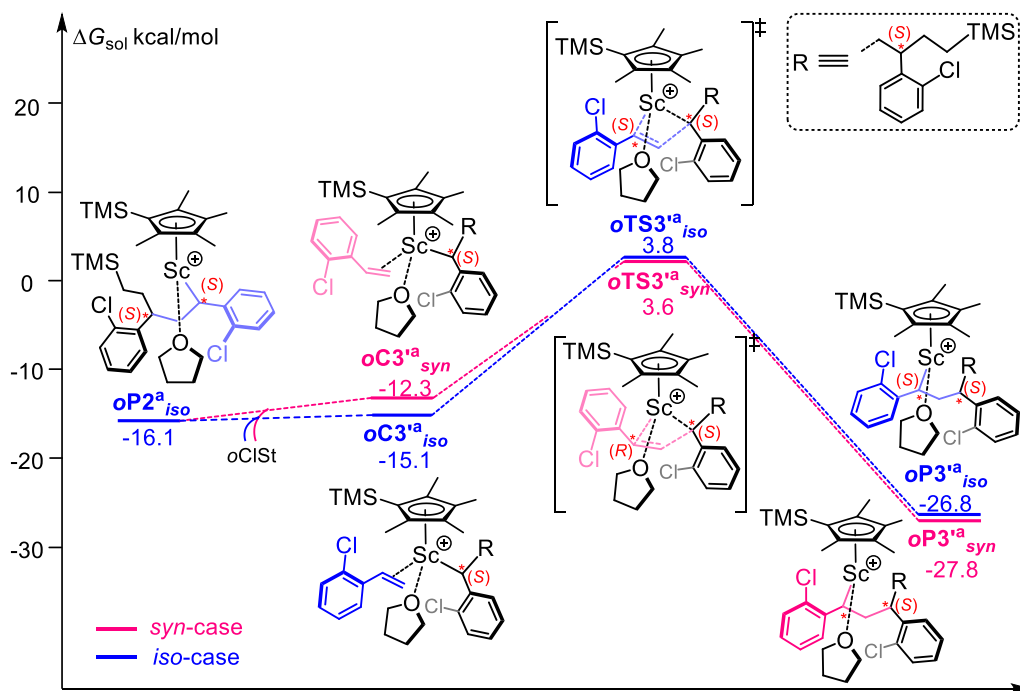


Fig. S15 Computed energy profiles (kcal mol⁻¹) for a mediated C=C insertion of the third molecule of *oClSt* based on *oP2^a_{iso}*. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

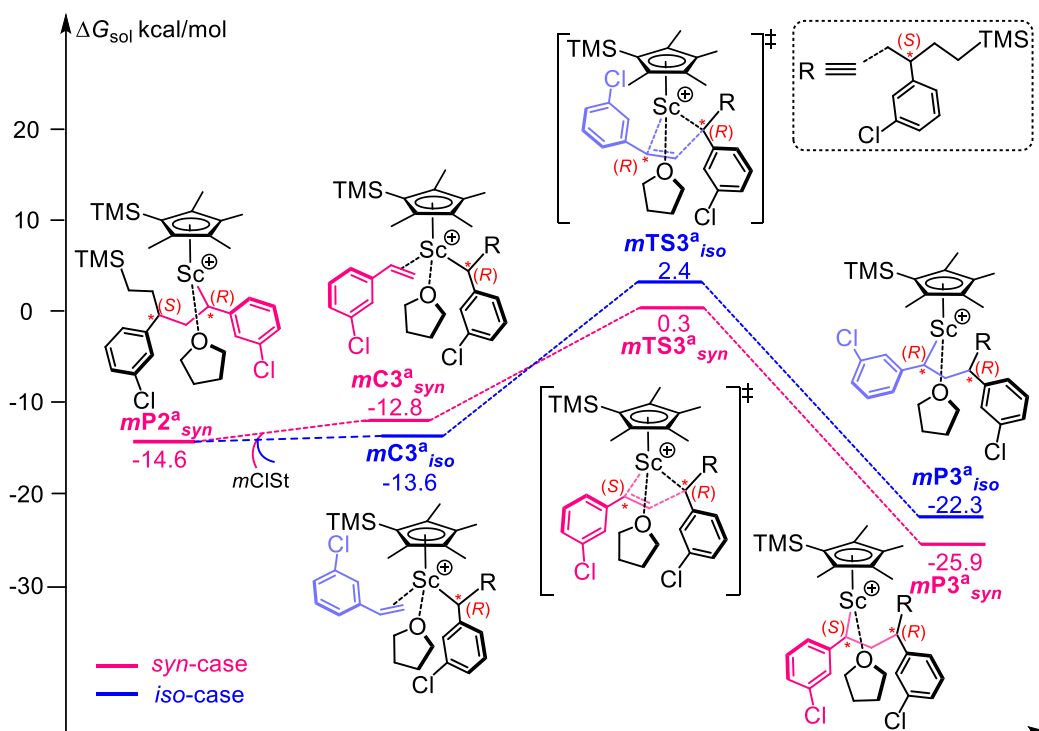


Fig. S16 Computed energy profiles (kcal mol⁻¹) for a mediated C=C insertion of the third molecule of *mClSt* based on *mP2^a_{syn}*. The syndiotactic polymerization pathway is in pink and the isospecific one is in blue.

Cartesian coordinates and single-point energies ($E_{(\text{SCF Done})}$, a.u.) obtained at the level of M06(SMD, chlorobenzene)/6-311+G(d,p)-SDD//B3PW91/6-31G(d)-SDD for all of the stationary points as well as the imaginary frequency (IF, cm^{-1}) of transition states.

THF, $E_{(\text{SCF Done})} = -232.3554321$ a.u.

C	1.155790000	-0.433519000	0.138716000
O	-0.003870000	-1.246317000	-0.009010000
C	-1.161887000	-0.424994000	-0.127361000
C	-0.724716000	0.997247000	0.226785000
C	0.735184000	0.988290000	-0.231929000
H	1.509795000	-0.479480000	1.181238000
H	1.948960000	-0.832816000	-0.504522000
H	-1.541885000	-0.475731000	-1.159935000
H	-1.942159000	-0.814053000	0.538077000
H	-1.334056000	1.764065000	-0.261751000
H	-0.781092000	1.157313000	1.310499000
H	0.794021000	1.134271000	-1.317499000
H	1.351162000	1.754826000	0.248707000

a, $E_{(\text{SCF Done})} = -1486.73266$ a.u.

Sc	0.292665000	-0.284660000	-0.123600000
Si	-3.392395000	0.707935000	-0.433727000
Si	1.750527000	3.023138000	0.112079000
O	2.299292000	-1.245732000	-0.326300000
C	-1.577815000	-0.811857000	1.394523000
C	-0.830815000	-2.019362000	1.378022000
C	-0.860553000	-2.543423000	0.054535000
C	-1.622140000	-1.660235000	-0.758704000
C	-2.089349000	-0.572256000	0.068881000
C	-1.868828000	-0.020062000	2.640206000
H	-1.758996000	1.057412000	2.491314000
H	-1.194461000	-0.306178000	3.454044000
H	-2.894676000	-0.196943000	2.996192000
C	-0.195887000	-2.661038000	2.580133000
H	-0.950750000	-3.119581000	3.233952000
H	0.359599000	-1.938840000	3.192056000
H	0.499578000	-3.459952000	2.299802000
C	-0.243676000	-3.832581000	-0.409721000
H	0.544572000	-4.181361000	0.266976000
H	0.201519000	-3.739172000	-1.408297000
H	-0.988775000	-4.638190000	-0.468610000
C	-2.009581000	-1.945728000	-2.183996000

H	-1.300610000	-2.633210000	-2.658571000
H	-2.042245000	-1.040878000	-2.795775000
H	-3.001876000	-2.418874000	-2.244585000
C	-3.383637000	2.254931000	0.671689000
H	-3.721605000	2.041778000	1.690463000
H	-4.070569000	2.995881000	0.243850000
H	-2.390895000	2.714803000	0.726986000
C	-3.189958000	1.321990000	-2.225330000
H	-2.149212000	1.575259000	-2.456099000
H	-3.791651000	2.229673000	-2.359135000
H	-3.537866000	0.588771000	-2.959956000
C	-5.109941000	-0.099937000	-0.282704000
H	-5.189828000	-0.979667000	-0.931500000
H	-5.903143000	0.602784000	-0.566487000
H	-5.299215000	-0.427479000	0.746052000
C	0.690943000	1.814590000	-0.843604000
H	1.104786000	1.727696000	-1.867465000
H	-0.300230000	2.285511000	-0.971544000
C	1.939278000	4.718913000	-0.749764000
H	2.396555000	4.605989000	-1.740540000
H	2.564623000	5.407041000	-0.166685000
H	0.960222000	5.192623000	-0.891259000
C	3.522720000	2.341105000	0.346770000
H	3.510512000	1.415650000	0.936088000
H	4.162070000	3.061564000	0.871282000
H	3.994461000	2.125394000	-0.620690000
C	1.027191000	3.348780000	1.845437000
H	0.012013000	3.758413000	1.775134000
H	1.636005000	4.066309000	2.409357000
H	0.970811000	2.418975000	2.424982000
C	3.105154000	-1.853863000	0.715426000
H	2.491550000	-2.604875000	1.216934000
H	3.381316000	-1.073638000	1.433293000
C	4.321113000	-2.420124000	-0.004697000
H	4.106964000	-3.423322000	-0.391230000
H	5.192926000	-2.485039000	0.652595000
C	4.504518000	-1.426756000	-1.155169000
H	4.999283000	-0.515740000	-0.801169000
H	5.085347000	-1.833378000	-1.988037000
C	3.066406000	-1.127261000	-1.556170000
H	2.912423000	-0.120329000	-1.950205000
H	2.674468000	-1.861158000	-2.269017000

pCISt, $E_{(\text{SCF Done})} = -769.0748779$ a.u.

C	-1.364794000	-0.014528000	0.000005000
C	-0.785210000	1.250693000	-0.000061000
C	0.602259000	1.357812000	0.000012000
C	1.430503000	0.225132000	0.000123000
C	0.811155000	-1.036075000	0.000220000
C	-0.571680000	-1.162574000	0.000155000
H	-1.411094000	2.137324000	-0.000155000
H	1.054454000	2.347172000	-0.000039000
H	1.416167000	-1.938228000	0.000397000
H	-1.037484000	-2.142953000	0.000245000
C	2.887371000	0.408400000	0.000144000
C	3.829024000	-0.542828000	-0.000388000
H	3.211955000	1.449367000	0.000614000
H	4.883041000	-0.281583000	-0.000298000
H	3.598085000	-1.605120000	-0.000943000
Cl	-3.102758000	-0.169540000	-0.000064000

pC1^a, $E_{(\text{SCF Done})} = -2255.829318$ a.u.

Sc	0.768090000	0.009751000	0.301975000
Si	1.233247000	3.703022000	0.155797000
C	1.785184000	1.899480000	-0.066680000
C	1.009259000	4.111749000	1.998788000
C	-0.387304000	4.075068000	-0.781517000
C	2.557475000	4.872209000	-0.541057000
C	1.108450000	-1.144931000	3.710245000
C	1.485106000	-1.359836000	2.270976000
C	2.641341000	-0.820662000	1.638804000
C	2.743101000	-1.372793000	0.315099000
C	1.639591000	-2.290413000	0.172861000
C	0.871112000	-2.278392000	1.364109000
C	3.624688000	0.070710000	2.342044000
C	1.406081000	-3.249083000	-0.961067000
C	-0.278525000	-3.199683000	1.665102000
C	-1.066845000	1.024766000	1.787233000
C	-1.984078000	0.032817000	1.902582000
H	2.754902000	1.853241000	0.453495000
H	2.047847000	1.797696000	-1.139268000
H	0.175649000	3.577190000	2.467914000
H	0.820272000	5.184019000	2.126869000
H	1.920760000	3.873297000	2.560207000
H	-0.233312000	4.011398000	-1.865889000
H	-0.719939000	5.097580000	-0.567067000
H	-1.214697000	3.403515000	-0.518795000
H	3.510494000	4.744047000	-0.014725000

H	2.256108000	5.921141000	-0.434437000
H	2.736829000	4.682353000	-1.605916000
H	1.318934000	-0.126184000	4.052728000
H	1.685802000	-1.817033000	4.358834000
H	0.051771000	-1.350976000	3.908652000
H	3.134163000	0.750325000	3.046915000
H	4.208207000	0.676324000	1.648887000
H	4.333053000	-0.533388000	2.925036000
H	2.039407000	-4.137725000	-0.842989000
H	1.638765000	-2.819989000	-1.939800000
H	0.372395000	-3.608600000	-0.983237000
H	-1.056721000	-3.187949000	0.891823000
H	-0.753226000	-2.961711000	2.621501000
H	0.072525000	-4.236855000	1.740752000
H	-1.245334000	1.924862000	1.204355000
H	-0.214531000	1.050832000	2.469245000
H	-1.744979000	-0.795091000	2.568630000
C	-1.453903000	-1.162288000	-1.812705000
O	-0.381326000	-0.204647000	-1.538945000
C	-0.165457000	0.642945000	-2.725431000
C	-1.057023000	0.051304000	-3.807056000
C	-2.194376000	-0.580709000	-3.002167000
H	-0.991404000	-2.124820000	-2.047928000
H	-2.059873000	-1.248598000	-0.908798000
H	-0.454081000	1.659445000	-2.449654000
H	0.898175000	0.613440000	-2.965236000
H	-1.400938000	0.817855000	-4.506619000
H	-0.518786000	-0.712673000	-4.378795000
H	-2.912546000	0.178246000	-2.673293000
H	-2.737641000	-1.349362000	-3.558499000
C	-3.856330000	0.988098000	0.512568000
C	-3.289866000	-0.062405000	1.260483000
C	-4.037485000	-1.242510000	1.425504000
C	-5.294282000	-1.388138000	0.851602000
C	-5.825258000	-0.335601000	0.104740000
C	-5.111373000	0.857040000	-0.062166000
H	-3.325952000	1.929425000	0.399829000
H	-3.629813000	-2.057203000	2.019420000
H	-5.865283000	-2.300726000	0.987055000
H	-5.551554000	1.674628000	-0.623880000
Cl	-7.389050000	-0.498211000	-0.613149000
Si	4.190711000	-1.253471000	-0.940576000
C	5.541081000	-0.025361000	-0.440539000
H	6.021870000	-0.284586000	0.507720000

H	6.315551000	-0.054020000	-1.217185000
H	5.178941000	1.006534000	-0.381921000
C	4.980489000	-2.972361000	-1.065668000
H	4.307240000	-3.721388000	-1.494014000
H	5.868780000	-2.921637000	-1.706536000
H	5.300359000	-3.328558000	-0.080088000
C	3.579934000	-0.705905000	-2.658085000
H	2.754263000	-1.308299000	-3.051408000
H	3.273814000	0.346709000	-2.642730000
H	4.408184000	-0.789168000	-3.372260000

***p*TS1^a**, $E_{(\text{SCF Done})} = -2255.818962$ a.u. $\text{IF} = i194.18$ cm^{-1}

Sc	0.272987000	-0.176721000	0.360955000
Si	1.452510000	3.643715000	-0.419184000
C	0.875237000	1.824108000	-0.271002000
C	2.362643000	4.210279000	1.140885000
C	-0.069343000	4.736790000	-0.724011000
C	2.605641000	3.786024000	-1.917079000
C	0.903725000	-0.900579000	3.859069000
C	1.232315000	-1.210863000	2.427115000
C	2.289783000	-0.627459000	1.678446000
C	2.409362000	-1.325550000	0.423464000
C	1.401609000	-2.354045000	0.435040000
C	0.670069000	-2.270642000	1.651489000
C	3.190141000	0.449022000	2.215977000
C	1.232187000	-3.446937000	-0.582615000
C	-0.401695000	-3.219535000	2.108322000
C	-0.469458000	1.920385000	1.664682000
C	-1.278715000	0.819117000	1.897801000
H	1.773695000	1.182571000	-0.452016000
H	0.169651000	1.668191000	-1.113047000
H	1.722785000	4.190912000	2.029743000
H	2.703306000	5.243809000	1.007288000
H	3.247391000	3.597354000	1.342932000
H	-0.643776000	4.393961000	-1.593080000
H	0.258451000	5.761022000	-0.937726000
H	-0.747276000	4.793906000	0.135140000
H	3.505808000	3.172018000	-1.800194000
H	2.930436000	4.825225000	-2.047350000
H	2.104014000	3.478468000	-2.841956000
H	0.910938000	0.172890000	4.079020000
H	1.646065000	-1.361303000	4.523799000
H	-0.071656000	-1.297896000	4.157288000
H	2.683811000	1.061344000	2.969178000

H	3. 555864000	1. 117740000	1. 435285000
H	4. 069225000	0. 009663000	2. 706096000
H	1. 898844000	-4. 287318000	-0. 350052000
H	1. 470246000	-3. 119654000	-1. 598359000
H	0. 216526000	-3. 854749000	-0. 588956000
H	-0. 998666000	-3. 608102000	1. 276654000
H	-1. 091943000	-2. 754578000	2. 819540000
H	0. 039460000	-4. 087905000	2. 615338000
H	-0. 850359000	2. 792532000	1. 147001000
H	0. 379364000	2. 107288000	2. 314004000
H	-1. 045684000	0. 189345000	2. 752730000
C	-2. 024541000	-1. 762468000	-1. 365761000
O	-0. 879765000	-0. 843027000	-1. 393605000
C	-0. 616226000	-0. 430575000	-2. 773439000
C	-1. 372376000	-1. 429104000	-3. 631000000
C	-2. 603744000	-1. 721408000	-2. 770973000
H	-1. 638967000	-2. 752831000	-1. 108466000
H	-2. 710873000	-1. 415479000	-0. 592036000
H	-1. 002493000	0. 587476000	-2. 897064000
H	0. 464835000	-0. 436026000	-2. 921164000
H	-1. 621413000	-1. 015484000	-4. 611957000
H	-0. 777296000	-2. 336522000	-3. 782199000
H	-3. 339400000	-0. 915044000	-2. 858791000
H	-3. 096169000	-2. 661746000	-3. 032624000
C	-3. 066321000	1. 368137000	0. 192908000
C	-2. 598056000	0. 608395000	1. 282511000
C	-3. 457172000	-0. 376791000	1. 806619000
C	-4. 727041000	-0. 591558000	1. 282153000
C	-5. 162243000	0. 178692000	0. 202565000
C	-4. 333465000	1. 161447000	-0. 342086000
H	-2. 444076000	2. 148260000	-0. 238375000
H	-3. 135087000	-0. 965545000	2. 662491000
H	-5. 382135000	-1. 342478000	1. 712291000
H	-4. 687110000	1. 767734000	-1. 170307000
Cl	-6. 742261000	-0. 082483000	-0. 464317000
Si	3. 853897000	-1. 261110000	-0. 837905000
C	5. 100175000	0. 118337000	-0. 471093000
H	5. 561904000	0. 019282000	0. 515797000
H	5. 901897000	0. 044632000	-1. 216341000
H	4. 673732000	1. 123825000	-0. 555078000
C	4. 772009000	-2. 915185000	-0. 744691000
H	4. 151973000	-3. 760369000	-1. 058849000
H	5. 650436000	-2. 886351000	-1. 400119000
H	5. 121625000	-3. 112295000	0. 274788000

C	3.246718000	-0.973580000	-2.617753000
H	2.534908000	-1.729601000	-2.965891000
H	2.794606000	0.018898000	-2.734166000
H	4.109408000	-1.012685000	-3.294072000

pP1^a, $E_{(\text{SCF Done})} = -2255.853597$ a.u.

Sc	0.217575000	-0.771272000	-0.351399000
Si	-1.366671000	4.412233000	-0.248180000
C	-0.616249000	2.646386000	-0.379836000
C	-2.820221000	4.572341000	-1.452247000
C	-0.029795000	5.692679000	-0.655610000
C	-1.965483000	4.655180000	1.535266000
C	0.030341000	-2.642413000	-3.408649000
C	-0.479116000	-2.492396000	-2.004706000
C	-1.621157000	-1.744353000	-1.621813000
C	-1.865174000	-1.953803000	-0.212949000
C	-0.841546000	-2.858316000	0.245109000
C	0.017325000	-3.170104000	-0.847713000
C	-2.481688000	-0.980618000	-2.587891000
C	-0.703427000	-3.466124000	1.613282000
C	1.160091000	-4.146044000	-0.822004000
C	-0.125877000	2.239255000	-1.781730000
C	0.544520000	0.874637000	-1.867074000
H	-1.392673000	1.941240000	-0.038422000
H	0.204773000	2.590105000	0.351799000
H	-2.500817000	4.445634000	-2.492772000
H	-3.278387000	5.564574000	-1.368732000
H	-3.599960000	3.830654000	-1.243123000
H	0.817677000	5.626059000	0.037011000
H	-0.439393000	6.706298000	-0.575361000
H	0.354079000	5.575913000	-1.675383000
H	-2.745692000	3.932362000	1.801536000
H	-2.389688000	5.657394000	1.665493000
H	-1.143748000	4.553696000	2.254557000
H	-0.010388000	-1.704796000	-3.973615000
H	-0.584616000	-3.368198000	-3.956908000
H	1.059324000	-3.014019000	-3.445702000
H	-1.885737000	-0.465963000	-3.348913000
H	-3.101317000	-0.230266000	-2.091625000
H	-3.157714000	-1.662220000	-3.120700000
H	-1.296023000	-4.387199000	1.688216000
H	-1.047475000	-2.799607000	2.406832000
H	0.332703000	-3.746020000	1.831824000
H	1.690115000	-4.149896000	0.136444000

H	1.896749000	-3.943747000	-1.605814000
H	0.795449000	-5.168592000	-0.985883000
H	0.544436000	3.019206000	-2.176915000
H	-0.986903000	2.232237000	-2.460159000
H	0.344391000	0.345450000	-2.805309000
C	1.944965000	-0.598081000	2.346334000
O	0.657077000	-0.270155000	1.722666000
C	-0.249272000	0.300628000	2.723528000
C	0.440444000	0.070851000	4.058827000
C	1.922599000	0.126166000	3.680951000
H	1.986427000	-1.685711000	2.468573000
H	2.731535000	-0.266226000	1.667046000
H	-0.364632000	1.362949000	2.490086000
H	-1.211646000	-0.205307000	2.624705000
H	0.157688000	0.828182000	4.794797000
H	0.181568000	-0.913215000	4.464688000
H	2.256679000	1.162671000	3.561249000
H	2.570154000	-0.358963000	4.416012000
C	2.683129000	1.663263000	-0.726952000
C	1.917694000	0.692686000	-1.430792000
C	2.491795000	-0.611348000	-1.516248000
C	3.759729000	-0.911124000	-0.988949000
C	4.477098000	0.079058000	-0.336537000
C	3.936642000	1.371911000	-0.216777000
H	2.305151000	2.677227000	-0.640214000
H	2.023712000	-1.351292000	-2.168749000
H	4.189711000	-1.899116000	-1.123113000
H	4.520213000	2.148050000	0.270124000
Cl	6.047801000	-0.261230000	0.319895000
Si	-3.534661000	-1.512801000	0.628869000
C	-3.846806000	0.360822000	0.697655000
H	-3.772980000	0.848691000	-0.279404000
H	-4.863557000	0.533564000	1.071370000
H	-3.161466000	0.871213000	1.384271000
C	-4.900860000	-2.350165000	-0.379378000
H	-5.868114000	-2.203215000	0.115644000
H	-4.983404000	-1.949217000	-1.394094000
H	-4.723937000	-3.428824000	-0.454731000
C	-3.662828000	-2.164329000	2.406055000
H	-3.541574000	-3.250392000	2.463043000
H	-2.959406000	-1.703438000	3.108292000
H	-4.672164000	-1.930998000	2.767306000

$pC2^a_{syn}$, $E_{(SCF Done)} = -3024.924855$ a.u.

Sc	-0.196073000	-1.021203000	-0.575308000
Si	-4.204743000	0.028614000	3.662716000
C	-3.212568000	0.342811000	2.050847000
C	-3.381800000	-1.359206000	4.665332000
C	-5.988758000	-0.454022000	3.241345000
C	-4.187594000	1.637235000	4.665884000
C	-2.134307000	-4.044965000	-0.234914000
C	-0.803974000	-3.434897000	-0.557665000
C	0.281642000	-3.266828000	0.340978000
C	1.452748000	-2.868745000	-0.404877000
C	1.040896000	-2.782129000	-1.778045000
C	-0.342618000	-3.100808000	-1.867777000
C	0.201320000	-3.599861000	1.806238000
C	1.922007000	-2.535370000	-2.970344000
C	-1.145841000	-3.217792000	-3.131836000
C	-3.109038000	-0.863088000	1.112928000
C	-2.387151000	-0.709644000	-0.261857000
H	-2.222079000	0.708666000	2.358671000
H	-3.704274000	1.180399000	1.538464000
H	-3.391136000	-2.313013000	4.124787000
H	-3.913491000	-1.515620000	5.611048000
H	-2.340879000	-1.115385000	4.910664000
H	-6.482568000	0.325857000	2.650199000
H	-6.573766000	-0.595908000	4.157399000
H	-6.036230000	-1.389205000	2.671805000
H	-3.165888000	1.939518000	4.924660000
H	-4.744888000	1.517672000	5.602020000
H	-4.651190000	2.458707000	4.107389000
H	-2.501631000	-3.764438000	0.755937000
H	-2.053936000	-5.140196000	-0.251502000
H	-2.903632000	-3.771376000	-0.963249000
H	-0.803799000	-3.428440000	2.205555000
H	0.905355000	-3.022113000	2.409740000
H	0.428667000	-4.660360000	1.978291000
H	2.182715000	-3.483916000	-3.457815000
H	2.859671000	-2.044737000	-2.698759000
H	1.432956000	-1.919085000	-3.732630000
H	-0.720307000	-2.626828000	-3.949062000
H	-2.185773000	-2.901383000	-2.997063000
H	-1.172815000	-4.260484000	-3.475547000
H	-4.135476000	-1.203722000	0.907392000
H	-2.635980000	-1.694854000	1.655295000
H	-2.740740000	-1.563345000	-0.860874000
C	0.069806000	0.938380000	-3.210102000

O	0.655187000	0.445140000	-1.955658000
C	2.035545000	0.917314000	-1.837047000
C	2.401839000	1.423240000	-3.221380000
C	1.063457000	1.963155000	-3.730453000
H	-0.029471000	0.080221000	-3.882708000
H	-0.913901000	1.343418000	-2.977567000
H	2.048375000	1.717540000	-1.091246000
H	2.642400000	0.080504000	-1.486531000
H	3.184824000	2.185388000	-3.180187000
H	2.756257000	0.601852000	-3.853821000
H	0.854624000	2.949713000	-3.302562000
H	1.021776000	2.050056000	-4.819456000
C	-2.351407000	1.818533000	-0.678204000
C	-2.703025000	0.507863000	-1.070673000
C	-3.353888000	0.389907000	-2.318756000
C	-3.638860000	1.489893000	-3.123245000
C	-3.275715000	2.765676000	-2.692326000
C	-2.635414000	2.932840000	-1.464529000
H	-1.867574000	1.980097000	0.280787000
H	-3.673522000	-0.594749000	-2.654326000
H	-4.155121000	1.363079000	-4.069990000
H	-2.369810000	3.929831000	-1.125738000
C	3.861045000	1.412741000	2.111184000
C	2.484313000	1.497269000	1.835007000
C	1.932942000	2.768056000	1.578147000
C	2.727552000	3.903430000	1.577208000
C	4.097647000	3.785931000	1.841706000
C	4.668997000	2.542604000	2.114261000
H	4.304365000	0.445731000	2.335683000
H	0.867637000	2.877990000	1.396022000
H	2.297259000	4.881571000	1.388321000
H	5.729251000	2.467422000	2.331743000
C	1.690206000	0.277580000	1.870466000
C	0.366006000	0.134936000	1.612279000
H	2.237914000	-0.613972000	2.173663000
H	-0.136653000	-0.790927000	1.905080000
H	-0.276722000	0.986271000	1.402010000
Si	3.279922000	-3.126183000	0.114483000
C	3.513202000	-3.416254000	1.976393000
H	3.220259000	-2.575779000	2.615304000
H	2.982867000	-4.306805000	2.326519000
H	4.583156000	-3.590314000	2.146344000
C	4.450332000	-1.701291000	-0.359369000
H	4.548893000	-1.557347000	-1.440441000

H	4.166121000	-0.743905000	0.090940000
H	5.451266000	-1.950008000	0.015074000
C	3.858973000	-4.698083000	-0.770814000
H	3.848094000	-4.587692000	-1.860019000
H	4.883962000	-4.946481000	-0.471161000
H	3.218041000	-5.548446000	-0.512864000
Cl	5.087124000	5.202533000	1.841613000
Cl	-3.624831000	4.151642000	-3.683476000

***p*TS2^a_{syn}, $E_{(\text{SCF Done})} = -3024.913664$ a.u. $\text{IF} = i170.63 \text{ cm}^{-1}$**

Sc	-0.469959000	-0.914313000	0.237279000
Si	5.787949000	-0.816589000	-1.638020000
C	4.136367000	-0.173551000	-0.888285000
C	5.418943000	-1.879645000	-3.165253000
C	6.710054000	-1.843541000	-0.338196000
C	6.816714000	0.695683000	-2.126361000
C	0.876163000	-4.154270000	-0.643475000
C	-0.321425000	-3.399274000	-0.145692000
C	-1.400090000	-2.933795000	-0.943061000
C	-2.433006000	-2.422883000	-0.081686000
C	-1.967928000	-2.626808000	1.265803000
C	-0.668699000	-3.201928000	1.225056000
C	-1.475941000	-3.172300000	-2.424869000
C	-2.792225000	-2.546853000	2.520936000
C	0.102297000	-3.715751000	2.407812000
C	3.174483000	-1.283572000	-0.457641000
C	1.820849000	-0.901080000	0.173534000
H	3.686227000	0.491866000	-1.638985000
H	4.400792000	0.460046000	-0.031206000
H	4.849635000	-2.780973000	-2.909877000
H	6.353571000	-2.207549000	-3.634849000
H	4.851600000	-1.320239000	-3.918385000
H	6.901260000	-1.261079000	0.570584000
H	7.680240000	-2.168974000	-0.731130000
H	6.155393000	-2.744879000	-0.052629000
H	6.302666000	1.308440000	-2.875898000
H	7.776804000	0.385929000	-2.554597000
H	7.030142000	1.330590000	-1.258834000
H	1.219916000	-3.804472000	-1.622593000
H	0.632703000	-5.219053000	-0.757854000
H	1.724520000	-4.096886000	0.046222000
H	-0.501789000	-3.075244000	-2.916270000
H	-2.174133000	-2.506630000	-2.933299000
H	-1.819544000	-4.197670000	-2.617039000

H	-3.187564000	-3.543505000	2.758368000
H	-3.652266000	-1.881820000	2.418780000
H	-2.215548000	-2.226446000	3.394824000
H	-0.110744000	-3.151288000	3.321708000
H	1.185804000	-3.697424000	2.245325000
H	-0.165614000	-4.760910000	2.613589000
H	3.697620000	-1.907866000	0.282390000
H	2.977070000	-1.950633000	-1.307359000
H	1.447131000	-1.842574000	0.635195000
C	-1.546458000	2.132894000	0.991029000
O	-1.415201000	0.724761000	1.402583000
C	-1.847134000	0.593869000	2.793740000
C	-1.911356000	2.009433000	3.336461000
C	-2.336850000	2.802059000	2.101199000
H	-0.535820000	2.537302000	0.896729000
H	-2.042189000	2.150531000	0.021788000
H	-2.828553000	0.116915000	2.789611000
H	-1.125975000	-0.045581000	3.306955000
H	-2.619873000	2.090876000	4.165581000
H	-0.928383000	2.336244000	3.690180000
H	-3.413135000	2.697709000	1.924998000
H	-2.104850000	3.868086000	2.173187000
C	2.130792000	1.503140000	0.957764000
C	1.838061000	0.147543000	1.229539000
C	1.608348000	-0.200036000	2.578165000
C	1.671369000	0.743256000	3.604703000
C	1.977871000	2.065288000	3.296288000
C	2.211313000	2.447877000	1.970889000
H	2.320453000	1.815608000	-0.063185000
H	1.449604000	-1.244029000	2.840705000
H	1.518852000	0.447029000	4.638124000
H	2.459263000	3.480170000	1.743867000
C	-2.238509000	1.673318000	-2.500969000
C	-0.894845000	1.390033000	-2.191159000
C	-0.006304000	2.477802000	-2.129741000
C	-0.437009000	3.782902000	-2.339946000
C	-1.780477000	4.030597000	-2.624702000
C	-2.684666000	2.972697000	-2.716752000
H	-2.949351000	0.855218000	-2.588257000
H	1.048846000	2.311697000	-1.934141000
H	0.266627000	4.608532000	-2.297422000
H	-3.723973000	3.166110000	-2.963197000
C	-0.484546000	-0.011893000	-2.008552000
C	0.830003000	-0.457802000	-1.878308000

H	-1.220271000	-0.741010000	-2.337538000
H	1.066147000	-1.481207000	-2.153970000
H	1.659865000	0.230158000	-1.987953000
Si	-4.254040000	-2.005631000	-0.514042000
C	-4.608058000	-1.961027000	-2.376895000
H	-4.029875000	-1.213786000	-2.931098000
H	-4.455103000	-2.935467000	-2.851129000
H	-5.667436000	-1.703858000	-2.500682000
C	-4.779233000	-0.317404000	0.186269000
H	-4.716912000	-0.262480000	1.278071000
H	-4.179013000	0.497955000	-0.232877000
H	-5.824949000	-0.129768000	-0.086433000
C	-5.349333000	-3.370897000	0.214532000
H	-5.315051000	-3.412140000	1.307391000
H	-6.392423000	-3.202363000	-0.078737000
H	-5.050859000	-4.353082000	-0.169060000
Cl	-2.323362000	5.659565000	-2.880776000
Cl	2.079084000	3.248257000	4.561046000

pP2^a_{syn}, $E_{(\text{SCF Done})} = -3024.962763$ a.u.

Sc	-0.679349000	-0.591112000	-0.315202000
Si	6.582240000	0.092931000	-0.900349000
C	4.741616000	0.440953000	-0.470884000
C	6.817238000	0.147918000	-2.781119000
C	7.069262000	-1.614323000	-0.232292000
C	7.627966000	1.439172000	-0.075137000
C	0.646862000	-3.872073000	-1.318789000
C	-0.492830000	-2.892219000	-1.335192000
C	-0.763073000	-1.987214000	-2.406353000
C	-2.043519000	-1.418788000	-2.182883000
C	-2.592615000	-1.957953000	-0.963385000
C	-1.605956000	-2.869304000	-0.447626000
C	0.088279000	-1.820179000	-3.629643000
C	-2.742650000	-0.508802000	-3.151272000
C	-1.750126000	-3.752405000	0.761405000
C	3.758020000	-0.592191000	-1.018906000
C	2.245647000	-0.323260000	-0.757197000
H	4.502993000	1.444074000	-0.851064000
H	4.675456000	0.495367000	0.624938000
H	6.229165000	-0.621850000	-3.294164000
H	7.869590000	-0.020284000	-3.037668000
H	6.529567000	1.123111000	-3.191004000
H	6.920860000	-1.678727000	0.852081000
H	8.128561000	-1.812720000	-0.432252000

H	6.491971000	-2.419066000	-0.702313000
H	7.348766000	2.437502000	-0.431267000
H	8.691265000	1.293903000	-0.297955000
H	7.513230000	1.424993000	1.014846000
H	1.607292000	-3.426401000	-1.602165000
H	0.451558000	-4.674471000	-2.042386000
H	0.773393000	-4.358038000	-0.346494000
H	1.148095000	-2.003745000	-3.425735000
H	0.003758000	-0.821962000	-4.069522000
H	-0.215319000	-2.536955000	-4.404430000
H	-2.034631000	-0.000781000	-3.812632000
H	-3.343169000	0.254909000	-2.650917000
H	-3.420584000	-1.082970000	-3.797076000
H	-2.249374000	-3.246289000	1.592214000
H	-0.781947000	-4.110608000	1.124823000
H	-2.345888000	-4.644264000	0.525870000
H	4.000371000	-1.584260000	-0.615429000
H	3.869006000	-0.666895000	-2.109438000
H	1.729089000	-1.163669000	-1.257948000
C	-1.823569000	-0.037482000	2.704598000
O	-1.773618000	0.365214000	1.297071000
C	-2.760466000	1.433917000	1.055723000
C	-3.625530000	1.460955000	2.302801000
C	-2.639858000	1.042104000	3.395291000
H	-2.308361000	-1.017411000	2.754568000
H	-0.797506000	-0.114830000	3.062233000
H	-2.201410000	2.359669000	0.910573000
H	-3.297843000	1.178959000	0.141373000
H	-4.050487000	2.454306000	2.470388000
H	-4.450143000	0.744410000	2.226162000
H	-1.998973000	1.883132000	3.681446000
H	-3.130325000	0.663873000	4.296283000
C	2.139578000	0.634829000	1.625221000
C	1.923394000	-0.427877000	0.726360000
C	1.536336000	-1.665027000	1.277788000
C	1.391614000	-1.850332000	2.657250000
C	1.643053000	-0.783304000	3.514746000
C	2.011384000	0.463778000	2.999722000
H	2.464581000	1.599818000	1.251722000
H	1.439884000	-2.529810000	0.626676000
H	1.122108000	-2.821730000	3.059628000
H	2.214760000	1.287463000	3.677194000
C	-1.522517000	2.841698000	-1.972414000
C	-0.425499000	2.369034000	-1.220620000

C	-0.005236000	3.190287000	-0.154142000
C	-0.635358000	4.395708000	0.148726000
C	-1.728712000	4.813598000	-0.607780000
C	-2.172309000	4.035386000	-1.676777000
H	-1.858852000	2.269552000	-2.833366000
H	0.842006000	2.895933000	0.458036000
H	-0.276311000	5.012825000	0.967016000
H	-3.004358000	4.375201000	-2.286120000
C	0.204644000	1.061881000	-1.556018000
C	1.740922000	0.970916000	-1.424666000
H	-0.073817000	0.810940000	-2.584909000
H	2.198014000	1.017015000	-2.422769000
H	2.139337000	1.841104000	-0.892280000
Cl	-2.527814000	6.312065000	-0.228548000
Cl	1.491918000	-0.996753000	5.228213000
Si	-4.467158000	-2.073584000	-0.575579000
C	-5.474912000	-0.555131000	-1.109514000
H	-5.506049000	-0.440749000	-2.196856000
H	-6.507554000	-0.712561000	-0.773811000
H	-5.138488000	0.392323000	-0.675841000
C	-5.081876000	-3.558024000	-1.581691000
H	-4.563046000	-4.479608000	-1.295675000
H	-6.155108000	-3.713054000	-1.419302000
H	-4.924595000	-3.405438000	-2.655132000
C	-4.853048000	-2.401979000	1.255306000
H	-4.551422000	-3.404586000	1.572456000
H	-4.401570000	-1.675100000	1.938379000
H	-5.940107000	-2.336665000	1.386560000

$pC2^a_{iso}$, $E_{(SCF Done)} = -3024.93264$ a.u.

Sc	-0.498003000	-0.559564000	0.241367000
Si	0.966748000	5.358668000	1.228410000
C	-0.338725000	3.962635000	1.330775000
C	1.283261000	5.813732000	-0.588303000
C	2.589665000	4.773620000	2.026359000
C	0.302047000	6.869838000	2.157149000
C	0.327994000	0.519590000	3.584426000
C	0.196888000	-0.629163000	2.631048000
C	1.264522000	-1.174935000	1.860787000
C	0.803301000	-2.379927000	1.253427000
C	-0.571326000	-2.584108000	1.616235000
C	-0.934326000	-1.471827000	2.459855000
C	2.669235000	-0.646134000	1.857878000
C	1.691944000	-3.319989000	0.486774000

C	0.037176000	2.631847000	0.657073000
C	-1.054810000	1.549970000	0.750543000
H	-1.274486000	4.339162000	0.893400000
H	-0.557312000	3.781768000	2.393446000
H	1.696905000	4.974925000	-1.160947000
H	1.998895000	6.641115000	-0.658248000
H	0.358677000	6.135107000	-1.081958000
H	2.438788000	4.492603000	3.075329000
H	3.340806000	5.571627000	2.004006000
H	3.015118000	3.908987000	1.502674000
H	-0.633813000	7.227110000	1.712444000
H	1.021697000	7.696022000	2.126710000
H	0.105684000	6.638078000	3.210265000
H	0.971064000	1.315504000	3.196778000
H	0.777163000	0.172207000	4.524558000
H	-0.636467000	0.967218000	3.839627000
H	2.699111000	0.448882000	1.863681000
H	3.246624000	-0.991254000	0.997086000
H	3.202156000	-0.980906000	2.758166000
H	2.529508000	-2.793981000	0.019487000
H	1.160561000	-3.868891000	-0.294879000
H	2.128325000	-4.070840000	1.159320000
H	0.966782000	2.253229000	1.108656000
H	0.284836000	2.830097000	-0.395089000
H	-1.378582000	1.483756000	1.796927000
C	-3.118868000	-1.214281000	-1.730593000
O	-1.710956000	-1.468516000	-1.378985000
C	-1.185008000	-2.531806000	-2.227095000
C	-2.407352000	-3.222377000	-2.803501000
C	-3.376706000	-2.050824000	-2.973661000
H	-3.725214000	-1.533766000	-0.879467000
H	-3.230840000	-0.142084000	-1.881456000
H	-0.581516000	-2.068192000	-3.016534000
H	-0.554073000	-3.168733000	-1.604296000
H	-2.182207000	-3.735265000	-3.742622000
H	-2.802723000	-3.958216000	-2.095230000
H	-3.139754000	-1.481125000	-3.879171000
H	-4.421777000	-2.365239000	-3.037113000
C	-2.217939000	2.270400000	-1.404864000
C	-2.265363000	1.767423000	-0.084842000
C	-3.548544000	1.455414000	0.419750000
C	-4.708110000	1.638437000	-0.327092000
C	-4.616905000	2.143429000	-1.624433000
C	-3.370209000	2.464163000	-2.163380000

H	-1.265474000	2.562910000	-1.840175000
H	-3.639843000	1.104682000	1.446021000
H	-5.680953000	1.414327000	0.100114000
H	-3.305262000	2.877055000	-3.165752000
C	4.208615000	-1.719523000	-2.223138000
C	3.441255000	-0.595812000	-1.865008000
C	4.107527000	0.525239000	-1.333747000
C	5.480482000	0.515710000	-1.146674000
C	6.215118000	-0.623982000	-1.493852000
C	5.584292000	-1.744539000	-2.036514000
H	3.718489000	-2.588340000	-2.656794000
H	3.552381000	1.423830000	-1.081263000
H	5.991145000	1.384520000	-0.744572000
H	6.167995000	-2.616136000	-2.313310000
C	2.005734000	-0.626141000	-2.101447000
C	1.072206000	0.283343000	-1.720238000
H	1.669344000	-1.480681000	-2.689806000
H	0.080974000	0.256920000	-2.175338000
H	1.346114000	1.200334000	-1.203855000
C	-2.258131000	-1.267188000	3.143485000
H	-3.104981000	-1.523184000	2.500090000
H	-2.337105000	-1.891249000	4.043384000
H	-2.389491000	-0.230620000	3.468090000
Cl	7.927351000	-0.635837000	-1.259754000
Cl	-6.058562000	2.386463000	-2.566635000
Si	-1.540439000	-4.235852000	1.606981000
C	-0.881174000	-5.515987000	0.368615000
H	0.147680000	-5.816580000	0.587905000
H	-1.505677000	-6.412752000	0.466937000
H	-0.933717000	-5.205110000	-0.680414000
C	-1.320656000	-4.971864000	3.339375000
H	-1.723235000	-4.315244000	4.117709000
H	-1.840184000	-5.934587000	3.413581000
H	-0.261512000	-5.143237000	3.561255000
C	-3.396551000	-4.021442000	1.261353000
H	-3.926932000	-3.547389000	2.092631000
H	-3.597694000	-3.442833000	0.353577000
H	-3.841369000	-5.014288000	1.121589000

***p*TS2^a_{iso}, $E_{(\text{SCF Done})} = -3024.91485$ a.u. IF = $i243.77$ cm⁻¹**

Sc	-0.186590000	-0.731526000	-0.085426000
Si	1.358427000	5.531286000	1.136407000
C	0.332669000	3.912051000	1.011068000
C	1.409265000	6.377406000	-0.560592000

C	3.120612000	5.124943000	1.709492000
C	0.502652000	6.651601000	2.399976000
C	1.991198000	-0.045841000	2.635920000
C	0.952882000	-0.991080000	2.104923000
C	1.211244000	-2.193478000	1.382810000
C	-0.032844000	-2.856372000	1.179420000
C	-1.081947000	-2.090337000	1.800147000
C	-0.442217000	-0.930879000	2.369682000
C	2.555648000	-2.817364000	1.168263000
C	-0.116486000	-4.227105000	0.566497000
C	0.869438000	2.860912000	0.029105000
C	-0.006667000	1.614036000	-0.066655000
H	-0.694863000	4.188849000	0.736374000
H	0.269696000	3.480575000	2.021378000
H	1.915163000	5.762899000	-1.314568000
H	1.955696000	7.325283000	-0.494835000
H	0.400649000	6.603679000	-0.925830000
H	3.118371000	4.601113000	2.672659000
H	3.700821000	6.046030000	1.837592000
H	3.656345000	4.501424000	0.984105000
H	-0.520532000	6.894630000	2.091237000
H	1.048190000	7.595485000	2.512794000
H	0.453168000	6.177655000	3.387061000
H	2.321881000	-0.362887000	3.634318000
H	1.611406000	0.976413000	2.740490000
H	2.879497000	-0.013729000	1.998646000
H	3.356210000	-2.079384000	1.089187000
H	2.593528000	-3.441007000	0.272247000
H	2.787951000	-3.465105000	2.025266000
H	0.503838000	-4.312131000	-0.333328000
H	-1.135299000	-4.510452000	0.304790000
H	0.256205000	-4.981789000	1.272174000
H	1.879962000	2.557625000	0.332272000
H	0.976833000	3.310684000	-0.966856000
H	-0.043589000	1.172562000	0.952990000
C	-1.636155000	-0.974383000	-3.011039000
O	-1.467413000	-1.587134000	-1.684576000
C	-2.397594000	-2.709828000	-1.561286000
C	-3.454948000	-2.461589000	-2.618691000
C	-2.625210000	-1.861538000	-3.753875000
H	-2.022695000	0.034999000	-2.852498000
H	-0.654566000	-0.927611000	-3.488822000
H	-1.837281000	-3.630268000	-1.752208000
H	-2.767099000	-2.709162000	-0.537098000

H	-3.969871000	-3.382721000	-2.904968000
H	-4.201500000	-1.744545000	-2.260417000
H	-2.101819000	-2.649089000	-4.307137000
H	-3.223357000	-1.286599000	-4.465631000
C	-1.638328000	2.547358000	-1.749075000
C	-1.374086000	1.774025000	-0.592510000
C	-2.467403000	1.104911000	-0.004066000
C	-3.752182000	1.170924000	-0.552935000
C	-3.971237000	1.937202000	-1.691189000
C	-2.913792000	2.640705000	-2.283389000
H	-0.836552000	3.111106000	-2.217461000
H	-2.343344000	0.595866000	0.950968000
H	-4.582802000	0.669866000	-0.067116000
H	-3.100918000	3.260425000	-3.155049000
C	3.535845000	-2.204994000	-1.990775000
C	3.010919000	-1.018976000	-1.451639000
C	3.900317000	-0.164100000	-0.779408000
C	5.248875000	-0.478823000	-0.643959000
C	5.737131000	-1.667546000	-1.185409000
C	4.881410000	-2.533013000	-1.864974000
H	2.881411000	-2.880296000	-2.538926000
H	3.544473000	0.768870000	-0.349118000
H	5.921940000	0.194637000	-0.122627000
H	5.268456000	-3.450314000	-2.297234000
C	1.593296000	-0.686955000	-1.677877000
C	1.133062000	0.641026000	-1.720350000
H	1.055272000	-1.420832000	-2.284582000
H	0.312411000	0.898627000	-2.387994000
H	1.863712000	1.434573000	-1.608630000
C	-1.075292000	0.100267000	3.265592000
H	-2.165678000	0.113070000	3.188200000
H	-0.829796000	-0.111673000	4.314181000
H	-0.719979000	1.117916000	3.064911000
Cl	7.420154000	-2.066225000	-1.017803000
Cl	-5.565689000	2.054776000	-2.365729000
Si	-2.789948000	-2.720270000	2.418392000
C	-3.222453000	-4.470360000	1.825033000
H	-2.470690000	-5.205309000	2.129034000
H	-4.163788000	-4.749127000	2.315131000
H	-3.385146000	-4.567214000	0.746626000
C	-2.688484000	-2.809259000	4.308581000
H	-2.579481000	-1.827348000	4.778158000
H	-3.604812000	-3.264942000	4.702335000
H	-1.844224000	-3.431865000	4.625030000

C	-4.237166000	-1.592038000	1.920045000
H	-4.139586000	-0.568598000	2.297910000
H	-4.371230000	-1.547060000	0.833437000
H	-5.161335000	-2.003365000	2.343654000

pP2^a_{iso}, $E_{(\text{SCF Done})} = -3024.958907$ a.u.

Sc	0.628146000	-0.458867000	0.340699000
Si	-6.297320000	1.645870000	0.521997000
C	-4.548738000	1.163807000	-0.113501000
C	-6.196940000	3.279197000	1.478996000
C	-6.964338000	0.270389000	1.644221000
C	-7.411942000	1.847289000	-0.996357000
C	-0.516597000	-0.966652000	3.742840000
C	0.630994000	-0.667903000	2.819335000
C	1.116676000	0.641044000	2.512586000
C	2.335856000	0.498003000	1.803481000
C	2.629075000	-0.908004000	1.653629000
C	1.558014000	-1.616609000	2.299979000
C	0.526533000	1.927984000	3.005520000
C	3.227843000	1.641600000	1.416976000
C	-3.506669000	0.937852000	0.980941000
C	-2.071029000	0.562415000	0.501368000
H	-4.228997000	1.961000000	-0.798628000
H	-4.668840000	0.256920000	-0.722979000
H	-5.577136000	3.192790000	2.378944000
H	-7.196672000	3.593645000	1.800052000
H	-5.782601000	4.081720000	0.857718000
H	-7.004112000	-0.691231000	1.119251000
H	-7.982457000	0.508499000	1.973150000
H	-6.352569000	0.141123000	2.544592000
H	-7.034689000	2.626933000	-1.668204000
H	-8.427469000	2.131295000	-0.697318000
H	-7.483840000	0.914727000	-1.567972000
H	-1.378144000	-0.307372000	3.586973000
H	-0.201944000	-0.824471000	4.785359000
H	-0.862030000	-2.002188000	3.661763000
H	-0.566608000	1.892836000	3.069027000
H	0.802869000	2.772209000	2.368961000
H	0.894451000	2.150277000	4.016524000
H	2.660618000	2.525163000	1.115981000
H	3.894472000	1.388549000	0.589480000
H	3.856707000	1.930356000	2.269262000
H	-3.850334000	0.146148000	1.659935000
H	-3.402674000	1.844966000	1.591908000

H	-1.500533000	0.422842000	1.441041000
C	1.436441000	-3.245138000	-1.109107000
O	1.170143000	-1.816777000	-1.294195000
C	1.332183000	-1.468589000	-2.711349000
C	1.914921000	-2.709774000	-3.369825000
C	1.365402000	-3.843751000	-2.502040000
H	2.432610000	-3.337883000	-0.669463000
H	0.686641000	-3.630197000	-0.415887000
H	0.340623000	-1.216306000	-3.097641000
H	1.986096000	-0.597060000	-2.767123000
H	1.612681000	-2.788313000	-4.417634000
H	3.009441000	-2.688669000	-3.333965000
H	0.330663000	-4.078301000	-2.770937000
H	1.954337000	-4.761882000	-2.577677000
C	-2.316092000	-0.892870000	-1.597780000
C	-2.072536000	-0.777687000	-0.216050000
C	-1.957064000	-1.967854000	0.526802000
C	-2.096873000	-3.224030000	-0.070736000
C	-2.359814000	-3.299014000	-1.435757000
C	-2.467639000	-2.135409000	-2.203784000
H	-2.423081000	0.003763000	-2.201596000
H	-1.836173000	-1.913091000	1.607083000
H	-2.039694000	-4.130490000	0.524197000
H	-2.689794000	-2.208166000	-3.264178000
C	1.919290000	2.463517000	-2.008389000
C	0.922626000	2.562330000	-1.018312000
C	0.829553000	3.798451000	-0.351311000
C	1.694693000	4.854498000	-0.628035000
C	2.684760000	4.704281000	-1.595680000
C	2.794191000	3.505006000	-2.296654000
H	2.002523000	1.548957000	-2.592290000
H	0.065394000	3.959989000	0.403141000
H	1.595156000	5.796352000	-0.097285000
H	3.547112000	3.395737000	-3.071196000
C	0.053294000	1.395088000	-0.707960000
C	-1.384789000	1.706951000	-0.266479000
H	-0.006587000	0.778121000	-1.634652000
H	-2.005000000	2.015567000	-1.121204000
H	-1.384553000	2.562887000	0.415608000
C	1.445645000	-3.098618000	2.531392000
H	2.022339000	-3.678758000	1.810140000
H	1.823062000	-3.361343000	3.528575000
H	0.407244000	-3.447536000	2.490738000
Cl	3.769827000	6.018505000	-1.945006000

Cl	-2.569361000	-4.847578000	-2.189739000
Si	4.374165000	-1.539331000	1.163450000
C	4.798076000	-1.139413000	-0.645727000
H	4.757001000	-0.067551000	-0.865446000
H	5.818568000	-1.477790000	-0.861717000
H	4.128174000	-1.655048000	-1.342669000
C	5.627335000	-0.703695000	2.312451000
H	5.359404000	-0.862099000	3.363125000
H	6.618371000	-1.144585000	2.151337000
H	5.712745000	0.373258000	2.142377000
C	4.603752000	-3.408737000	1.411994000
H	4.402200000	-3.713650000	2.443905000
H	4.013153000	-4.045500000	0.744821000
H	5.659338000	-3.629762000	1.209909000

b, $E_{(\text{SCF Done})} = -1210.614978$ a.u.

Sc	-0.050578000	0.258986000	-0.236087000
N	-1.454355000	2.073349000	-0.141882000
C	-1.115873000	0.030494000	-2.144439000
H	-0.898726000	0.951280000	-2.697703000
H	-1.081272000	-0.828447000	-2.813920000
C	-2.303298000	0.054362000	-1.281083000
C	-2.456985000	1.015756000	-0.230537000
C	-3.524968000	0.930095000	0.680725000
H	-3.646778000	1.682713000	1.452831000
C	-4.447282000	-0.099058000	0.588277000
H	-5.275094000	-0.147806000	1.289165000
C	-4.311347000	-1.062398000	-0.420885000
H	-5.037894000	-1.865800000	-0.505186000
C	-3.262553000	-0.988681000	-1.318899000
H	-3.171016000	-1.731454000	-2.106450000
C	-1.343695000	2.713091000	1.182949000
H	-2.218866000	3.333176000	1.415870000
H	-0.463972000	3.363452000	1.184842000
H	-1.235601000	1.959792000	1.970963000
C	-1.614357000	3.119764000	-1.178333000
H	-1.778810000	2.665055000	-2.154792000
H	-0.712867000	3.738160000	-1.214932000
H	-2.477666000	3.753930000	-0.940318000
C	1.962817000	-0.758380000	0.385462000
C	1.192737000	-0.595331000	1.594470000
C	0.058346000	-1.450940000	1.524598000
C	0.125731000	-2.171741000	0.289192000
C	1.293905000	-1.758816000	-0.404577000

C	1.527229000	0.305678000	2.754770000
H	0.750552000	0.271468000	3.523632000
H	1.662191000	1.358324000	2.472233000
H	2.463008000	-0.009721000	3.229934000
C	-0.977156000	-1.671160000	2.590775000
H	-0.729496000	-2.555333000	3.192509000
H	-1.972310000	-1.838577000	2.166363000
H	-1.052243000	-0.825395000	3.280908000
C	-0.812168000	-3.270565000	-0.113244000
H	-0.885911000	-3.378168000	-1.199087000
H	-1.822245000	-3.104872000	0.271872000
H	-0.465376000	-4.232580000	0.286743000
C	1.747956000	-2.319478000	-1.724210000
H	2.703624000	-2.845076000	-1.614443000
H	1.884978000	-1.553517000	-2.494810000
H	1.024673000	-3.039994000	-2.113483000
Si	3.282176000	0.458238000	-0.231336000
C	4.377498000	-0.212493000	-1.612694000
H	3.836656000	-0.421527000	-2.539298000
H	5.153229000	0.528554000	-1.838790000
H	4.882029000	-1.132580000	-1.298112000
C	4.386882000	1.157629000	1.130857000
H	4.904999000	0.346488000	1.654773000
H	5.152099000	1.795951000	0.673646000
H	3.854815000	1.756161000	1.875130000
C	2.174897000	1.873059000	-0.943137000
H	2.786671000	2.684313000	-1.355984000
H	1.541454000	1.548291000	-1.788723000
H	1.547433000	2.360940000	-0.175884000

pC1^b, $E_{(\text{SCF Done})} = -1979.702425$ a.u.

Sc	-0.664290000	0.152427000	-0.082986000
N	0.775712000	1.951428000	-0.191828000
C	-1.284398000	1.037769000	-1.994295000
H	-0.402067000	0.938712000	-2.640044000
H	-2.177790000	0.793414000	-2.570465000
C	-1.398265000	2.332548000	-1.292251000
C	-0.422397000	2.773516000	-0.350686000
C	-0.600326000	3.959537000	0.378738000
H	0.163907000	4.294121000	1.072415000
C	-1.742140000	4.726877000	0.206421000
H	-1.864379000	5.649030000	0.766641000
C	-2.721767000	4.311361000	-0.703559000
H	-3.613338000	4.913509000	-0.855239000

C	-2.552154000	3.140988000	-1.422211000
H	-3.309275000	2.833703000	-2.138654000
C	1.480929000	2.125806000	1.092587000
H	1.977489000	3.102778000	1.158788000
H	2.250212000	1.352759000	1.174654000
H	0.780173000	2.033156000	1.927038000
C	1.736932000	2.162031000	-1.298160000
H	1.234111000	2.067219000	-2.260984000
H	2.538357000	1.422412000	-1.227929000
H	2.168826000	3.169250000	-1.230961000
C	-1.901012000	0.278725000	2.032171000
C	-2.844244000	0.003978000	0.995283000
C	-2.567840000	-1.292391000	0.447129000
C	-1.453797000	-1.820268000	1.191963000
C	-1.041217000	-0.852969000	2.154132000
C	-4.009921000	0.895564000	0.679509000
H	-4.237570000	0.931644000	-0.386650000
H	-3.836871000	1.919937000	1.018542000
H	-4.908543000	0.531552000	1.195311000
C	-0.956385000	-3.239379000	1.146308000
H	0.024150000	-3.355213000	1.618553000
H	-0.893714000	-3.645850000	0.132553000
H	-1.640439000	-3.890099000	1.705403000
C	0.012109000	-1.041029000	3.209805000
H	-0.431649000	-1.441200000	4.130976000
H	0.508003000	-0.102784000	3.481509000
H	0.788866000	-1.748436000	2.902478000
C	-1.928033000	1.471522000	2.946712000
H	-2.729878000	1.364231000	3.689069000
H	-0.994936000	1.579097000	3.509301000
H	-2.107778000	2.409260000	2.411201000
C	5.944428000	-0.582983000	-0.190685000
C	5.288033000	-1.042350000	0.952377000
C	3.951582000	-1.411002000	0.862905000
C	3.245551000	-1.312134000	-0.349341000
C	3.938388000	-0.864275000	-1.490166000
C	5.275305000	-0.501309000	-1.416639000
H	5.824631000	-1.120000000	1.892211000
H	3.446962000	-1.787044000	1.750092000
H	3.439843000	-0.832763000	-2.455062000
H	5.809229000	-0.171623000	-2.301952000
C	1.844629000	-1.721508000	-0.386579000
C	0.934613000	-1.478550000	-1.361071000
H	1.518262000	-2.309371000	0.470744000

H	-0.026813000	-1.997007000	-1.353287000
H	1.184692000	-0.945804000	-2.275127000
Cl	7.609301000	-0.127973000	-0.096939000
Si	-3.608950000	-2.300219000	-0.810172000
C	-4.430740000	-3.724088000	0.132843000
H	-5.109416000	-4.267428000	-0.535331000
H	-3.706839000	-4.445548000	0.525198000
H	-5.022343000	-3.346122000	0.974084000
C	-2.529118000	-2.998172000	-2.212497000
H	-1.754203000	-3.695153000	-1.875523000
H	-3.173935000	-3.555064000	-2.903519000
H	-2.054607000	-2.197447000	-2.792687000
C	-4.968325000	-1.280262000	-1.646166000
H	-5.710293000	-0.895691000	-0.940248000
H	-4.571911000	-0.442025000	-2.229130000
H	-5.494356000	-1.941798000	-2.345545000

pTS1^b, $E_{(\text{SCF Done})} = -1979.681813$ a.u. **IF** = $i308.61$ cm⁻¹

Sc	-0.144068000	-0.101646000	0.068072000
N	0.978408000	1.844200000	0.711147000
C	-0.040091000	1.186134000	-1.985791000
H	0.976087000	1.531598000	-2.170784000
H	-0.590790000	1.182277000	-2.924640000
C	-0.750021000	2.094406000	-1.027520000
C	-0.238902000	2.481779000	0.244172000
C	-0.903861000	3.450397000	1.011545000
H	-0.491499000	3.760135000	1.965723000
C	-2.071711000	4.038924000	0.552156000
H	-2.559727000	4.804722000	1.147772000
C	-2.613922000	3.644269000	-0.675665000
H	-3.526508000	4.103604000	-1.044061000
C	-1.972259000	2.679511000	-1.432667000
H	-2.380232000	2.399757000	-2.400075000
C	1.172727000	1.868760000	2.174962000
H	1.450384000	2.869536000	2.531007000
H	1.989827000	1.185696000	2.422814000
H	0.266591000	1.545774000	2.688034000
C	2.202261000	2.411639000	0.090212000
H	2.099454000	2.485314000	-0.989939000
H	3.052408000	1.767053000	0.320097000
H	2.381189000	3.418086000	0.490344000
C	-1.048355000	-1.011989000	2.209700000
C	-2.100964000	-0.346717000	1.519944000
C	-2.373911000	-1.061600000	0.295323000

C	-1.486037000	-2.193878000	0.282682000
C	-0.660112000	-2.147411000	1.434078000
C	-2.900705000	0.790682000	2.089027000
H	-3.250900000	1.481809000	1.321147000
H	-2.328549000	1.371330000	2.819050000
H	-3.785189000	0.406720000	2.614316000
C	-1.520799000	-3.348997000	-0.676577000
H	-0.531881000	-3.781746000	-0.864127000
H	-1.955353000	-3.083340000	-1.643046000
H	-2.133815000	-4.159180000	-0.260910000
C	0.305469000	-3.207282000	1.875402000
H	-0.214933000	-3.978012000	2.460211000
H	1.097599000	-2.806989000	2.517097000
H	0.779056000	-3.721881000	1.032553000
C	-0.573585000	-0.756025000	3.613386000
H	-0.993543000	-1.512568000	4.289161000
H	0.516265000	-0.816019000	3.716556000
H	-0.896491000	0.215582000	3.998057000
C	5.332676000	-0.401164000	-0.394014000
C	4.620082000	-1.245916000	0.458380000
C	3.292655000	-1.544394000	0.172560000
C	2.636533000	-1.017181000	-0.960098000
C	3.389334000	-0.172912000	-1.799862000
C	4.720321000	0.128879000	-1.529703000
H	5.107739000	-1.674344000	1.328501000
H	2.756969000	-2.228080000	0.826603000
H	2.950399000	0.228151000	-2.709737000
H	5.288051000	0.763223000	-2.203454000
C	1.231580000	-1.372135000	-1.221758000
C	0.462299000	-0.756547000	-2.251739000
H	0.921628000	-2.359201000	-0.894619000
H	-0.488701000	-1.235979000	-2.486920000
H	0.949572000	-0.390686000	-3.152760000
Cl	6.989814000	-0.018590000	-0.046326000
Si	-3.931996000	-0.962130000	-0.820866000
C	-4.954289000	-2.525708000	-0.497645000
H	-5.902354000	-2.464877000	-1.045297000
H	-4.447504000	-3.441790000	-0.815985000
H	-5.191004000	-2.622543000	0.567925000
C	-3.494228000	-0.872897000	-2.670573000
H	-2.956590000	-1.754402000	-3.035636000
H	-4.423700000	-0.805532000	-3.249053000
H	-2.897669000	0.014186000	-2.910780000
C	-5.049658000	0.519073000	-0.440287000

H	-5.441447000	0.494285000	0.581184000
H	-4.563258000	1.485376000	-0.602091000
H	-5.909066000	0.463778000	-1.119905000

pP1^b, $E_{(\text{SCF Done})} = -1979.705534$ a.u.

Sc	-0.277075000	-0.203993000	0.188997000
N	0.787365000	1.543710000	1.316764000
C	0.648123000	1.802724000	-1.755015000
H	1.682650000	1.985034000	-1.463969000
H	0.498318000	2.382944000	-2.669818000
C	-0.329522000	2.403369000	-0.739503000
C	-0.229463000	2.368274000	0.683363000
C	-1.158576000	3.074599000	1.466427000
H	-1.068434000	3.068156000	2.546363000
C	-2.180445000	3.814395000	0.886516000
H	-2.869732000	4.366278000	1.518762000
C	-2.302272000	3.851238000	-0.500941000
H	-3.092041000	4.428800000	-0.971765000
C	-1.387887000	3.159098000	-1.282333000
H	-1.465454000	3.222420000	-2.364804000
C	0.569033000	1.270932000	2.752699000
H	0.726750000	2.166634000	3.368016000
H	1.293480000	0.515048000	3.066236000
H	-0.439828000	0.891966000	2.930837000
C	2.172023000	2.066344000	1.178354000
H	2.391426000	2.355106000	0.155661000
H	2.877231000	1.287172000	1.473305000
H	2.294802000	2.944152000	1.825575000
C	-1.067101000	-1.872386000	1.798813000
C	-2.164151000	-1.021538000	1.475606000
C	-2.484583000	-1.193209000	0.079157000
C	-1.589080000	-2.204976000	-0.419778000
C	-0.715638000	-2.606538000	0.621087000
C	-2.926201000	-0.191581000	2.473489000
H	-3.156025000	0.813857000	2.109954000
H	-2.386045000	-0.093576000	3.420624000
H	-3.882058000	-0.671752000	2.717027000
C	-1.617778000	-2.849096000	-1.775814000
H	-0.616205000	-3.113387000	-2.131952000
H	-2.085042000	-2.216692000	-2.533991000
H	-2.190904000	-3.784796000	-1.736717000
C	0.280248000	-3.725869000	0.552495000
H	-0.225825000	-4.692946000	0.675250000
H	1.031971000	-3.660085000	1.345168000

H	0.806728000	-3.759915000	-0.406659000
C	-0.468804000	-2.119456000	3.156734000
H	-0.831662000	-3.072195000	3.563342000
H	0.625308000	-2.188134000	3.128277000
H	-0.734162000	-1.346196000	3.882822000
C	5.423532000	-0.321140000	-0.390618000
C	4.616176000	-1.163923000	0.373597000
C	3.262971000	-1.272759000	0.068361000
C	2.675146000	-0.565766000	-0.998531000
C	3.528258000	0.248248000	-1.764468000
C	4.883641000	0.379726000	-1.466342000
H	5.046453000	-1.728269000	1.195334000
H	2.644094000	-1.944565000	0.660547000
H	3.146298000	0.768149000	-2.639692000
H	5.522931000	1.009260000	-2.077681000
C	1.217761000	-0.738514000	-1.272869000
C	0.512777000	0.298330000	-2.158823000
H	1.017871000	-1.738081000	-1.672280000
H	-0.570625000	0.047489000	-2.225806000
H	0.832665000	0.220238000	-3.207530000
Cl	7.111202000	-0.158022000	-0.007284000
Si	-4.053767000	-0.610630000	-0.861140000
C	-5.138922000	-2.138659000	-1.129883000
H	-6.073059000	-1.853601000	-1.628040000
H	-4.646790000	-2.893326000	-1.751583000
H	-5.398326000	-2.606795000	-0.173765000
C	-3.635711000	0.185347000	-2.536239000
H	-3.122201000	-0.483179000	-3.234500000
H	-4.571860000	0.492640000	-3.018728000
H	-3.026594000	1.087520000	-2.409316000
C	-5.054565000	0.675157000	0.104705000
H	-5.436924000	0.291079000	1.054916000
H	-4.491424000	1.593801000	0.300772000
H	-5.922367000	0.948775000	-0.508166000

pC2^b_{syn}, E_(SCF Done) = -2748.794083

Sc	-0.362444000	-0.309386000	-0.574877000
N	5.801482000	0.385853000	-1.485963000
C	3.760342000	2.215347000	-0.502871000
H	4.399061000	2.660129000	-1.271549000
H	3.356649000	3.046368000	0.089681000
C	4.544778000	1.300059000	0.407654000
C	5.485531000	0.368634000	-0.094603000
C	6.074637000	-0.547161000	0.787387000

H	6.796977000	-1.265693000	0.411509000
C	5.774288000	-0.536844000	2.149406000
H	6.256378000	-1.251317000	2.811785000
C	4.888412000	0.408604000	2.656406000
H	4.668764000	0.446760000	3.720001000
C	4.284580000	1.312353000	1.781674000
H	3.585010000	2.049440000	2.172364000
C	6.222297000	-0.880481000	-2.062116000
H	7.244694000	-1.185563000	-1.775647000
H	6.204022000	-0.792657000	-3.154481000
H	5.531065000	-1.676323000	-1.769512000
C	6.736663000	1.447958000	-1.857423000
H	6.441644000	2.398751000	-1.408205000
H	6.742814000	1.566140000	-2.946991000
H	7.766557000	1.227125000	-1.527422000
C	0.669454000	-2.158877000	0.637857000
C	-0.755664000	-2.229005000	0.839561000
C	-1.330339000	-2.553362000	-0.439755000
C	-0.287199000	-2.637278000	-1.404620000
C	0.952092000	-2.375323000	-0.737707000
C	-2.772263000	-2.889914000	-0.695993000
H	-3.031644000	-3.844668000	-0.221603000
H	-2.977866000	-2.999072000	-1.763288000
H	-3.459355000	-2.135806000	-0.302636000
C	-0.404550000	-3.142089000	-2.814442000
H	0.320440000	-2.674867000	-3.489801000
H	-1.404670000	-2.994478000	-3.232563000
H	-0.207390000	-4.221917000	-2.841590000
C	2.310977000	-2.455765000	-1.368218000
H	2.691254000	-3.485712000	-1.334459000
H	3.041069000	-1.822072000	-0.857042000
H	2.293784000	-2.155554000	-2.420997000
C	1.719799000	-2.003140000	1.700579000
H	1.847839000	-2.952444000	2.237379000
H	2.695770000	-1.741976000	1.283275000
H	1.469532000	-1.248076000	2.450560000
C	-0.276125000	1.336307000	1.359669000
C	0.564101000	1.860612000	0.331700000
C	0.236612000	3.167779000	-0.132619000
C	-0.823199000	3.884278000	0.396168000
C	-1.638252000	3.325092000	1.396880000
C	-1.358902000	2.059435000	1.887574000
H	0.029093000	0.425163000	1.878476000
H	0.861760000	3.640073000	-0.885066000

H	-1.028224000	4.891620000	0.045322000
H	-1.949154000	1.645061000	2.699178000
C	1.517147000	0.972302000	-0.299192000
C	2.596120000	1.493696000	-1.226059000
H	1.923595000	0.250928000	0.420851000
H	2.175489000	2.190370000	-1.964077000
H	3.026835000	0.665815000	-1.800891000
C	-3.600333000	-0.440723000	-2.971829000
C	-2.504468000	0.292261000	-2.478958000
C	-2.722517000	1.161849000	-1.390384000
C	-3.984422000	1.291595000	-0.813772000
C	-5.054263000	0.563846000	-1.336694000
C	-4.865974000	-0.297464000	-2.423091000
H	-3.459891000	-1.108504000	-3.817989000
H	-1.931837000	1.823673000	-1.029525000
H	-4.143341000	1.974220000	0.014422000
H	-5.708997000	-0.848729000	-2.827026000
C	-1.188942000	0.127668000	-3.107423000
C	-0.116271000	0.935281000	-2.942885000
H	-1.091494000	-0.729612000	-3.769836000
H	0.816988000	0.729243000	-3.456701000
H	-0.172459000	1.877652000	-2.401708000
Cl	-6.625380000	0.732811000	-0.641324000
Cl	-2.969997000	4.240191000	2.033444000
Si	-1.703134000	-2.366803000	2.504302000
C	-3.383453000	-1.482881000	2.426502000
H	-4.123057000	-2.038340000	1.841876000
H	-3.781565000	-1.391333000	3.444352000
H	-3.312207000	-0.471090000	2.010874000
C	-1.966739000	-4.212788000	2.835860000
H	-2.501487000	-4.352271000	3.782831000
H	-2.553893000	-4.695815000	2.047851000
H	-1.008632000	-4.738771000	2.911160000
C	-0.747222000	-1.644709000	3.975783000
H	-1.389410000	-1.743437000	4.859943000
H	0.175554000	-2.193594000	4.184948000
H	-0.500260000	-0.581390000	3.879828000

$pTS2^b_{syn}$, $E_{(SCF_{Done})} = -2748.781328$ a.u. $IF = i178.46$ cm^{-1}

Sc	-0.483360000	-0.409476000	-0.571415000
N	5.613450000	0.185549000	-1.573362000
C	3.730662000	2.173391000	-0.571999000
H	4.449373000	2.694499000	-1.213382000
H	3.260602000	2.946595000	0.048138000

C	4. 421818000	1. 174180000	0. 327722000
C	5. 294540000	0. 181840000	-0. 182448000
C	5. 817778000	-0. 779094000	0. 692970000
H	6. 485054000	-1. 545693000	0. 310490000
C	5. 527213000	-0. 751368000	2. 056661000
H	5. 962015000	-1. 499680000	2. 714238000
C	4. 711925000	0. 251688000	2. 571326000
H	4. 501107000	0. 301531000	3. 636094000
C	4. 165811000	1. 196924000	1. 702377000
H	3. 520521000	1. 978797000	2. 099393000
C	5. 934330000	-1. 106614000	-2. 159136000
H	6. 926299000	-1. 495144000	-1. 868858000
H	5. 930974000	-1. 007287000	-3. 250439000
H	5. 178173000	-1. 845826000	-1. 878644000
C	6. 629432000	1. 174442000	-1. 937249000
H	6. 411467000	2. 142121000	-1. 480630000
H	6. 644248000	1. 300415000	-3. 025644000
H	7. 638306000	0. 870453000	-1. 609775000
C	0. 454031000	-2. 075787000	0. 953567000
C	-0. 964742000	-2. 016002000	1. 181371000
C	-1. 589274000	-2. 509284000	-0. 020382000
C	-0. 576609000	-2. 848578000	-0. 960985000
C	0. 688651000	-2. 552759000	-0. 367478000
C	-3. 059949000	-2. 760084000	-0. 213841000
H	-3. 431212000	-3. 471725000	0. 532754000
H	-3. 263056000	-3. 192664000	-1. 196133000
H	-3. 665573000	-1. 852633000	-0. 124722000
C	-0. 772301000	-3. 593198000	-2. 248152000
H	0. 056954000	-3. 440640000	-2. 946185000
H	-1. 699882000	-3. 318199000	-2. 758268000
H	-0. 823741000	-4. 672317000	-2. 051710000
C	2. 028750000	-2. 842357000	-0. 980680000
H	2. 322563000	-3. 883141000	-0. 789294000
H	2. 819218000	-2. 207500000	-0. 568338000
H	2. 024206000	-2. 706778000	-2. 067451000
C	1. 546854000	-1. 830818000	1. 956060000
H	1. 774078000	-2. 763999000	2. 489323000
H	2. 481727000	-1. 499320000	1. 494311000
H	1. 274263000	-1. 094985000	2. 715027000
C	-0. 027346000	1. 441048000	1. 184636000
C	0. 613582000	1. 891917000	0. 001974000
C	0. 262980000	3. 186801000	-0. 464372000
C	-0. 689274000	3. 954289000	0. 183632000
C	-1. 353513000	3. 451753000	1. 315127000

C	-1.016625000	2.205244000	1.823168000
H	0.349708000	0.557319000	1.696668000
H	0.761720000	3.600100000	-1.336135000
H	-0.931660000	4.948160000	-0.180509000
H	-1.481240000	1.847486000	2.736019000
C	1.462796000	0.986196000	-0.771461000
C	2.671709000	1.543641000	-1.502394000
H	1.761736000	0.100585000	-0.180276000
H	2.357350000	2.303487000	-2.230998000
H	3.165039000	0.749234000	-2.072029000
C	-3.124493000	-0.770741000	-3.108058000
C	-2.062485000	-0.002242000	-2.575677000
C	-2.402678000	1.019826000	-1.656036000
C	-3.732561000	1.266619000	-1.289604000
C	-4.746031000	0.495980000	-1.843145000
C	-4.440283000	-0.516755000	-2.766045000
H	-2.903838000	-1.546137000	-3.836376000
H	-1.648591000	1.737315000	-1.318874000
H	-3.970717000	2.070720000	-0.600966000
H	-5.243887000	-1.096426000	-3.209565000
C	-0.672410000	-0.314121000	-2.883127000
C	0.383284000	0.595296000	-2.733819000
H	-0.475904000	-1.257416000	-3.383104000
H	1.330569000	0.328377000	-3.188120000
H	0.174303000	1.663065000	-2.709706000
Cl	-6.395769000	0.790571000	-1.410148000
Cl	-2.559681000	4.416991000	2.098673000
Si	-1.903533000	-1.814972000	2.843315000
C	-3.499124000	-0.810577000	2.621729000
H	-4.261869000	-1.357558000	2.059711000
H	-3.920409000	-0.592660000	3.610592000
H	-3.331117000	0.148598000	2.118674000
C	-2.323494000	-3.557868000	3.457288000
H	-2.869652000	-3.498007000	4.406231000
H	-2.947370000	-4.114013000	2.750230000
H	-1.412633000	-4.141344000	3.631580000
C	-0.873849000	-0.980183000	4.203761000
H	-1.530009000	-0.840341000	5.071911000
H	-0.039576000	-1.608254000	4.531335000
H	-0.475731000	0.006170000	3.941664000

$pP2^b_{\text{syn}}, E_{(\text{SCF Done})} = -2748.815854 \text{ a.u.}$

Sc	0.879924000	-0.163000000	-0.405393000
N	-5.972313000	-1.350121000	-0.486230000

C	-4.367583000	-0.570296000	1.844466000
H	-5.264515000	-1.020738000	2.284161000
H	-3.901716000	0.009711000	2.651784000
C	-4.718041000	0.379095000	0.717528000
C	-5.444874000	-0.029156000	-0.428252000
C	-5.613316000	0.875794000	-1.485845000
H	-6.165089000	0.568240000	-2.368917000
C	-5.114869000	2.175799000	-1.416788000
H	-5.279085000	2.859756000	-2.245612000
C	-4.448697000	2.601011000	-0.271012000
H	-4.092419000	3.624340000	-0.184792000
C	-4.257207000	1.698769000	0.776497000
H	-3.733388000	2.026217000	1.673089000
C	-6.129381000	-1.923239000	-1.812789000
H	-6.978046000	-1.505506000	-2.382859000
H	-6.304256000	-3.000041000	-1.710507000
H	-5.214615000	-1.777383000	-2.395208000
C	-7.185409000	-1.542755000	0.307506000
H	-7.076392000	-1.096742000	1.298018000
H	-7.376222000	-2.614711000	0.430257000
H	-8.069088000	-1.085962000	-0.170231000
C	0.624690000	1.875013000	-1.707966000
C	2.027043000	1.633932000	-1.492469000
C	2.346370000	0.429179000	-2.216744000
C	1.164244000	-0.056207000	-2.848140000
C	0.095150000	0.824585000	-2.516131000
C	3.714734000	-0.161348000	-2.415112000
H	4.173902000	0.245304000	-3.325414000
H	3.679589000	-1.248085000	-2.529795000
H	4.391403000	0.057935000	-1.585519000
C	1.087536000	-1.182615000	-3.832710000
H	0.116746000	-1.687099000	-3.815403000
H	1.864182000	-1.933220000	-3.663694000
H	1.230145000	-0.797646000	-4.851315000
C	-1.307949000	0.725862000	-3.040807000
H	-1.404535000	1.284071000	-3.981836000
H	-2.051737000	1.136783000	-2.350615000
H	-1.589575000	-0.310278000	-3.251011000
C	-0.164112000	3.091789000	-1.307948000
H	-0.027639000	3.885112000	-2.054558000
H	-1.239712000	2.891165000	-1.263363000
H	0.145533000	3.510005000	-0.347926000
C	-0.751213000	0.824119000	1.304206000
C	-1.260299000	-0.416771000	1.726509000

C	-0.890890000	-0.855518000	3.009837000
C	-0.041652000	-0.109295000	3.820943000
C	0.481740000	1.103998000	3.359846000
C	0.123068000	1.583162000	2.101576000
H	-1.135097000	1.266709000	0.380636000
H	-1.277642000	-1.797687000	3.388783000
H	0.221618000	-0.463705000	4.813033000
H	0.474969000	2.554251000	1.769221000
C	-2.102214000	-1.269217000	0.802119000
C	-3.432145000	-1.719266000	1.427606000
H	-2.348144000	-0.661850000	-0.080826000
H	-3.241818000	-2.360081000	2.299957000
H	-3.956515000	-2.336930000	0.691138000
C	2.125089000	-3.313202000	-1.129843000
C	1.257708000	-2.591058000	-0.270682000
C	1.852287000	-2.068650000	0.914696000
C	3.201646000	-2.284358000	1.239358000
C	3.999445000	-3.014579000	0.370947000
C	3.453483000	-3.539663000	-0.811357000
H	1.717056000	-3.745615000	-2.039134000
H	1.212309000	-1.617692000	1.681830000
H	3.610805000	-1.904552000	2.170429000
H	4.080275000	-4.134529000	-1.469196000
C	-0.095438000	-2.183955000	-0.648254000
C	-1.260157000	-2.477638000	0.321833000
H	-0.337874000	-2.500394000	-1.663971000
H	-1.947131000	-3.171579000	-0.179827000
H	-0.886977000	-3.017197000	1.203933000
Cl	5.666898000	-3.297524000	0.747586000
Cl	1.540089000	2.027771000	4.370481000
Si	3.352731000	2.735779000	-0.647425000
C	4.128338000	1.798338000	0.814291000
H	4.600023000	0.853584000	0.522948000
H	4.906563000	2.419361000	1.274311000
H	3.389173000	1.586502000	1.597632000
C	4.672486000	3.183008000	-1.928503000
H	5.384911000	3.888361000	-1.484474000
H	5.239575000	2.317356000	-2.282522000
H	4.219438000	3.670670000	-2.798972000
C	2.648688000	4.362675000	0.023599000
H	3.493994000	4.956504000	0.392774000
H	2.149369000	4.954641000	-0.749683000
H	1.958629000	4.237328000	0.864862000

$pC2^{b_{iso}}$, $E_{(SCF Done)} = -2748.790207$ a.u.

Sc	-0.863129000	-0.400170000	-0.129653000
N	5.310444000	0.564949000	-0.343202000
C	3.545894000	-0.596850000	1.653547000
H	4.190935000	0.195827000	2.043542000
H	3.282408000	-1.238348000	2.503996000
C	4.256510000	-1.428312000	0.612695000
C	5.063677000	-0.840775000	-0.389747000
C	5.587491000	-1.651025000	-1.405067000
H	6.209844000	-1.208524000	-2.177230000
C	5.343081000	-3.023658000	-1.434057000
H	5.769087000	-3.629367000	-2.229807000
C	4.582899000	-3.613415000	-0.428980000
H	4.407118000	-4.685803000	-0.425329000
C	4.050889000	-2.811374000	0.580911000
H	3.452743000	-3.268017000	1.367592000
C	5.539647000	1.212714000	-1.624276000
H	6.529426000	0.997114000	-2.064808000
H	5.475574000	2.298329000	-1.486281000
H	4.771058000	0.909454000	-2.341411000
C	6.353155000	0.941369000	0.610998000
H	6.200546000	0.439052000	1.568909000
H	6.323327000	2.024295000	0.778414000
H	7.362058000	0.675393000	0.250707000
C	-0.752016000	-1.534905000	-2.265091000
C	-2.103779000	-1.076856000	-2.082182000
C	-2.051154000	0.362278000	-2.126280000
C	-0.694075000	0.769261000	-2.282944000
C	0.110449000	-0.404400000	-2.380863000
C	-3.225707000	1.296201000	-2.216718000
H	-3.554881000	1.373595000	-3.261050000
H	-2.970325000	2.309964000	-1.895223000
H	-4.089418000	0.959019000	-1.636702000
C	-0.194903000	2.175375000	-2.452122000
H	0.814186000	2.304695000	-2.046787000
H	-0.843418000	2.910713000	-1.967519000
H	-0.145944000	2.438448000	-3.517203000
C	1.569047000	-0.432772000	-2.725099000
H	1.696714000	-0.452598000	-3.815921000
H	2.084304000	-1.311157000	-2.326461000
H	2.094723000	0.452064000	-2.355076000
C	-0.276053000	-2.950677000	-2.434662000
H	-0.251772000	-3.211117000	-3.501341000
H	0.742229000	-3.091787000	-2.056455000

H	-0.925068000	-3.679306000	-1.946187000
C	-0.626268000	-2.506112000	1.221741000
C	0.363143000	-1.585070000	1.680916000
C	0.296578000	-1.241618000	3.059679000
C	-0.657067000	-1.784625000	3.902669000
C	-1.622373000	-2.680571000	3.410518000
C	-1.600069000	-3.053096000	2.075686000
H	-0.523174000	-2.937611000	0.221819000
H	1.037068000	-0.564463000	3.475527000
H	-0.661499000	-1.527380000	4.957948000
H	-2.307023000	-3.787741000	1.702404000
C	1.171782000	-0.898215000	0.687478000
C	2.261732000	0.071751000	1.099650000
H	1.496227000	-1.574659000	-0.112324000
H	1.883899000	0.775213000	1.857732000
H	2.558591000	0.685683000	0.241138000
C	-2.456088000	4.382738000	0.256212000
C	-1.767858000	3.351796000	0.922358000
C	-0.505677000	3.640743000	1.476821000
C	0.051900000	4.903198000	1.358744000
C	-0.653878000	5.908412000	0.686137000
C	-1.911476000	5.654753000	0.136807000
H	-3.441986000	4.188809000	-0.159837000
H	0.048999000	2.876314000	2.013736000
H	1.023977000	5.122354000	1.787991000
H	-2.452559000	6.445949000	-0.371372000
C	-2.408380000	2.049830000	1.033543000
C	-1.966792000	0.949892000	1.701457000
H	-3.376617000	1.975486000	0.539599000
H	-2.642375000	0.105435000	1.854980000
H	-1.084006000	0.974213000	2.337505000
Si	-3.742763000	-2.070218000	-1.974909000
C	-4.824963000	-1.619816000	-3.460772000
H	-5.741067000	-2.222011000	-3.444021000
H	-5.120543000	-0.566474000	-3.470520000
H	-4.302351000	-1.833576000	-4.399787000
C	-4.635161000	-1.638779000	-0.348598000
H	-4.876296000	-0.574795000	-0.249214000
H	-5.583751000	-2.186950000	-0.297076000
H	-4.046599000	-1.942372000	0.526649000
C	-3.489970000	-3.946902000	-1.980922000
H	-4.481564000	-4.414646000	-1.942064000
H	-2.997833000	-4.304254000	-2.890831000
H	-2.928656000	-4.314141000	-1.114599000

Cl	0.041872000	7.482509000	0.541851000
Cl	-2.812462000	-3.340231000	4.485500000

***p*TS2^b_{iso}, $E_{(\text{SCF Done})} = -2748.771727$ a.u. $\text{IF} = i-215.81\text{cm}^{-1}$**

Sc	-0.555652000	-0.590506000	-0.040972000
N	3.591401000	3.536366000	-0.386709000
C	0.829216000	3.807728000	-1.311142000
H	1.442870000	4.414196000	-1.985657000
H	-0.200829000	4.163709000	-1.435903000
C	1.238523000	3.989014000	0.134326000
C	2.571843000	3.800982000	0.574152000
C	2.850960000	3.867800000	1.946424000
H	3.870226000	3.726954000	2.293093000
C	1.851161000	4.144263000	2.877797000
H	2.102147000	4.205879000	3.933539000
C	0.548288000	4.376447000	2.447646000
H	-0.233248000	4.628619000	3.159430000
C	0.258377000	4.294121000	1.085168000
H	-0.759241000	4.474405000	0.742899000
C	4.733431000	2.770936000	0.087982000
H	5.417433000	3.345584000	0.736578000
H	5.313591000	2.433391000	-0.778219000
H	4.392230000	1.890956000	0.642343000
C	4.044206000	4.725444000	-1.111588000
H	3.195323000	5.327184000	-1.441763000
H	4.616777000	4.420373000	-1.994416000
H	4.686520000	5.368302000	-0.486232000
C	-1.747465000	-0.971714000	2.066293000
C	-1.997235000	-2.073911000	1.179479000
C	-0.739519000	-2.769910000	1.024905000
C	0.260326000	-2.072801000	1.756212000
C	-0.354904000	-0.937209000	2.370057000
C	-0.540675000	-4.104129000	0.368079000
H	-0.820700000	-4.907988000	1.060623000
H	0.503654000	-4.265625000	0.092960000
H	-1.151103000	-4.230670000	-0.531595000
C	1.666094000	-2.523784000	2.018015000
H	2.365201000	-1.686425000	2.102639000
H	2.045855000	-3.191730000	1.242906000
H	1.701809000	-3.067453000	2.971926000
C	0.320024000	0.010230000	3.322326000
H	0.223362000	-0.349270000	4.355619000
H	-0.108241000	1.017282000	3.291949000
H	1.390613000	0.103344000	3.116352000

C	-2.761632000	-0.115729000	2.767035000
H	-3.041114000	-0.595985000	3.714432000
H	-2.368120000	0.872178000	3.028396000
H	-3.677601000	0.013998000	2.192191000
C	-2.225752000	1.654212000	0.043224000
C	-1.426143000	1.596548000	-1.117143000
C	-2.089408000	1.690993000	-2.369379000
C	-3.461090000	1.839683000	-2.448033000
C	-4.230987000	1.886790000	-1.273330000
C	-3.619698000	1.798427000	-0.032639000
H	-1.748506000	1.737840000	1.017333000
H	-1.512996000	1.686292000	-3.290121000
H	-3.949457000	1.932264000	-3.413152000
H	-4.210384000	1.893196000	0.872039000
C	0.033998000	1.386138000	-1.033855000
C	0.930014000	2.347354000	-1.799151000
H	0.364906000	1.416694000	0.038228000
H	0.677816000	2.316718000	-2.867250000
H	1.976602000	2.037026000	-1.704731000
C	2.396074000	-3.492359000	-1.541061000
C	2.041817000	-2.143813000	-1.365824000
C	3.033047000	-1.265194000	-0.895404000
C	4.317470000	-1.710274000	-0.598040000
C	4.634115000	-3.057055000	-0.767544000
C	3.675660000	-3.950997000	-1.245537000
H	1.669148000	-4.190754000	-1.948395000
H	2.808922000	-0.208161000	-0.760694000
H	5.072139000	-1.018561000	-0.237524000
H	3.935788000	-4.993553000	-1.398995000
C	0.695380000	-1.664531000	-1.736310000
C	0.531302000	-0.386468000	-2.293618000
H	-0.041166000	-2.428237000	-1.995752000
H	-0.343093000	-0.202972000	-2.916523000
H	1.416883000	0.167563000	-2.586246000
Si	-3.633217000	-2.663346000	0.367377000
C	-3.938264000	-4.491118000	0.752546000
H	-4.928456000	-4.772223000	0.374432000
H	-3.206767000	-5.164308000	0.297877000
H	-3.936134000	-4.666298000	1.834274000
C	-3.446874000	-2.397144000	-1.511697000
H	-2.603975000	-2.954342000	-1.938278000
H	-4.349977000	-2.737508000	-2.032713000
H	-3.327243000	-1.333163000	-1.761505000
C	-5.159633000	-1.708383000	0.947291000

H	-6.036746000	-2.168219000	0.475515000
H	-5.303590000	-1.771745000	2.030771000
H	-5.152657000	-0.654463000	0.652904000
Cl	6.232916000	-3.621530000	-0.393302000
Cl	-5.945670000	2.091830000	-1.385960000

$pP2^b_{iso}$, $E_{(SCF Done)} = -2748.807625$ a.u.

Sc	1.351612000	0.210350000	0.125552000
N	-5.453012000	-0.790675000	-1.927764000
C	-3.681737000	-2.662308000	-0.466746000
H	-4.265803000	-3.404471000	-1.025731000
H	-3.169833000	-3.235426000	0.317763000
C	-4.587615000	-1.649864000	0.206501000
C	-5.393895000	-0.727442000	-0.506911000
C	-6.109203000	0.244116000	0.208621000
H	-6.723136000	0.958677000	-0.330522000
C	-6.075265000	0.298373000	1.600126000
H	-6.650322000	1.057899000	2.123269000
C	-5.335019000	-0.641369000	2.309828000
H	-5.326264000	-0.635140000	3.396466000
C	-4.604417000	-1.597564000	1.605516000
H	-4.025628000	-2.336898000	2.157493000
C	-5.763499000	0.450675000	-2.617577000
H	-6.823238000	0.751248000	-2.540038000
H	-5.537965000	0.325274000	-3.682603000
H	-5.142617000	1.262834000	-2.227663000
C	-6.265345000	-1.889433000	-2.446747000
H	-6.033550000	-2.822574000	-1.929843000
H	-6.056752000	-2.026255000	-3.513765000
H	-7.345465000	-1.698224000	-2.326988000
C	3.638885000	-0.179855000	0.884436000
C	3.641354000	-0.064554000	-0.550482000
C	3.277270000	1.299438000	-0.850850000
C	3.034395000	1.986393000	0.371412000
C	3.229900000	1.063621000	1.442922000
C	3.319679000	1.964764000	-2.195541000
H	4.289120000	2.457263000	-2.345453000
H	2.551875000	2.738180000	-2.292818000
H	3.183138000	1.255684000	-3.015342000
C	2.808254000	3.457733000	0.547308000
H	2.009998000	3.681839000	1.261694000
H	2.557911000	3.949055000	-0.394453000
H	3.724105000	3.927843000	0.929223000
C	3.139509000	1.403977000	2.903867000

H	4. 109496000	1. 757068000	3. 278801000
H	2. 857908000	0. 543595000	3. 520318000
H	2. 416493000	2. 204497000	3. 092550000
C	4. 122064000	-1. 333770000	1. 713944000
H	5. 197597000	-1. 223278000	1. 907871000
H	3. 632567000	-1. 373885000	2. 691335000
H	3. 984267000	-2. 299146000	1. 227161000
C	-1. 034659000	-1. 471617000	1. 552583000
C	-0. 765713000	-1. 583081000	0. 175413000
C	0. 390119000	-2. 301564000	-0. 194564000
C	1. 200975000	-2. 930219000	0. 757959000
C	0. 873536000	-2. 841264000	2. 114493000
C	-0. 232711000	-2. 088857000	2. 514923000
H	-1. 923555000	-0. 933486000	1. 874668000
H	0. 631000000	-2. 426719000	-1. 247878000
H	2. 056251000	-3. 518218000	0. 443104000
H	-0. 482534000	-2. 013432000	3. 569027000
C	-1. 702658000	-0. 999354000	-0. 863001000
C	-2. 646854000	-2. 078103000	-1. 442142000
H	-2. 338241000	-0. 258075000	-0. 362198000
H	-2. 044347000	-2. 899839000	-1. 853936000
H	-3. 185272000	-1. 617012000	-2. 276089000
C	-0. 093126000	3. 242960000	-1. 440064000
C	-0. 244769000	1. 939039000	-0. 905684000
C	-0. 647141000	1. 872335000	0. 454646000
C	-0. 903682000	3. 019254000	1. 222792000
C	-0. 761433000	4. 269268000	0. 642404000
C	-0. 364585000	4. 379928000	-0. 699591000
H	0. 193394000	3. 347651000	-2. 483423000
H	-0. 933885000	0. 918751000	0. 901623000
H	-1. 247068000	2. 928678000	2. 248791000
H	-0. 280358000	5. 363422000	-1. 152407000
C	0. 136411000	0. 728375000	-1. 659224000
C	-0. 949747000	-0. 306489000	-2. 012927000
H	0. 655788000	1. 010799000	-2. 578907000
H	-0. 476944000	-1. 074669000	-2. 641024000
H	-1. 711962000	0. 160197000	-2. 654513000
Si	4. 370459000	-1. 261354000	-1. 865422000
C	5. 860942000	-0. 398624000	-2. 653954000
H	6. 364553000	-1. 092784000	-3. 337264000
H	5. 585504000	0. 490760000	-3. 228214000
H	6. 586337000	-0. 097886000	-1. 889760000
C	3. 093775000	-1. 702300000	-3. 204565000
H	2. 571302000	-0. 832239000	-3. 615125000

H	3.607708000	-2.198762000	-4.036692000
H	2.339847000	-2.406181000	-2.832184000
C	4.997241000	-2.893508000	-1.130687000
H	5.455846000	-3.464352000	-1.947728000
H	5.767910000	-2.742516000	-0.368603000
H	4.209319000	-3.525059000	-0.706036000
Cl	-1.092412000	5.701210000	1.562005000
Cl	1.808817000	-3.691386000	3.293235000

pC1^a, $E_{(\text{SCF Done})} = -2023.442292$ a.u.

Sc	0.975432000	0.702958000	0.598819000
Si	0.640906000	3.089975000	-1.074405000
C	1.611830000	2.770513000	0.502349000
H	1.207569000	3.349891000	1.346768000
H	2.669145000	3.029940000	0.390679000
C	-0.245855000	1.356765000	-1.453312000
H	0.401459000	0.475370000	-1.645765000
H	-0.742775000	1.500080000	-2.419716000
H	-1.068083000	1.060326000	-0.775500000
C	-0.779696000	4.326084000	-0.913370000
H	-1.418183000	4.115247000	-0.047858000
H	-1.410232000	4.333975000	-1.809534000
H	-0.372172000	5.334546000	-0.779922000
C	1.716108000	3.438115000	-2.584672000
H	2.198932000	4.415780000	-2.475023000
H	1.122139000	3.457704000	-3.505165000
H	2.507326000	2.690189000	-2.702179000
C	3.105218000	-0.272537000	0.022005000
C	3.198137000	0.069817000	1.398302000
C	2.260049000	-0.739530000	2.113329000
C	1.603724000	-1.586983000	1.177043000
C	2.101152000	-1.295442000	-0.141680000
C	0.646273000	-2.688577000	1.542068000
H	1.124789000	-3.667603000	1.412079000
H	0.343662000	-2.631344000	2.592100000
H	-0.257723000	-2.694695000	0.925258000
C	3.980953000	0.309254000	-1.050991000
H	3.468051000	0.395023000	-2.011286000
H	4.351131000	1.301425000	-0.777604000
H	4.861183000	-0.327176000	-1.212867000
C	4.183514000	1.005804000	2.031845000
H	4.588862000	1.724529000	1.315492000
H	3.743364000	1.576501000	2.855913000
H	5.032174000	0.443059000	2.442925000

C	2.120661000	-0.764410000	3.609466000
H	1.135284000	-1.107999000	3.940350000
H	2.858024000	-1.448274000	4.050148000
H	2.301143000	0.219101000	4.056625000
C	-3.364116000	-1.348465000	1.213799000
C	-2.822417000	-0.060225000	1.379342000
C	-3.509546000	1.031995000	0.813043000
C	-4.676899000	0.841912000	0.091510000
C	-5.182567000	-0.453773000	-0.072602000
C	-4.532279000	-1.552592000	0.491795000
H	-2.865073000	-2.202544000	1.665231000
H	-3.147007000	2.045624000	0.959198000
H	-5.209770000	1.686176000	-0.333397000
H	-4.944065000	-2.548912000	0.370374000
C	-1.597128000	0.087196000	2.151655000
C	-0.843626000	1.205296000	2.327693000
H	-1.260318000	-0.822883000	2.648165000
H	-0.036899000	1.203354000	3.062444000
H	-1.146401000	2.180037000	1.947952000
Cl	-6.637246000	-0.689099000	-0.971621000
Si	1.770992000	-2.387929000	-1.685474000
C	2.269035000	-1.549861000	-3.312776000
H	3.350852000	-1.416114000	-3.405231000
H	1.953879000	-2.207649000	-4.132214000
H	1.784857000	-0.580269000	-3.476665000
C	2.794525000	-3.966987000	-1.479367000
H	2.518098000	-4.519249000	-0.574925000
H	2.640960000	-4.632191000	-2.337159000
H	3.863988000	-3.737564000	-1.419138000
C	-0.071203000	-2.837278000	-1.836640000
H	-0.380475000	-3.595833000	-1.111253000
H	-0.736310000	-1.971268000	-1.733452000
H	-0.243930000	-3.258941000	-2.834179000

***p*TS1^{a'}**, $E_{(\text{SCF Done})} = -2023.431289$ a.u. **IF = *i*211.80 cm⁻¹**

Sc	0.670289000	0.517097000	0.519006000
Si	1.204542000	2.901303000	-1.275675000
C	1.600328000	2.520505000	0.558489000
H	1.826106000	3.472321000	1.043904000
H	2.527530000	1.923278000	0.660076000
C	0.300580000	1.359581000	-2.006075000
H	0.919777000	0.455938000	-2.093020000
H	0.046595000	1.619625000	-3.041588000
H	-0.674421000	1.103591000	-1.558625000

C	0.073223000	4.408219000	-1.388268000
H	-0.850768000	4.316484000	-0.808515000
H	-0.204925000	4.593711000	-2.432015000
H	0.603974000	5.296714000	-1.027222000
C	2.771720000	3.173220000	-2.293316000
H	3.341351000	4.020245000	-1.895686000
H	2.516919000	3.400014000	-3.335374000
H	3.423250000	2.293853000	-2.287277000
C	2.456972000	-0.983802000	-0.155231000
C	2.764529000	-0.592490000	1.180698000
C	1.757706000	-1.124543000	2.039784000
C	0.830966000	-1.843094000	1.235222000
C	1.238517000	-1.750365000	-0.144186000
C	-0.269219000	-2.707178000	1.781599000
H	0.101367000	-3.729258000	1.931126000
H	-0.622300000	-2.358884000	2.756471000
H	-1.132611000	-2.767909000	1.114750000
C	3.374218000	-0.739822000	-1.321620000
H	2.847182000	-0.625019000	-2.270772000
H	3.996646000	0.147641000	-1.171403000
H	4.061532000	-1.587478000	-1.442279000
C	4.018177000	0.087186000	1.652798000
H	4.479603000	0.710926000	0.880574000
H	3.842823000	0.717869000	2.530803000
H	4.767616000	-0.661364000	1.942230000
C	1.807149000	-1.077356000	3.538841000
H	0.847947000	-1.331399000	3.999243000
H	2.538863000	-1.804140000	3.915552000
H	2.114243000	-0.096392000	3.918954000
C	-2.653562000	-0.240328000	1.901296000
C	-1.820817000	0.856637000	1.583557000
C	-2.200513000	1.658007000	0.484494000
C	-3.352360000	1.386583000	-0.255330000
C	-4.151470000	0.301452000	0.092586000
C	-3.804770000	-0.510576000	1.179593000
H	-2.410553000	-0.860280000	2.758824000
H	-1.631626000	2.551414000	0.239775000
H	-3.639075000	2.028975000	-1.082040000
H	-4.446683000	-1.340370000	1.458113000
C	-0.610252000	1.125019000	2.364109000
C	0.118260000	2.310377000	2.282375000
H	-0.358460000	0.415747000	3.147259000
H	0.901543000	2.483847000	3.013207000
H	-0.330427000	3.211316000	1.876367000

Cl	-5.588285000	-0.038042000	-0.808974000
Si	0.422447000	-2.767592000	-1.557112000
C	1.290853000	-2.553140000	-3.227924000
H	2.343593000	-2.851004000	-3.202451000
H	0.783900000	-3.212690000	-3.943328000
H	1.224213000	-1.536844000	-3.631518000
C	0.524982000	-4.599959000	-1.089993000
H	-0.089350000	-4.855316000	-0.221592000
H	0.174925000	-5.208415000	-1.932401000
H	1.558423000	-4.892893000	-0.874257000
C	-1.388614000	-2.246088000	-1.796929000
H	-1.969972000	-2.238312000	-0.869329000
H	-1.462629000	-1.250783000	-2.250402000
H	-1.878805000	-2.947317000	-2.483115000

$pP1^a$, $E_{(\text{SCF Done})} = -2023.458019$ a.u.

Sc	-0.280418000	-0.467558000	0.446874000
Si	-1.613735000	-2.735036000	-1.317574000
C	-1.393178000	-2.776556000	0.611478000
H	-2.054600000	-3.629376000	0.820675000
H	-1.948944000	-1.964998000	1.131338000
C	-1.073403000	-1.045441000	-2.061178000
H	-1.676605000	-0.191705000	-1.721274000
H	-1.285382000	-1.120293000	-3.135660000
H	-0.003495000	-0.786098000	-2.024613000
C	-0.620264000	-4.137421000	-2.091276000
H	0.460219000	-4.059468000	-1.931730000
H	-0.795322000	-4.162074000	-3.172974000
H	-0.947299000	-5.100461000	-1.682745000
C	-3.458608000	-2.911074000	-1.655587000
H	-3.831502000	-3.872946000	-1.286342000
H	-3.657008000	-2.869987000	-2.732572000
H	-4.040259000	-2.116162000	-1.176697000
C	-2.167803000	0.983337000	0.891310000
C	-1.694038000	0.565160000	2.170814000
C	-0.381312000	1.089189000	2.349196000
C	-0.036158000	1.814145000	1.173410000
C	-1.140668000	1.761077000	0.247347000
C	1.222182000	2.624483000	1.025246000
H	1.104349000	3.596628000	1.521426000
H	2.085949000	2.133740000	1.482649000
H	1.473180000	2.821744000	-0.019207000
C	-3.561635000	0.721650000	0.388860000
H	-3.614748000	0.625853000	-0.698063000

H	-3.993934000	-0.183519000	0.828326000
H	-4.227317000	1.549475000	0.666119000
C	-2.462756000	-0.185209000	3.220200000
H	-3.303961000	-0.748591000	2.804879000
H	-1.827146000	-0.888214000	3.769784000
H	-2.882961000	0.511284000	3.957604000
C	0.406798000	1.046138000	3.622184000
H	0.208543000	0.140799000	4.203610000
H	1.483812000	1.108165000	3.443862000
H	0.138309000	1.901007000	4.257374000
C	2.984211000	-0.657681000	1.630468000
C	1.930541000	-1.418197000	1.048630000
C	1.953187000	-1.539976000	-0.368511000
C	2.960465000	-0.948835000	-1.155047000
C	3.957644000	-0.212242000	-0.541203000
C	3.977442000	-0.085702000	0.861321000
H	3.028363000	-0.566875000	2.712144000
H	1.299590000	-2.268610000	-0.849360000
H	2.976577000	-1.098769000	-2.230439000
H	4.789667000	0.458543000	1.334041000
C	0.776593000	-1.855653000	1.796586000
C	-0.035762000	-3.071738000	1.342808000
H	0.855289000	-1.742204000	2.874953000
H	-0.289016000	-3.635134000	2.246359000
H	0.562362000	-3.748616000	0.718476000
Si	-1.260543000	2.888950000	-1.305700000
C	-2.906546000	2.706498000	-2.227822000
H	-3.772675000	2.932249000	-1.598316000
H	-2.900829000	3.436906000	-3.046449000
H	-3.054154000	1.720973000	-2.683400000
C	-1.130978000	4.677270000	-0.699532000
H	-0.162718000	4.896634000	-0.239661000
H	-1.261201000	5.364322000	-1.544023000
H	-1.912872000	4.898299000	0.035491000
C	0.118164000	2.524196000	-2.563048000
H	1.127441000	2.562704000	-2.141217000
H	-0.014204000	1.548292000	-3.044065000
H	0.072749000	3.279967000	-3.356814000
Cl	5.210336000	0.525055000	-1.485407000

$pC2^a_{\text{syn}}, E_{(\text{SCF Done})} = -2792.555247 \text{ a.u.}$

Sc	0.665751000	0.629997000	-0.221214000
Si	5.572584000	-1.376879000	1.185905000
C	3.836495000	-0.884374000	0.518837000

C	6. 760466000	0. 086305000	0. 983291000
C	6. 211665000	-2. 879335000	0. 223615000
C	5. 379130000	-1. 814519000	3. 019901000
C	3. 171859000	3. 119094000	-0. 627234000
C	1. 759474000	2. 821411000	-0. 223118000
C	1. 295817000	2. 589822000	1. 106786000
C	-0. 131078000	2. 551371000	1. 080076000
C	-0. 572970000	2. 712764000	-0. 278406000
C	0. 616504000	2. 889567000	-1. 070559000
C	2. 156638000	2. 546797000	2. 338089000
C	-0. 983644000	2. 551009000	2. 317418000
C	0. 680854000	3. 217685000	-2. 536478000
C	3. 787971000	-0. 444783000	-0. 955213000
C	2. 411699000	-0. 059724000	-1. 482819000
H	3. 464204000	-0. 067924000	1. 161566000
H	3. 172197000	-1. 744943000	0. 689564000
H	6. 888162000	0. 366243000	-0. 068628000
H	7. 751052000	-0. 171063000	1. 375528000
H	6. 411123000	0. 969971000	1. 530692000
H	5. 531533000	-3. 734589000	0. 313481000
H	7. 186031000	-3. 193172000	0. 615649000
H	6. 343485000	-2. 659726000	-0. 841885000
H	5. 006021000	-0. 963241000	3. 601641000
H	6. 343094000	-2. 109041000	3. 450427000
H	4. 686180000	-2. 652278000	3. 161728000
H	3. 902684000	2. 615450000	0. 011769000
H	3. 365622000	4. 197630000	-0. 553416000
H	3. 376212000	2. 827452000	-1. 661807000
H	3. 185600000	2. 254478000	2. 108591000
H	1. 775970000	1. 854450000	3. 097168000
H	2. 203903000	3. 537951000	2. 808382000
H	-0. 445497000	2. 146261000	3. 180336000
H	-1. 914199000	1. 994210000	2. 195083000
H	-1. 256903000	3. 581483000	2. 580137000
H	-0. 237033000	2. 948657000	-3. 065129000
H	1. 517111000	2. 721860000	-3. 042402000
H	0. 828040000	4. 296611000	-2. 675820000
H	4. 228301000	-1. 234175000	-1. 584851000
H	4. 448940000	0. 419309000	-1. 082262000
H	2. 441344000	0. 757407000	-2. 212875000
C	1. 604587000	-2. 471942000	-1. 637737000
C	1. 453382000	-1. 078773000	-1. 871624000
C	0. 170460000	-0. 656254000	-2. 331530000
C	-0. 876037000	-1. 560910000	-2. 573610000

C	-0.672591000	-2.912056000	-2.336373000
C	0.576995000	-3.366934000	-1.881176000
H	2.564890000	-2.853644000	-1.305221000
H	0.042936000	0.374230000	-2.683709000
H	-1.821337000	-1.210407000	-2.975528000
H	0.733571000	-4.431311000	-1.731686000
C	-3.277316000	-0.584288000	2.790002000
C	-2.344439000	-1.115256000	1.879080000
C	-2.819496000	-1.937406000	0.838442000
C	-4.171819000	-2.206128000	0.704663000
C	-5.077555000	-1.657991000	1.621270000
C	-4.634962000	-0.849502000	2.669613000
H	-2.931119000	0.034184000	3.614676000
H	-2.128684000	-2.384782000	0.130439000
H	-4.531337000	-2.844592000	-0.095496000
H	-5.346590000	-0.442428000	3.380133000
C	-0.934591000	-0.828350000	2.087472000
C	0.137005000	-1.271445000	1.374386000
H	-0.725835000	-0.201125000	2.953343000
H	1.138906000	-1.129543000	1.784864000
H	0.042606000	-2.012165000	0.580367000
Cl	-6.763102000	-1.995984000	1.455026000
Cl	-1.949200000	-4.053015000	-2.629826000
Si	-2.349613000	3.032668000	-0.938918000
C	-3.674273000	2.891794000	0.406294000
H	-3.523060000	3.600200000	1.226423000
H	-4.639573000	3.131302000	-0.056823000
H	-3.757104000	1.882971000	0.824443000
C	-2.817948000	1.783471000	-2.293223000
H	-2.128901000	1.771308000	-3.144578000
H	-2.887251000	0.769096000	-1.882528000
H	-3.809159000	2.040430000	-2.685898000
C	-2.394640000	4.796951000	-1.624102000
H	-3.411884000	5.035723000	-1.956583000
H	-2.118646000	5.521234000	-0.849556000
H	-1.724690000	4.943609000	-2.476660000

***p*TS2^{a'}_{syn}, $E_{(\text{SCF Done})} = -2792.533793$ a.u. IF = $i144.69$ cm⁻¹**

Sc	-0.178968000	-0.685259000	0.054823000
Si	6.283937000	0.125146000	-0.616909000
C	4.467481000	0.641266000	-0.242556000
C	6.292195000	-1.230001000	-1.944031000
C	7.103179000	-0.510319000	0.968838000
C	7.179168000	1.665283000	-1.257102000

C	1.071154000	-3.379357000	2.081933000
C	-0.045021000	-2.880904000	1.208097000
C	-0.188181000	-3.145325000	-0.185051000
C	-1.469396000	-2.671577000	-0.593214000
C	-2.119482000	-2.060516000	0.536661000
C	-1.222900000	-2.216638000	1.652980000
C	0.792048000	-3.916718000	-1.020698000
C	-2.084529000	-2.966624000	-1.929808000
C	-1.536673000	-1.940682000	3.097321000
C	3.600200000	-0.476438000	0.347568000
C	2.100982000	-0.260602000	0.580125000
H	4.054602000	1.031884000	-1.182302000
H	4.522195000	1.486633000	0.455234000
H	5.796049000	-2.147220000	-1.605806000
H	7.323474000	-1.497803000	-2.201779000
H	5.801917000	-0.895125000	-2.865827000
H	7.079664000	0.244340000	1.763452000
H	8.154357000	-0.756612000	0.779624000
H	6.618724000	-1.417571000	1.347656000
H	6.706497000	2.054681000	-2.166207000
H	8.222137000	1.432774000	-1.500530000
H	7.185039000	2.466483000	-0.509224000
H	2.003093000	-3.521108000	1.525516000
H	0.806040000	-4.355178000	2.509889000
H	1.281785000	-2.713062000	2.925765000
H	1.830975000	-3.687718000	-0.758825000
H	0.670195000	-3.724682000	-2.090704000
H	0.657642000	-4.996721000	-0.875253000
H	-1.330180000	-3.121840000	-2.707615000
H	-2.763959000	-2.181467000	-2.262830000
H	-2.665421000	-3.896626000	-1.872578000
H	-2.185991000	-1.071712000	3.232055000
H	-0.636098000	-1.786918000	3.701856000
H	-2.054697000	-2.801875000	3.537979000
H	4.022965000	-0.739612000	1.329451000
H	3.704529000	-1.388711000	-0.255731000
H	1.741793000	-1.166879000	1.105388000
C	1.808494000	2.263125000	0.806069000
C	1.517260000	0.925560000	1.195416000
C	0.443063000	0.752924000	2.113008000
C	-0.341109000	1.831061000	2.553756000
C	-0.035885000	3.114726000	2.126959000
C	1.063152000	3.329755000	1.276741000
H	2.631962000	2.461258000	0.130155000

H	0.318134000	-0.204882000	2.612369000
H	-1.144818000	1.668899000	3.264919000
H	1.314513000	4.342993000	0.977521000
C	-1.896441000	0.256735000	-3.157295000
C	-0.826949000	0.435828000	-2.250383000
C	-0.924712000	1.508860000	-1.334727000
C	-2.024890000	2.374616000	-1.334182000
C	-3.045753000	2.179834000	-2.255809000
C	-2.976003000	1.122604000	-3.175927000
H	-1.844446000	-0.544364000	-3.888718000
H	-0.079580000	1.774149000	-0.692573000
H	-2.067965000	3.205866000	-0.637905000
H	-3.769527000	0.994485000	-3.905625000
C	0.309302000	-0.482057000	-2.227968000
C	1.563119000	-0.142207000	-1.727124000
H	0.192160000	-1.430579000	-2.743381000
H	2.391078000	-0.815074000	-1.918487000
H	1.829368000	0.903409000	-1.602772000
Si	-3.949180000	-1.502295000	0.732219000
C	-4.911658000	-1.509427000	-0.897338000
H	-4.977004000	-2.505197000	-1.346466000
H	-5.935279000	-1.183492000	-0.675070000
H	-4.502500000	-0.814860000	-1.637712000
C	-4.795934000	-2.723508000	1.907717000
H	-4.398248000	-2.682034000	2.926258000
H	-5.866718000	-2.493528000	1.962420000
H	-4.694616000	-3.752512000	1.545026000
C	-4.049752000	0.258418000	1.439216000
H	-3.628407000	0.349585000	2.445631000
H	-3.549786000	0.985055000	0.788647000
H	-5.103928000	0.553938000	1.504761000
Cl	-4.406042000	3.248665000	-2.281441000
Cl	-0.975318000	4.464446000	2.670357000

$pP2^{a'}_{\text{syn}}, E_{(\text{SCF Done})} = -2792.569233 \text{ a.u.}$

Sc	-0.613021000	-0.628179000	0.008753000
Si	6.489916000	-0.266847000	-0.614128000
C	4.640431000	0.261243000	-0.689599000
C	6.738427000	-1.845769000	-1.633402000
C	6.984446000	-0.567267000	1.190964000
C	7.508563000	1.150820000	-1.346142000
C	0.609724000	-3.232345000	2.143001000
C	-0.550348000	-2.685336000	1.359587000
C	-0.897005000	-3.074758000	0.028908000

C	-2.151911000	-2.483223000	-0.286048000
C	-2.588998000	-1.688758000	0.833272000
C	-1.587262000	-1.845594000	1.856739000
C	-0.143275000	-4.069648000	-0.802615000
C	-2.918782000	-2.784693000	-1.540945000
C	-1.667784000	-1.344998000	3.272665000
C	3.663566000	-0.761675000	-0.113069000
C	2.145593000	-0.435368000	-0.250374000
H	4.409375000	0.470713000	-1.743820000
H	4.564616000	1.215555000	-0.151471000
H	6.182445000	-2.696710000	-1.223026000
H	7.798385000	-2.124992000	-1.643096000
H	6.426422000	-1.705834000	-2.674977000
H	6.820400000	0.325585000	1.805537000
H	8.049243000	-0.819464000	1.254614000
H	6.425705000	-1.396395000	1.640301000
H	7.230330000	1.349113000	-2.387597000
H	8.576702000	0.905639000	-1.330202000
H	7.373858000	2.078091000	-0.777441000
H	1.485459000	-3.428537000	1.515417000
H	0.332340000	-4.189163000	2.604850000
H	0.924026000	-2.574151000	2.960239000
H	0.939292000	-3.999968000	-0.653540000
H	-0.338299000	-3.948121000	-1.871339000
H	-0.437988000	-5.093281000	-0.535293000
H	-2.253797000	-3.054394000	-2.366506000
H	-3.541695000	-1.951911000	-1.867533000
H	-3.581211000	-3.644497000	-1.373389000
H	-2.205082000	-0.396579000	3.356005000
H	-0.679922000	-1.214675000	3.728062000
H	-2.200705000	-2.071888000	3.898976000
H	3.876845000	-0.919543000	0.951941000
H	3.809130000	-1.732918000	-0.605512000
H	1.657361000	-1.338678000	0.183612000
C	2.009605000	2.081861000	0.224036000
C	1.722650000	0.753207000	0.593093000
C	1.003358000	0.558275000	1.786512000
C	0.556426000	1.630787000	2.570288000
C	0.856839000	2.929562000	2.173442000
C	1.598164000	3.153971000	1.006925000
H	2.563870000	2.284395000	-0.686671000
H	0.862366000	-0.454596000	2.168862000
H	0.010951000	1.453077000	3.491314000
H	1.840878000	4.170713000	0.713427000

C	-1.850008000	-0.039843000	-3.236475000
C	-0.790027000	0.220751000	-2.325663000
C	-0.912393000	1.406478000	-1.548917000
C	-1.993206000	2.293400000	-1.700956000
C	-2.988519000	2.003475000	-2.618479000
C	-2.909179000	0.833250000	-3.394498000
H	-1.798506000	-0.929347000	-3.858139000
H	-0.071110000	1.748479000	-0.942364000
H	-2.029556000	3.213896000	-1.126536000
H	-3.681330000	0.628087000	-4.130054000
C	0.239628000	-0.761770000	-2.031781000
C	1.688638000	-0.338487000	-1.741546000
H	0.172973000	-1.654929000	-2.650463000
H	2.341789000	-1.010564000	-2.309677000
H	1.889454000	0.672026000	-2.119044000
Si	-4.270534000	-0.803200000	1.126327000
C	-5.423947000	-0.895634000	-0.369752000
H	-5.656048000	-1.925050000	-0.659383000
H	-6.368758000	-0.413231000	-0.090371000
H	-5.035620000	-0.362515000	-1.243552000
C	-5.129916000	-1.654169000	2.583736000
H	-4.585975000	-1.543842000	3.526689000
H	-6.126352000	-1.218389000	2.723738000
H	-5.259176000	-2.724734000	2.389345000
C	-3.983526000	1.036321000	1.510180000
H	-3.396097000	1.214016000	2.417338000
H	-3.491053000	1.545906000	0.673377000
H	-4.953630000	1.526816000	1.656050000
Cl	-4.324120000	3.087246000	-2.834044000
Cl	0.327059000	4.270685000	3.127466000

pC2^{a'}_{iso}, $E_{(\text{SCF Done})} = -2792.549432$ a.u.

Sc	-0.848154000	-0.258586000	0.156297000
Si	3.507853000	3.972876000	0.062776000
C	1.782850000	3.446261000	0.710169000
C	3.596545000	3.682000000	-1.813801000
C	4.847563000	2.945425000	0.931684000
C	3.750844000	5.811362000	0.440895000
C	-1.326276000	0.016414000	3.686303000
C	-1.506837000	-0.819691000	2.455451000
C	-0.608248000	-1.835699000	2.014171000
C	-1.232341000	-2.539449000	0.943828000
C	-2.507644000	-1.932471000	0.667069000
C	-2.673505000	-0.880965000	1.634634000

C	0.714156000	-2.163728000	2.646077000
C	-0.725209000	-3.836890000	0.380419000
C	-3.925234000	-0.086966000	1.882318000
C	1.357235000	1.999379000	0.401407000
C	-0.019119000	1.643292000	0.988754000
H	1.035023000	4.138368000	0.297424000
H	1.767662000	3.602149000	1.798606000
H	3.497862000	2.620966000	-2.075291000
H	4.558575000	4.025544000	-2.211132000
H	2.808335000	4.233150000	-2.340264000
H	4.831643000	3.112484000	2.014902000
H	5.844644000	3.222441000	0.570232000
H	4.719185000	1.869733000	0.760085000
H	2.990779000	6.424088000	-0.057112000
H	4.733192000	6.154534000	0.096802000
H	3.687849000	6.007050000	1.517387000
H	-0.270575000	0.198411000	3.907561000
H	-1.755123000	-0.496931000	4.557267000
H	-1.822937000	0.988077000	3.611573000
H	1.206943000	-1.271305000	3.045528000
H	1.406512000	-2.635642000	1.941724000
H	0.582642000	-2.860480000	3.484581000
H	0.365389000	-3.909562000	0.422605000
H	-1.047296000	-4.011381000	-0.650516000
H	-1.116661000	-4.670374000	0.978246000
H	-4.359730000	0.331908000	0.971842000
H	-3.745056000	0.739694000	2.572693000
H	-4.687603000	-0.729136000	2.341106000
H	2.107417000	1.304533000	0.804312000
H	1.372727000	1.862885000	-0.690310000
H	-0.025226000	1.808779000	2.068172000
C	-1.469319000	1.933890000	-1.030503000
C	-1.214799000	2.189717000	0.347570000
C	-2.277599000	2.789072000	1.070846000
C	-3.471604000	3.141752000	0.466832000
C	-3.684334000	2.871421000	-0.894564000
C	-2.683947000	2.275749000	-1.648157000
H	-0.648147000	1.625623000	-1.681144000
H	-2.126673000	3.020248000	2.121962000
H	-4.250787000	3.635093000	1.040151000
H	-2.826887000	2.109233000	-2.711566000
C	3.046636000	-3.382994000	-0.977636000
C	2.566087000	-2.087000000	-1.245956000
C	3.465074000	-1.007140000	-1.144496000

C	4.784694000	-1.211934000	-0.777311000
C	5.232100000	-2.511419000	-0.507701000
C	4.367271000	-3.602159000	-0.610438000
H	2.377504000	-4.234672000	-1.074339000
H	3.137251000	0.004246000	-1.364575000
H	5.475708000	-0.378639000	-0.706000000
H	4.730407000	-4.604692000	-0.410769000
C	1.179511000	-1.937764000	-1.654219000
C	0.503827000	-0.803126000	-1.987250000
H	0.629356000	-2.874049000	-1.726629000
H	-0.467464000	-0.897561000	-2.477150000
H	1.015258000	0.151705000	-2.092853000
Cl	6.877828000	-2.764784000	-0.051982000
Cl	-5.189615000	3.309500000	-1.634423000
Si	-3.768916000	-2.604223000	-0.613181000
C	-3.024449000	-2.486423000	-2.363880000
H	-2.066715000	-3.008189000	-2.472481000
H	-3.717201000	-2.936675000	-3.085131000
H	-2.890843000	-1.440051000	-2.669273000
C	-4.164291000	-4.407995000	-0.194700000
H	-4.565051000	-4.491849000	0.821665000
H	-4.928347000	-4.783609000	-0.885625000
H	-3.295267000	-5.068270000	-0.270559000
C	-5.391843000	-1.633198000	-0.647075000
H	-5.914754000	-1.648636000	0.313800000
H	-5.265029000	-0.590371000	-0.955975000
H	-6.048761000	-2.112221000	-1.383662000

***p*TS2^a_{iso}, $E_{(\text{SCF Done})} = -2792.52955$ a.u. IF = *i*180.37 cm⁻¹**

Sc	0.321610000	-0.608313000	0.198765000
Si	-2.623679000	5.063190000	-0.666991000
C	-2.165309000	3.193288000	-0.658911000
C	-1.051654000	6.092537000	-0.921169000
C	-3.446083000	5.513040000	0.980229000
C	-3.827955000	5.337797000	-2.101150000
C	0.656113000	-1.889979000	3.453683000
C	0.836696000	-2.177639000	1.988803000
C	2.051438000	-1.984806000	1.256122000
C	1.855338000	-2.490268000	-0.058591000
C	0.500266000	-2.974316000	-0.170931000
C	-0.100223000	-2.819141000	1.127444000
C	3.342490000	-1.485628000	1.837272000
C	2.950692000	-2.677593000	-1.065262000
C	-1.421622000	-3.371899000	1.574763000

C	-1.205098000	2.778983000	0.457824000
C	-0.801415000	1.296081000	0.515091000
H	-1.750206000	2.959541000	-1.648657000
H	-3.106055000	2.632259000	-0.575656000
H	-0.340503000	5.972581000	-0.095561000
H	-1.301754000	7.158032000	-0.981557000
H	-0.540949000	5.822384000	-1.852927000
H	-4.333113000	4.896260000	1.165813000
H	-3.770031000	6.560104000	0.967920000
H	-2.764586000	5.393425000	1.830400000
H	-3.374654000	5.071883000	-3.063068000
H	-4.127807000	6.390468000	-2.156728000
H	-4.738814000	4.740341000	-1.979559000
H	1.229915000	-1.015172000	3.778077000
H	1.006199000	-2.737662000	4.057322000
H	-0.391502000	-1.720054000	3.720012000
H	3.183516000	-0.756759000	2.638205000
H	3.983672000	-1.017371000	1.086667000
H	3.904277000	-2.321602000	2.275367000
H	3.752958000	-1.948456000	-0.933241000
H	2.596800000	-2.610431000	-2.098400000
H	3.398948000	-3.672135000	-0.943635000
H	-2.224779000	-3.199875000	0.856009000
H	-1.731355000	-2.951208000	2.533890000
H	-1.338910000	-4.457548000	1.713416000
H	-1.665945000	3.026816000	1.425920000
H	-0.286791000	3.381643000	0.413651000
H	-0.166038000	1.193221000	1.436943000
C	-2.658921000	-0.098327000	-0.515044000
C	-1.964830000	0.346034000	0.630882000
C	-2.477954000	-0.031962000	1.890045000
C	-3.648137000	-0.772243000	2.007106000
C	-4.319583000	-1.180461000	0.851877000
C	-3.821860000	-0.857183000	-0.412062000
H	-2.314795000	0.195252000	-1.503562000
H	-1.975880000	0.308337000	2.793223000
H	-4.046129000	-1.030006000	2.983482000
H	-4.355351000	-1.174692000	-1.302229000
C	4.118304000	0.572312000	-1.385846000
C	2.881051000	0.952430000	-0.835304000
C	2.902238000	1.810489000	0.280100000
C	4.098928000	2.256841000	0.834725000
C	5.307882000	1.851505000	0.272887000
C	5.319809000	1.014821000	-0.845099000

H	4.139459000	-0.049665000	-2.276802000
H	1.970565000	2.161228000	0.721018000
H	4.095919000	2.921154000	1.693119000
H	6.264765000	0.725910000	-1.294252000
C	1.614780000	0.503005000	-1.443764000
C	0.477138000	1.312140000	-1.405126000
H	1.670735000	-0.278170000	-2.201876000
H	-0.341217000	1.091970000	-2.087939000
H	0.568354000	2.359885000	-1.143526000
Cl	6.804914000	2.401239000	0.955572000
Cl	-5.777350000	-2.097878000	0.988441000
Si	-0.184015000	-3.870168000	-1.726011000
C	-0.213959000	-2.652694000	-3.190801000
H	0.776781000	-2.272270000	-3.461682000
H	-0.616423000	-3.158772000	-4.076714000
H	-0.870220000	-1.794682000	-2.992248000
C	0.923897000	-5.350875000	-2.125269000
H	0.998930000	-6.024802000	-1.264568000
H	0.486851000	-5.918593000	-2.955314000
H	1.937004000	-5.061630000	-2.418490000
C	-1.952997000	-4.504222000	-1.500823000
H	-2.040207000	-5.233855000	-0.690074000
H	-2.678872000	-3.703513000	-1.325565000
H	-2.244210000	-5.011067000	-2.429088000

pP2^a_{iso}, $E_{(\text{SCF Done})} = -2792.571073$ a.u.

Sc	1.136439000	-0.150007000	0.121454000
Si	-6.161639000	0.809859000	-0.761052000
C	-4.259391000	0.551090000	-0.674736000
C	-6.573966000	2.121259000	-2.065819000
C	-6.798633000	1.359683000	0.938625000
C	-6.936258000	-0.851457000	-1.240872000
C	3.784067000	-0.900707000	2.311284000
C	3.166109000	-1.219346000	0.979011000
C	3.508946000	-0.608603000	-0.264131000
C	2.753738000	-1.248602000	-1.290153000
C	1.932046000	-2.271677000	-0.692343000
C	2.228903000	-2.258956000	0.717217000
C	4.604034000	0.397348000	-0.457934000
C	2.945603000	-0.990069000	-2.756219000
C	1.804819000	-3.252178000	1.762226000
C	-3.450903000	1.809748000	-0.357967000
C	-1.907244000	1.636175000	-0.226002000
H	-3.951289000	0.122531000	-1.638476000

H	-4.082165000	-0.226563000	0.083265000
H	-6.160108000	3.102600000	-1.807034000
H	-7.660175000	2.238334000	-2.155964000
H	-6.189850000	1.841217000	-3.053616000
H	-6.549001000	0.628701000	1.716626000
H	-7.889787000	1.462040000	0.920692000
H	-6.385098000	2.329576000	1.238375000
H	-6.577199000	-1.190794000	-2.219389000
H	-8.027438000	-0.767163000	-1.300254000
H	-6.704223000	-1.631504000	-0.506418000
H	4.130648000	0.136314000	2.366901000
H	4.660186000	-1.538030000	2.491241000
H	3.094847000	-1.071190000	3.145510000
H	4.636125000	1.145319000	0.340472000
H	4.511087000	0.928037000	-1.407547000
H	5.577820000	-0.110386000	-0.461097000
H	3.121966000	0.069344000	-2.965520000
H	2.087440000	-1.308664000	-3.351279000
H	3.822638000	-1.537630000	-3.125318000
H	0.902425000	-3.798096000	1.487940000
H	1.642074000	-2.789992000	2.741393000
H	2.598496000	-3.999331000	1.898482000
H	-3.814168000	2.258133000	0.576297000
H	-3.615588000	2.564486000	-1.138190000
H	-1.519994000	2.638799000	0.006294000
C	-1.304906000	-0.623508000	0.834919000
C	-1.569257000	0.755161000	0.957134000
C	-1.547738000	1.296907000	2.255108000
C	-1.272431000	0.520155000	3.376230000
C	-1.013110000	-0.845669000	3.226335000
C	-1.036234000	-1.424443000	1.957298000
H	-1.390631000	-1.105564000	-0.140981000
H	-1.760203000	2.355494000	2.389880000
H	-1.266372000	0.964553000	4.366933000
H	-0.885126000	-2.491933000	1.845942000
C	2.150894000	2.599374000	-2.021147000
C	1.185083000	2.029546000	-1.152807000
C	1.302132000	2.391245000	0.218847000
C	2.284159000	3.281112000	0.684948000
C	3.187229000	3.825486000	-0.213862000
C	3.111254000	3.490155000	-1.575418000
H	2.097514000	2.365583000	-3.081348000
H	0.516931000	2.117623000	0.930337000
H	2.317160000	3.564179000	1.732639000

H	3.807965000	3.941509000	-2.275607000
C	0.260175000	0.971054000	-1.592118000
C	-1.267548000	1.183888000	-1.544289000
H	0.525565000	0.638400000	-2.599692000
H	-1.737454000	0.250276000	-1.877859000
H	-1.550251000	1.931775000	-2.301125000
Cl	4.402108000	4.933273000	0.332573000
Cl	-0.693800000	-1.821191000	4.619096000
Si	0.952040000	-3.563159000	-1.726091000
C	-0.371022000	-2.730950000	-2.808465000
H	0.017965000	-1.947515000	-3.465666000
H	-0.833745000	-3.493972000	-3.446363000
H	-1.173676000	-2.294377000	-2.201760000
C	2.201063000	-4.488667000	-2.805987000
H	2.975478000	-4.957215000	-2.188359000
H	1.692434000	-5.283632000	-3.364119000
H	2.697575000	-3.837789000	-3.532173000
C	0.035758000	-4.843713000	-0.669745000
H	0.707742000	-5.459428000	-0.064066000
H	-0.728266000	-4.410129000	-0.014025000
H	-0.486561000	-5.518025000	-1.359892000

***o*C1st**, $E_{(\text{SCF Done})} = -769.0727791$ a.u.

C	-2.357935000	-0.717382000	0.000016000
C	-1.770739000	0.542866000	-0.000086000
C	-0.381950000	0.660249000	0.000005000
C	0.465892000	-0.464118000	0.000193000
C	-0.167894000	-1.720531000	0.000328000
C	-1.548824000	-1.854101000	0.000226000
H	-2.379736000	1.441112000	-0.000244000
H	-1.994977000	-2.844837000	0.000346000
C	1.928702000	-0.329883000	0.000300000
C	2.826584000	-1.322832000	-0.000467000
H	2.300350000	0.691135000	0.001049000
H	3.889749000	-1.101498000	-0.000261000
H	2.558393000	-2.376148000	-0.001371000
H	-3.440669000	-0.807687000	-0.000049000
H	0.448253000	-2.614780000	0.000586000
Cl	0.273860000	2.285123000	-0.000185000

***o*C1^a**, $E_{(\text{SCF Done})} = -2255.82822$ a.u.

Sc	-0.613310000	0.016630000	-0.225465000
Si	-0.989007000	3.721161000	-0.299867000
C	-1.549276000	1.954726000	0.109626000

C	-0.716135000	3.933815000	-2.169956000
C	0.610951000	4.168295000	0.640028000
C	-2.315891000	4.967639000	0.238793000
C	-0.899256000	-0.986399000	-3.675974000
C	-1.332529000	-1.244876000	-2.259721000
C	-2.484655000	-0.689112000	-1.634476000
C	-2.634367000	-1.284931000	-0.334361000
C	-1.569032000	-2.248917000	-0.203511000
C	-0.772918000	-2.219069000	-1.376598000
C	-3.417649000	0.263081000	-2.325288000
C	-1.399748000	-3.259995000	0.896233000
C	0.344912000	-3.169700000	-1.697061000
C	1.407941000	0.894045000	-1.596760000
C	2.419969000	0.000511000	-1.486024000
H	-2.565700000	1.890188000	-0.308466000
H	-1.702135000	1.944767000	1.207951000
H	0.106318000	3.325652000	-2.564092000
H	-0.488793000	4.980357000	-2.404501000
H	-1.624827000	3.667872000	-2.723450000
H	0.430453000	4.179755000	1.722245000
H	0.947671000	5.173614000	0.360761000
H	1.444826000	3.481303000	0.448234000
H	-3.261545000	4.787356000	-0.285624000
H	-2.005122000	5.996445000	0.020762000
H	-2.513249000	4.898398000	1.315007000
H	-1.081425000	0.047427000	-3.988849000
H	-1.460821000	-1.626072000	-4.369606000
H	0.161831000	-1.203824000	-3.838228000
H	-2.883595000	0.956455000	-2.983353000
H	-4.004696000	0.856435000	-1.624451000
H	-4.125407000	-0.292625000	-2.955226000
H	-2.019790000	-4.143262000	0.695121000
H	-1.697835000	-2.878579000	1.876941000
H	-0.367679000	-3.617890000	0.968397000
H	1.027527000	-3.327901000	-0.854812000
H	0.942648000	-2.834777000	-2.549755000
H	-0.059207000	-4.154878000	-1.965358000
H	1.432304000	1.873148000	-1.125220000
H	0.637008000	0.735084000	-2.353999000
H	2.331907000	-0.935063000	-2.034474000
C	1.411742000	-1.321742000	1.970798000
O	0.462066000	-0.258303000	1.648020000
C	0.429063000	0.720393000	2.748228000
C	1.353838000	0.154359000	3.818215000

C	2.327480000	-0.710486000	3.013475000
H	0.846303000	-2.169695000	2.367234000
H	1.909097000	-1.612071000	1.042946000
H	0.782633000	1.670573000	2.341174000
H	-0.608010000	0.821129000	3.072193000
H	1.851254000	0.949319000	4.380146000
H	0.790920000	-0.460824000	4.528518000
H	3.099253000	-0.096787000	2.536401000
H	2.820290000	-1.475087000	3.620083000
C	4.071914000	1.448335000	-0.287932000
C	3.659837000	0.175411000	-0.731799000
C	4.528576000	-0.906907000	-0.472982000
C	5.733894000	-0.730574000	0.201656000
C	6.102368000	0.540467000	0.633346000
C	5.268905000	1.633778000	0.387781000
H	3.453699000	2.311250000	-0.515728000
H	6.377372000	-1.586087000	0.378484000
H	5.564001000	2.629763000	0.703625000
Si	-4.080383000	-1.130656000	0.918394000
C	-4.918373000	-2.825997000	1.044042000
H	-4.262434000	-3.595728000	1.461762000
H	-5.799437000	-2.753576000	1.692706000
H	-5.256722000	-3.167275000	0.059299000
C	-5.399635000	0.132097000	0.421218000
H	-5.869504000	-0.100356000	-0.539465000
H	-6.186697000	0.101823000	1.185059000
H	-5.020469000	1.159011000	0.388677000
C	-3.438329000	-0.597870000	2.629216000
H	-4.264731000	-0.625848000	3.349642000
H	-2.643232000	-1.240235000	3.022772000
H	-3.072188000	0.434996000	2.596438000
Cl	4.120740000	-2.525999000	-0.977517000
H	7.048231000	0.676160000	1.149807000

***o*TS1^a**, $E_{(\text{SCF Done})} = -2255.819407$ a.u. **IF** = $i188.37$ cm⁻¹

Sc	-0.050011000	-0.195243000	-0.138432000
Si	-1.528204000	3.595900000	-0.084539000
C	-0.844692000	1.820665000	0.120397000
C	-2.175282000	3.888619000	-1.839632000
C	-0.140739000	4.829068000	0.312540000
C	-2.935211000	3.850148000	1.160761000
C	0.174888000	-1.643485000	-3.446596000
C	-0.494439000	-1.666648000	-2.102883000
C	-1.699476000	-0.995168000	-1.756414000

C	-2.111964000	-1.431746000	-0.446896000
C	-1.131578000	-2.393995000	-0.013167000
C	-0.137550000	-2.527096000	-1.019956000
C	-2.448665000	-0.093060000	-2.696417000
C	-1.198898000	-3.236773000	1.229999000
C	0.999037000	-3.509694000	-1.029514000
C	0.806300000	1.750422000	-1.606613000
C	1.735027000	0.728792000	-1.502728000
H	-1.729648000	1.149216000	0.250896000
H	-0.279770000	1.825668000	1.075917000
H	-1.393296000	3.781609000	-2.599157000
H	-2.566522000	4.910015000	-1.916157000
H	-2.993582000	3.206288000	-2.094084000
H	0.287036000	4.647925000	1.305981000
H	-0.551373000	5.845680000	0.318215000
H	0.674977000	4.820079000	-0.419287000
H	-3.769122000	3.162355000	0.980363000
H	-3.328233000	4.871179000	1.086499000
H	-2.591789000	3.702309000	2.191244000
H	0.158723000	-0.653910000	-3.916180000
H	-0.341136000	-2.325299000	-4.135545000
H	1.216702000	-1.973781000	-3.393678000
H	-1.786026000	0.348502000	-3.447719000
H	-2.956952000	0.723352000	-2.181282000
H	-3.212896000	-0.657309000	-3.247161000
H	-1.688732000	-4.195377000	1.015290000
H	-1.769517000	-2.756939000	2.029079000
H	-0.207550000	-3.477308000	1.628056000
H	1.212248000	-3.902117000	-0.030638000
H	1.925506000	-3.081693000	-1.426472000
H	0.750189000	-4.373693000	-1.659934000
H	1.007960000	2.736580000	-1.206233000
H	0.058209000	1.717503000	-2.392196000
H	1.714236000	-0.056746000	-2.252153000
C	2.072435000	-1.341498000	2.078105000
O	0.862201000	-0.551723000	1.822225000
C	0.274796000	-0.120170000	3.091660000
C	0.940857000	-0.987487000	4.145213000
C	2.344250000	-1.178525000	3.565184000
H	1.848500000	-2.377035000	1.806425000
H	2.864944000	-0.951198000	1.437835000
H	0.511385000	0.941458000	3.224117000
H	-0.807238000	-0.248292000	3.020023000
H	0.943849000	-0.504000000	5.125845000

H	0.422653000	-1.948194000	4.238228000
H	2.962239000	-0.292439000	3.745119000
H	2.863814000	-2.046884000	3.978984000
C	3.038191000	1.740698000	0.397782000
C	2.935914000	0.809407000	-0.656737000
C	4.056045000	-0.024031000	-0.866140000
C	5.203308000	0.068652000	-0.081009000
C	5.266747000	1.002202000	0.950370000
C	4.178515000	1.842880000	1.186056000
H	2.201584000	2.406387000	0.593406000
H	6.045419000	-0.582287000	-0.293270000
H	4.221823000	2.586161000	1.977246000
Si	-3.812210000	-1.186842000	0.407643000
C	-4.689232000	-2.865339000	0.409691000
H	-4.161529000	-3.612883000	1.010478000
H	-5.699027000	-2.758594000	0.823100000
H	-4.783997000	-3.256833000	-0.609245000
C	-4.919445000	0.059869000	-0.491960000
H	-5.146750000	-0.241438000	-1.518873000
H	-5.870673000	0.111232000	0.052066000
H	-4.503815000	1.073137000	-0.512944000
C	-3.641076000	-0.559078000	2.196351000
H	-4.644631000	-0.452053000	2.626419000
H	-3.088453000	-1.241592000	2.850700000
H	-3.168270000	0.429451000	2.240374000
H	6.166189000	1.077480000	1.554238000
Cl	4.067787000	-1.189669000	-2.167811000

pP1^a, $E_{(\text{SCF Done})} = -2255.855935$ a.u.

Sc	0.070551000	-0.415825000	-0.149343000
Si	-1.199536000	3.816780000	-0.087650000
C	-0.450077000	2.023157000	-0.218462000
C	-1.976909000	4.264164000	-1.749033000
C	0.209621000	4.997419000	0.351792000
C	-2.493031000	3.800253000	1.291240000
C	0.145841000	-1.958253000	-3.381432000
C	-0.539668000	-1.864526000	-2.051877000
C	-1.672143000	-1.064112000	-1.743171000
C	-2.138401000	-1.399740000	-0.419612000
C	-1.265940000	-2.437055000	0.062643000
C	-0.277890000	-2.704058000	-0.924462000
C	-2.305928000	-0.118112000	-2.725190000
C	-1.411606000	-3.210324000	1.343777000
C	0.781698000	-3.767211000	-0.862908000

C	0.545062000	1.878787000	-1.422985000
C	1.459680000	0.638455000	-1.460160000
H	-1.349935000	1.374801000	-0.291480000
H	0.028671000	1.865827000	0.766715000
H	-1.239755000	4.265456000	-2.559143000
H	-2.406418000	5.271308000	-1.694777000
H	-2.785549000	3.576984000	-2.022191000
H	0.673159000	4.738013000	1.310694000
H	-0.185463000	6.015800000	0.445805000
H	0.992274000	5.022092000	-0.413959000
H	-3.326147000	3.125205000	1.066834000
H	-2.912742000	4.804952000	1.419118000
H	-2.061019000	3.504210000	2.254397000
H	0.164145000	-1.002627000	-3.914058000
H	-0.380727000	-2.674567000	-4.026433000
H	1.178320000	-2.301838000	-3.285042000
H	-1.581451000	0.235413000	-3.465277000
H	-2.753120000	0.757803000	-2.249816000
H	-3.105411000	-0.621465000	-3.284708000
H	-1.922884000	-4.163933000	1.158781000
H	-2.000852000	-2.671056000	2.089787000
H	-0.445126000	-3.458078000	1.796660000
H	0.970151000	-4.102596000	0.161878000
H	1.732810000	-3.432752000	-1.290960000
H	0.467839000	-4.652052000	-1.432386000
H	1.159319000	2.790425000	-1.441488000
H	-0.058237000	1.898758000	-2.335449000
H	1.596618000	0.260078000	-2.471839000
C	2.194562000	-1.295468000	2.172289000
O	0.898579000	-0.674154000	1.853295000
C	0.190919000	-0.339861000	3.088205000
C	0.924871000	-1.098971000	4.179978000
C	2.367136000	-1.087337000	3.667611000
H	2.120025000	-2.354639000	1.906250000
H	2.953542000	-0.806885000	1.560060000
H	0.259754000	0.744807000	3.228602000
H	-0.853962000	-0.629212000	2.960376000
H	0.811441000	-0.618243000	5.155378000
H	0.546294000	-2.124123000	4.257633000
H	2.843103000	-0.120950000	3.865801000
H	2.985329000	-1.869966000	4.115449000
C	2.954903000	1.719864000	0.284310000
C	2.734128000	0.748471000	-0.720414000
C	3.820171000	-0.133223000	-0.945491000

C	5.017639000	-0.055223000	-0.241042000
C	5.184758000	0.913441000	0.747776000
C	4.144765000	1.804341000	1.003402000
H	2.183556000	2.458286000	0.484362000
H	5.818027000	-0.748914000	-0.479354000
H	4.264326000	2.584747000	1.750486000
Si	-3.819145000	-0.962205000	0.390505000
C	-4.852592000	-2.547741000	0.443079000
H	-4.394734000	-3.326764000	1.060942000
H	-5.845331000	-2.334743000	0.856817000
H	-4.989584000	-2.955075000	-0.564734000
C	-4.793994000	0.343898000	-0.575588000
H	-5.020344000	0.032500000	-1.599609000
H	-5.751384000	0.488633000	-0.059812000
H	-4.298109000	1.320125000	-0.612830000
C	-3.618827000	-0.279157000	2.157121000
H	-4.606269000	0.021231000	2.528652000
H	-3.226499000	-1.015246000	2.867288000
H	-2.981189000	0.612717000	2.187976000
H	6.122005000	0.976986000	1.292340000
Cl	3.701786000	-1.366541000	-2.181896000

oC2_{syn}, $E_{(\text{SCF Done})} = -3024.932504$ a.u.

Sc	1.103764000	-0.931544000	0.211790000
Si	1.829283000	5.284991000	-0.853842000
C	2.189826000	3.683563000	0.132553000
C	0.037492000	5.838527000	-0.546067000
C	2.080455000	4.968001000	-2.708717000
C	3.024330000	6.629712000	-0.260028000
C	2.773005000	-2.037077000	-1.130410000
C	2.313440000	-0.916337000	-1.909829000
C	0.940309000	-1.110581000	-2.218281000
C	0.538329000	-2.376621000	-1.683754000
C	1.657876000	-2.944752000	-1.020673000
C	3.159280000	0.203909000	-2.445225000
C	0.072335000	-0.214608000	-3.055264000
C	-0.806487000	-3.007906000	-1.903686000
C	1.671877000	-4.297377000	-0.361624000
C	1.351462000	2.448538000	-0.246041000
C	1.640207000	1.196374000	0.580074000
H	2.075161000	3.911694000	1.201711000
H	3.255255000	3.443804000	-0.001012000
H	-0.687369000	5.085344000	-0.877284000
H	-0.177354000	6.762345000	-1.095572000

H	-0.142058000	6.039472000	0.516890000
H	3.096203000	4.613020000	-2.919073000
H	1.928427000	5.890603000	-3.280754000
H	1.374075000	4.223823000	-3.095241000
H	2.900941000	6.828318000	0.810860000
H	2.851691000	7.570807000	-0.794774000
H	4.067378000	6.338232000	-0.428693000
H	3.731416000	0.721145000	-1.669951000
H	2.553756000	0.949135000	-2.967161000
H	3.880583000	-0.183751000	-3.175921000
H	0.316203000	0.843939000	-2.923528000
H	-0.990036000	-0.343307000	-2.823162000
H	0.193992000	-0.445503000	-4.121998000
H	-0.891890000	-3.370281000	-2.936330000
H	-1.634855000	-2.308926000	-1.744592000
H	-0.970989000	-3.870703000	-1.252393000
H	0.661900000	-4.698194000	-0.236383000
H	2.152280000	-4.285637000	0.621581000
H	2.224006000	-5.020812000	-0.974803000
H	1.536862000	2.213708000	-1.300028000
H	0.278947000	2.687246000	-0.195010000
H	2.718362000	0.955193000	0.525900000
C	-1.134352000	-2.582540000	1.864454000
O	-0.818876000	-1.376074000	1.100812000
C	-1.950998000	-0.436016000	1.156536000
C	-3.067601000	-1.209512000	1.840861000
C	-2.303794000	-2.180128000	2.745095000
H	-1.401907000	-3.369244000	1.152617000
H	-0.235748000	-2.872500000	2.415770000
H	-1.618015000	0.428908000	1.736753000
H	-2.189473000	-0.134257000	0.133983000
H	-3.733739000	-0.543798000	2.395646000
H	-3.666989000	-1.753089000	1.103796000
H	-1.945780000	-1.673381000	3.647873000
H	-2.901234000	-3.044820000	3.046483000
C	0.319491000	2.156035000	2.543542000
C	1.213192000	1.198163000	1.995874000
C	1.580978000	0.190978000	2.916345000
C	1.179677000	0.124605000	4.246090000
C	0.329458000	1.111341000	4.732631000
C	-0.101080000	2.120584000	3.865989000
H	-0.013092000	2.969792000	1.907475000
H	1.536147000	-0.676978000	4.885669000
H	-0.761245000	2.901831000	4.233241000

C	-6.019578000	-0.879547000	-0.965494000
C	-5.768921000	0.502947000	-1.008394000
C	-6.669581000	1.327794000	-0.311534000
C	-7.744597000	0.805670000	0.397179000
C	-7.961341000	-0.571994000	0.418941000
C	-7.095851000	-1.419879000	-0.266819000
H	-6.531955000	2.404077000	-0.364462000
H	-8.426119000	1.474608000	0.914766000
H	-7.252045000	-2.493892000	-0.267992000
C	-4.646382000	1.070779000	-1.770064000
C	-4.018710000	2.220040000	-1.487396000
H	-4.326056000	0.500205000	-2.639745000
H	-3.232621000	2.600191000	-2.133719000
H	-4.275536000	2.828979000	-0.623434000
Si	4.615344000	-2.426485000	-0.761988000
C	5.352153000	-3.127927000	-2.360406000
H	6.409593000	-3.377217000	-2.212827000
H	4.832133000	-4.040466000	-2.672313000
H	5.291212000	-2.409299000	-3.184750000
C	4.831007000	-3.719834000	0.612084000
H	4.345940000	-3.449074000	1.556918000
H	4.475889000	-4.711364000	0.316063000
H	5.904596000	-3.809070000	0.818797000
C	5.588643000	-0.880945000	-0.246501000
H	6.575723000	-1.198908000	0.110854000
H	5.753935000	-0.193070000	-1.080902000
H	5.111309000	-0.326147000	0.568839000
H	0.015982000	1.094497000	5.771755000
H	-8.807974000	-0.989294000	0.956533000
Cl	2.625727000	-1.145383000	2.327645000
Cl	-4.944664000	-1.998139000	-1.788920000

***o*TS2^a_{syn}, $E_{(\text{SCF Done})} = -3024.911323$ a.u. $\text{IF} = i$ 185.05 cm⁻¹**

Sc	0.864906000	0.607629000	0.228578000
Si	-5.064915000	-1.731096000	-1.029132000
C	-3.283950000	-1.627709000	-0.314666000
C	-5.089337000	-1.019381000	-2.787548000
C	-6.248470000	-0.754626000	0.083923000
C	-5.556756000	-3.560233000	-1.058016000
C	0.287817000	2.893544000	-0.478650000
C	1.449748000	2.536577000	-1.248602000
C	2.556514000	2.380919000	-0.369006000
C	2.106571000	2.659079000	0.955357000
C	0.722516000	2.969883000	0.895160000

C	1. 553779000	2. 518920000	-2. 748037000
C	3. 995520000	2. 194758000	-0. 751744000
C	3. 004735000	2. 798108000	2. 148495000
C	-0. 077433000	3. 470421000	2. 065403000
C	-2. 730270000	-0. 205952000	-0. 185790000
C	-1. 295038000	-0. 061553000	0. 364310000
H	-2. 643869000	-2. 261189000	-0. 946492000
H	-3. 300266000	-2. 113400000	0. 670301000
H	-4. 809567000	0. 040566000	-2. 806042000
H	-6. 095543000	-1. 098846000	-3. 214951000
H	-4. 406633000	-1. 562418000	-3. 451734000
H	-6. 223316000	-1. 123194000	1. 115967000
H	-7. 278709000	-0. 853874000	-0. 277094000
H	-6. 009456000	0. 314907000	0. 100865000
H	-4. 884083000	-4. 148333000	-1. 693036000
H	-6. 572784000	-3. 681873000	-1. 450511000
H	-5. 535786000	-3. 993623000	-0. 051428000
H	0. 721692000	2. 000346000	-3. 232472000
H	2. 481125000	2. 048167000	-3. 087292000
H	1. 560666000	3. 545118000	-3. 138046000
H	4. 112781000	1. 687276000	-1. 710719000
H	4. 557477000	1. 625998000	-0. 003132000
H	4. 489113000	3. 172503000	-0. 837754000
H	3. 518005000	3. 768795000	2. 119758000
H	3. 786072000	2. 030908000	2. 176135000
H	2. 454237000	2. 763578000	3. 093228000
H	0. 282076000	3. 067705000	3. 017810000
H	-1. 135853000	3. 221871000	1. 985609000
H	-0. 001535000	4. 564170000	2. 135201000
H	-3. 399186000	0. 357299000	0. 478979000
H	-2. 777493000	0. 311875000	-1. 153150000
H	-1. 211291000	1. 010710000	0. 675071000
C	2. 224977000	-0. 537637000	2. 994401000
O	2. 277789000	-0. 461655000	1. 532388000
C	3. 409011000	-1. 247931000	1. 036086000
C	4. 303780000	-1. 439108000	2. 246796000
C	3. 284673000	-1. 558730000	3. 382260000
H	2. 450262000	0. 459603000	3. 379882000
H	1. 212820000	-0. 826748000	3. 279488000
H	3. 016312000	-2. 196105000	0. 657395000
H	3. 866056000	-0. 691583000	0. 216111000
H	4. 938630000	-2. 323575000	2. 145956000
H	4. 952339000	-0. 568007000	2. 393390000
H	2. 853830000	-2. 565312000	3. 407233000

H	3.710974000	-1.345188000	4.366190000
C	-0.408487000	-2.212479000	1.387743000
C	-1.023226000	-0.956926000	1.549379000
C	-1.485053000	-0.658462000	2.853761000
C	-1.347219000	-1.553963000	3.914051000
C	-0.736787000	-2.788759000	3.704724000
C	-0.263295000	-3.117544000	2.436271000
H	-0.044105000	-2.487796000	0.404284000
H	-1.736490000	-1.285640000	4.891158000
H	0.203201000	-4.081710000	2.255041000
C	2.958460000	-2.295780000	-2.298522000
C	1.613173000	-2.072859000	-1.934242000
C	0.836824000	-3.238454000	-1.760315000
C	1.363115000	-4.518169000	-1.890887000
C	2.706100000	-4.691995000	-2.219769000
C	3.500979000	-3.570775000	-2.436557000
H	-0.225340000	-3.141743000	-1.556014000
H	0.715761000	-5.379934000	-1.754591000
H	4.541299000	-3.675314000	-2.727846000
C	1.036623000	-0.719297000	-1.841695000
C	-0.328672000	-0.470586000	-1.675118000
H	1.630995000	0.069106000	-2.295945000
H	-0.718791000	0.488963000	-2.005013000
H	-1.056209000	-1.270674000	-1.716894000
Si	-1.263277000	3.774621000	-1.186150000
C	-0.750563000	5.583414000	-1.430221000
H	-1.588822000	6.169369000	-1.825317000
H	-0.440473000	6.038171000	-0.482779000
H	0.083348000	5.674872000	-2.134882000
C	-2.762864000	3.727582000	-0.021562000
H	-2.996919000	2.726874000	0.356548000
H	-2.645780000	4.399769000	0.833987000
H	-3.637499000	4.074215000	-0.585764000
C	-1.837994000	3.086936000	-2.861132000
H	-2.752591000	3.625362000	-3.139705000
H	-1.112634000	3.252089000	-3.662777000
H	-2.092568000	2.021487000	-2.840817000
Cl	-2.330803000	0.830839000	3.183981000
Cl	4.023874000	-0.948759000	-2.645955000
H	-0.644112000	-3.488761000	4.530286000
H	3.128763000	-5.685893000	-2.331663000

oP2^a_{syn}, $E_{(\text{SCF Done})} = -3024.956343$ a.u.

Sc	-1.252554000	-0.087440000	-0.306219000
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Si	6.388255000	-0.816019000	-0.661240000
C	4.833385000	0.103252000	-0.009093000
C	6.051208000	-1.471248000	-2.410272000
C	6.815178000	-2.252188000	0.500867000
C	7.814167000	0.431010000	-0.706692000
C	-2.079738000	-2.379157000	-0.654857000
C	-0.865284000	-2.236528000	-1.424123000
C	-1.078699000	-1.281700000	-2.452995000
C	-2.421871000	-0.803090000	-2.332570000
C	-3.037191000	-1.489740000	-1.249730000
C	0.397592000	-3.038784000	-1.279329000
C	-0.142945000	-0.953898000	-3.577826000
C	-3.105651000	0.119505000	-3.300487000
C	-4.494169000	-1.371423000	-0.902480000
C	3.574907000	-0.766880000	0.081906000
C	2.191646000	-0.092148000	0.320601000
H	4.669004000	0.963831000	-0.672882000
H	5.105213000	0.510211000	0.972956000
H	5.249661000	-2.218958000	-2.425185000
H	6.949795000	-1.949431000	-2.817082000
H	5.772015000	-0.659977000	-3.092907000
H	7.000785000	-1.895883000	1.520811000
H	7.721632000	-2.765566000	0.159933000
H	6.012192000	-2.996983000	0.544175000
H	7.585976000	1.273583000	-1.369689000
H	8.732784000	-0.040765000	-1.073933000
H	8.025035000	0.834922000	0.290306000
H	0.649162000	-3.249515000	-0.237390000
H	1.250908000	-2.528921000	-1.736222000
H	0.298012000	-4.005570000	-1.790262000
H	0.907619000	-1.007663000	-3.278054000
H	-0.322745000	0.045769000	-3.984093000
H	-0.280082000	-1.667024000	-4.401866000
H	-3.387994000	-0.429902000	-4.208662000
H	-2.467921000	0.951508000	-3.613782000
H	-4.028509000	0.540268000	-2.889078000
H	-4.864420000	-0.345104000	-0.997474000
H	-4.707808000	-1.711306000	0.113084000
H	-5.098939000	-1.985232000	-1.582797000
H	3.715977000	-1.533403000	0.855371000
H	3.459754000	-1.316098000	-0.863565000
H	1.481183000	-0.911781000	0.154086000
C	-3.354040000	0.750030000	2.058031000
O	-2.768920000	1.063510000	0.752322000

C	-3.442429000	2.234356000	0.176387000
C	-4.737943000	2.351815000	0.957270000
C	-4.311882000	1.895559000	2.354613000
H	-3.865171000	-0.211871000	1.965716000
H	-2.537900000	0.664004000	2.778347000
H	-2.785316000	3.094813000	0.320756000
H	-3.573461000	2.044984000	-0.891658000
H	-5.125848000	3.373892000	0.942738000
H	-5.506326000	1.687087000	0.547254000
H	-3.792626000	2.704253000	2.879850000
H	-5.151424000	1.569364000	2.974336000
C	2.834334000	1.356225000	2.319730000
C	1.985255000	0.396123000	1.738656000
C	0.938529000	-0.026650000	2.563118000
C	0.740516000	0.393874000	3.875430000
C	1.630407000	1.316619000	4.415471000
C	2.671900000	1.803863000	3.626483000
H	3.635913000	1.766114000	1.716170000
H	-0.083002000	-0.000026000	4.462650000
H	3.362039000	2.539101000	4.030127000
C	-0.682626000	3.587475000	-1.517334000
C	-0.094736000	2.657988000	-0.626997000
C	0.029942000	3.113964000	0.705713000
C	-0.383083000	4.376602000	1.118419000
C	-0.960421000	5.257523000	0.203714000
C	-1.106523000	4.855808000	-1.120993000
H	0.492163000	2.452502000	1.431931000
H	-0.242762000	4.675622000	2.153929000
H	-1.529652000	5.528607000	-1.860499000
C	0.374851000	1.300419000	-1.038050000
C	1.868525000	0.989008000	-0.738684000
H	0.253621000	1.234736000	-2.123204000
H	2.324348000	0.640949000	-1.674786000
H	2.398226000	1.916138000	-0.481882000
Si	-2.558042000	-3.817874000	0.524137000
C	-3.746304000	-4.932196000	-0.443726000
H	-4.019627000	-5.804205000	0.162114000
H	-4.671393000	-4.415038000	-0.719022000
H	-3.277572000	-5.296895000	-1.364431000
C	-3.419239000	-3.237189000	2.119831000
H	-2.786772000	-2.576862000	2.723548000
H	-4.378380000	-2.738335000	1.946625000
H	-3.630781000	-4.123989000	2.730180000
C	-1.075522000	-4.864260000	1.068770000

H	-1.458672000	-5.668207000	1.709564000
H	-0.561468000	-5.338555000	0.227794000
H	-0.339139000	-4.305838000	1.656359000
Cl	-0.273081000	-1.186857000	1.932088000
Cl	-0.858789000	3.211723000	-3.223231000
H	1.503279000	1.652616000	5.440207000
H	-1.279067000	6.250340000	0.507750000

oC2_{iso}, $E_{(\text{SCF Done})} = -3024.93383$ a.u.

Sc	-0.955257000	0.959456000	-0.195881000
Si	-3.807395000	-3.807984000	-1.285342000
C	-2.948179000	-2.206894000	-0.663151000
C	-4.173317000	-3.667522000	-3.140120000
C	-5.419687000	-4.065107000	-0.320086000
C	-2.630578000	-5.261112000	-0.965579000
C	-1.759070000	3.180373000	-2.768498000
C	-0.730835000	2.195612000	-2.285477000
C	-0.727530000	0.819766000	-2.642364000
C	0.432174000	0.219707000	-2.057700000
C	1.155207000	1.233956000	-1.372244000
C	0.435117000	2.472951000	-1.481928000
C	-1.656526000	0.151884000	-3.611252000
C	0.885980000	-1.197975000	-2.257774000
C	2.506252000	1.020005000	-0.749799000
C	-3.712389000	-0.896612000	-0.919023000
C	-3.116213000	0.361865000	-0.284483000
H	-1.954151000	-2.152553000	-1.135990000
H	-2.761337000	-2.346315000	0.411889000
H	-4.849826000	-2.833541000	-3.358813000
H	-4.652139000	-4.583195000	-3.505867000
H	-3.255643000	-3.521719000	-3.722254000
H	-5.231142000	-4.156846000	0.756310000
H	-5.918139000	-4.985801000	-0.644718000
H	-6.124790000	-3.240280000	-0.473171000
H	-1.686343000	-5.140424000	-1.509789000
H	-3.081599000	-6.204606000	-1.293767000
H	-2.396547000	-5.361847000	0.100953000
H	-2.708676000	2.689983000	-3.003290000
H	-1.418475000	3.669992000	-3.690367000
H	-1.964933000	3.968481000	-2.041792000
H	-2.652108000	0.604146000	-3.613304000
H	-1.775071000	-0.915498000	-3.404551000
H	-1.261107000	0.240802000	-4.632205000
H	0.048078000	-1.881787000	-2.426032000

H	1.464553000	-1.575146000	-1.408114000
H	1.536298000	-1.268877000	-3.140139000
H	3.286132000	1.043393000	-1.522078000
H	2.592334000	0.047189000	-0.254383000
H	2.758036000	1.791847000	-0.018744000
H	-4.762180000	-1.014725000	-0.604005000
H	-3.763868000	-0.735537000	-2.000372000
H	-3.437942000	1.256109000	-0.846351000
C	-0.359368000	-1.282658000	2.053625000
O	-0.036303000	0.058779000	1.543928000
C	0.813177000	0.764153000	2.509552000
C	0.662790000	-0.023872000	3.797644000
C	0.520235000	-1.457608000	3.281345000
H	-1.425711000	-1.284810000	2.296562000
H	-0.154981000	-1.997437000	1.253441000
H	1.837387000	0.740703000	2.128117000
H	0.459295000	1.796047000	2.568814000
H	1.526349000	0.109139000	4.454725000
H	-0.237258000	0.287539000	4.338825000
H	1.497603000	-1.863972000	3.001708000
H	0.061794000	-2.130480000	4.011043000
C	-4.060617000	-0.369968000	1.981953000
C	-3.412407000	0.580705000	1.154193000
C	-3.028965000	1.750594000	1.843814000
C	-3.267388000	2.015559000	3.186584000
C	-3.922519000	1.049396000	3.944105000
C	-4.313127000	-0.142529000	3.329523000
H	-4.410746000	-1.292450000	1.531319000
H	-2.957214000	2.959578000	3.623947000
H	-4.839237000	-0.899285000	3.905350000
C	5.351164000	-1.525899000	0.859408000
C	4.976138000	-2.694708000	0.175083000
C	5.624864000	-2.940522000	-1.048146000
C	6.574331000	-2.067601000	-1.564711000
C	6.918540000	-0.915168000	-0.858277000
C	6.305632000	-0.643082000	0.361701000
H	5.393974000	-3.859612000	-1.579281000
H	7.061887000	-2.297047000	-2.507862000
H	6.566460000	0.243267000	0.931121000
C	3.983390000	-3.635655000	0.715343000
C	3.193905000	-4.432830000	-0.015583000
H	3.910177000	-3.678973000	1.800332000
H	2.516666000	-5.136675000	0.459736000
H	3.201772000	-4.424289000	-1.103100000

Si	1.165428000	4.175341000	-0.979747000
C	1.564731000	4.272038000	0.878518000
H	0.658390000	4.211200000	1.492310000
H	2.268377000	3.506899000	1.221614000
H	2.025354000	5.246277000	1.083333000
C	0.006681000	5.626600000	-1.352147000
H	0.534950000	6.548080000	-1.077378000
H	-0.249704000	5.702022000	-2.413081000
H	-0.922505000	5.603762000	-0.772234000
C	2.753294000	4.414858000	-1.984342000
H	3.193410000	5.393661000	-1.759982000
H	3.507191000	3.651923000	-1.765964000
H	2.540950000	4.381399000	-3.058719000
H	7.671640000	-0.234451000	-1.244855000
H	-4.132890000	1.233032000	4.993139000
Cl	4.597411000	-1.117952000	2.394348000
Cl	-2.147043000	3.006992000	0.915243000

***o*TS2^a_{iso}, $E_{(\text{SCF Done})} = -3024.91696$ a.u. $\text{IF} = i252.09$ cm⁻¹**

Sc	-0.720713000	0.024360000	0.068541000
Si	5.507607000	-0.701876000	-1.184698000
C	3.749704000	-1.283384000	-0.674728000
C	6.438778000	-0.095753000	0.354313000
C	5.388097000	0.705992000	-2.450897000
C	6.404518000	-2.184983000	-1.945903000
C	1.163954000	0.972127000	-2.843942000
C	-0.182921000	0.628785000	-2.280555000
C	-1.150308000	1.577345000	-1.833943000
C	-2.361305000	0.875750000	-1.570556000
C	-2.168509000	-0.519617000	-1.862093000
C	-0.797185000	-0.651851000	-2.295756000
C	-1.022019000	3.065421000	-1.941942000
C	-3.631449000	1.585497000	-1.192633000
C	2.875987000	-0.242944000	0.043604000
C	1.532318000	-0.790899000	0.532236000
H	3.873363000	-2.167714000	-0.034433000
H	3.237342000	-1.643084000	-1.579620000
H	5.959722000	0.779334000	0.809167000
H	7.461210000	0.196365000	0.088113000
H	6.510496000	-0.879967000	1.117160000
H	4.850845000	0.390971000	-3.352999000
H	6.390168000	1.025030000	-2.760405000
H	4.877706000	1.585028000	-2.040604000
H	6.492579000	-3.008859000	-1.228521000

H	7.417450000	-1.906545000	-2.258452000
H	5.876813000	-2.562794000	-2.829173000
H	1.063411000	1.258351000	-3.900014000
H	1.859114000	0.128624000	-2.809520000
H	1.626416000	1.820160000	-2.329454000
H	-0.004685000	3.418013000	-1.758016000
H	-1.688549000	3.591731000	-1.255222000
H	-1.296897000	3.373525000	-2.960705000
H	-3.463567000	2.329815000	-0.406215000
H	-4.408295000	0.900478000	-0.855459000
H	-4.034146000	2.128382000	-2.058359000
H	2.684057000	0.600392000	-0.628340000
H	3.437132000	0.179368000	0.887319000
H	1.031867000	-1.209830000	-0.371933000
C	-1.981824000	-0.363964000	3.135041000
O	-2.269372000	-0.264465000	1.700447000
C	-3.637353000	-0.722147000	1.458838000
C	-4.042007000	-1.466973000	2.717259000
C	-3.314365000	-0.670126000	3.799631000
H	-1.262201000	-1.177953000	3.272351000
H	-1.541778000	0.581221000	3.459096000
H	-4.256106000	0.163847000	1.292136000
H	-3.622660000	-1.336013000	0.558706000
H	-5.127220000	-1.482831000	2.849992000
H	-3.682947000	-2.501902000	2.687507000
H	-3.853279000	0.255969000	4.027857000
H	-3.181849000	-1.226200000	4.731581000
C	2.644925000	-1.922147000	2.510464000
C	1.602861000	-1.854023000	1.565324000
C	0.611572000	-2.838485000	1.703719000
C	0.641937000	-3.851996000	2.651479000
C	1.700943000	-3.887654000	3.557628000
C	2.694125000	-2.913194000	3.487059000
H	3.445752000	-1.191156000	2.463914000
H	-0.147164000	-4.596763000	2.682234000
H	3.521664000	-2.928363000	4.190440000
C	-0.432530000	4.343679000	1.089950000
C	0.394839000	3.210905000	0.963254000
C	1.681814000	3.444035000	0.442437000
C	2.114335000	4.712448000	0.072534000
C	1.264823000	5.809184000	0.210841000
C	-0.014335000	5.620170000	0.725815000
H	2.360898000	2.604027000	0.326098000
H	3.117554000	4.844121000	-0.323315000

H	-0.692053000	6.458375000	0.852279000
C	-0.043747000	1.883179000	1.415679000
C	0.856817000	0.884870000	1.828369000
H	-1.035630000	1.867422000	1.866315000
H	0.541057000	0.176843000	2.591619000
H	1.915095000	1.116221000	1.889078000
C	-0.147660000	-1.889149000	-2.853360000
H	-0.642763000	-2.804898000	-2.522560000
H	-0.181545000	-1.873067000	-3.950411000
H	0.908962000	-1.970787000	-2.575871000
Si	-3.518577000	-1.803038000	-2.349632000
C	-5.290107000	-1.210606000	-2.009893000
H	-5.525176000	-0.280907000	-2.537177000
H	-5.963221000	-1.983580000	-2.401757000
H	-5.537581000	-1.080084000	-0.951052000
C	-3.378543000	-2.019724000	-4.227366000
H	-2.437366000	-2.487102000	-4.531509000
H	-4.195885000	-2.657009000	-4.585444000
H	-3.459061000	-1.053892000	-4.738449000
C	-3.342108000	-3.504399000	-1.521036000
H	-2.376662000	-3.984273000	-1.708755000
H	-3.505010000	-3.477524000	-0.437603000
H	-4.114114000	-4.160122000	-1.942850000
H	1.591418000	6.804812000	-0.073805000
H	1.741612000	-4.670381000	4.308871000
Cl	-0.768384000	-2.790174000	0.594348000
Cl	-2.058509000	4.189345000	1.736158000

oP2_{iso}, $E_{(\text{SCF Done})} = -3024.957615$ a.u.

Sc	1.386749000	0.398805000	-0.193726000
Si	-5.896625000	-0.034595000	1.313417000
C	-4.209329000	-0.694812000	0.688018000
C	-7.165666000	-0.082038000	-0.096565000
C	-5.702831000	1.747821000	1.936987000
C	-6.466966000	-1.156435000	2.730309000
C	-1.008660000	1.415826000	2.240250000
C	0.378359000	0.897223000	2.006598000
C	1.542578000	1.711602000	1.893658000
C	2.682193000	0.856781000	1.850546000
C	2.241057000	-0.507711000	1.939868000
C	0.801860000	-0.460653000	2.035861000
C	1.561613000	3.204954000	2.028164000
C	4.092976000	1.376651000	1.848270000
C	-3.536547000	0.122762000	-0.419756000

C	-2.192968000	-0.433443000	-0.927249000
H	-4.363427000	-1.732554000	0.362407000
H	-3.540292000	-0.759282000	1.559426000
H	-6.874691000	0.562910000	-0.933826000
H	-8.143521000	0.264247000	0.257789000
H	-7.297490000	-1.100075000	-0.481671000
H	-4.952567000	1.815553000	2.733561000
H	-6.651508000	2.115124000	2.345185000
H	-5.406465000	2.430945000	1.132589000
H	-6.579569000	-2.193965000	2.395039000
H	-7.435993000	-0.827590000	3.122930000
H	-5.751968000	-1.147822000	3.561213000
H	-1.104168000	1.789512000	3.268821000
H	-1.763608000	0.636905000	2.109976000
H	-1.259315000	2.244373000	1.569781000
H	0.658929000	3.668993000	1.622946000
H	2.425034000	3.660076000	1.534701000
H	1.619803000	3.476287000	3.091404000
H	4.185788000	2.298603000	1.263533000
H	4.810196000	0.653743000	1.457403000
H	4.411155000	1.622035000	2.870353000
H	-3.340443000	1.135727000	-0.046061000
H	-4.219302000	0.257568000	-1.270761000
H	-1.537075000	-0.513238000	-0.050235000
C	2.769846000	-0.535052000	-2.989906000
O	2.958845000	-0.371122000	-1.540672000
C	4.376059000	-0.530873000	-1.217469000
C	4.972373000	-1.240130000	-2.418494000
C	4.171658000	-0.634512000	-3.572732000
H	2.187369000	-1.448372000	-3.135215000
H	2.205709000	0.325912000	-3.355135000
H	4.806265000	0.466773000	-1.076819000
H	4.432707000	-1.090940000	-0.284674000
H	6.048011000	-1.063591000	-2.503712000
H	4.805396000	-2.320958000	-2.350531000
H	4.555993000	0.359022000	-3.828519000
H	4.188706000	-1.248618000	-4.477031000
C	-3.466438000	-2.311063000	-2.124135000
C	-2.289733000	-1.818600000	-1.539631000
C	-1.182396000	-2.666089000	-1.637909000
C	-1.205430000	-3.921024000	-2.236261000
C	-2.400253000	-4.372781000	-2.789652000
C	-3.529186000	-3.559622000	-2.737116000
H	-4.359329000	-1.694783000	-2.095603000

H	-0.308905000	-4.531810000	-2.267274000
H	-4.465219000	-3.896814000	-3.172823000
C	0.797095000	3.561539000	-1.212251000
C	-0.346449000	2.743924000	-1.250795000
C	-1.555087000	3.443911000	-1.059342000
C	-1.597056000	4.824998000	-0.885147000
C	-0.428384000	5.584380000	-0.898897000
C	0.796237000	4.938790000	-1.062342000
H	-2.487055000	2.888517000	-1.069326000
H	-2.558176000	5.313466000	-0.749774000
H	1.729171000	5.493573000	-1.061286000
C	-0.237441000	1.280476000	-1.480901000
C	-1.493422000	0.526230000	-1.945655000
H	0.508801000	1.170713000	-2.297028000
H	-1.205408000	-0.068483000	-2.819850000
H	-2.250036000	1.223303000	-2.333379000
C	-0.109756000	-1.620471000	2.325566000
H	0.327475000	-2.576115000	2.028640000
H	-0.318430000	-1.671903000	3.402130000
H	-1.076379000	-1.533077000	1.819515000
Si	3.262402000	-2.061449000	2.417289000
C	5.126854000	-1.725998000	2.549580000
H	5.352560000	-0.926854000	3.262544000
H	5.590290000	-2.643652000	2.933035000
H	5.624359000	-1.490950000	1.602681000
C	2.701585000	-2.594924000	4.147249000
H	1.663521000	-2.938471000	4.172906000
H	3.333246000	-3.419578000	4.498514000
H	2.803226000	-1.769800000	4.861061000
C	3.026769000	-3.503575000	1.202000000
H	1.991235000	-3.854702000	1.157010000
H	3.335260000	-3.248808000	0.181367000
H	3.645066000	-4.348002000	1.530213000
H	-0.460435000	6.662659000	-0.778178000
H	-2.439296000	-5.351217000	-3.258987000
Cl	0.410331000	-2.183352000	-0.984189000
Cl	2.383832000	2.748399000	-1.331785000

oC1^b, $E_{(\text{SCF Done})} = -1979.702112$ a.u.

Sc	-0.513019000	0.247042000	-0.097288000
N	0.866864000	2.088918000	-0.240994000
C	-1.183066000	1.096639000	-2.008456000
H	-0.302323000	1.034017000	-2.660601000
H	-2.071592000	0.816157000	-2.575701000

C	-1.340548000	2.381738000	-1.299555000
C	-0.364050000	2.863647000	-0.378096000
C	-0.575384000	4.042195000	0.354497000
H	0.190078000	4.409950000	1.029863000
C	-1.753313000	4.758627000	0.210256000
H	-1.902177000	5.675393000	0.772831000
C	-2.737576000	4.297425000	-0.672822000
H	-3.659443000	4.858233000	-0.800241000
C	-2.534099000	3.136037000	-1.397383000
H	-3.294717000	2.794632000	-2.094173000
C	1.579834000	2.280568000	1.036550000
H	2.046450000	3.272282000	1.101705000
H	2.371312000	1.530072000	1.112380000
H	0.892520000	2.163898000	1.879458000
C	1.804463000	2.335638000	-1.359558000
H	1.287267000	2.239897000	-2.314706000
H	2.624532000	1.614789000	-1.314742000
H	2.212454000	3.352500000	-1.287739000
C	-1.907648000	0.328499000	1.903812000
C	-2.736540000	-0.125552000	0.831206000
C	-2.265162000	-1.406442000	0.390575000
C	-1.141769000	-1.736840000	1.228155000
C	-0.921587000	-0.672703000	2.150738000
C	-3.975644000	0.592809000	0.382456000
H	-4.145079000	0.507692000	-0.692020000
H	-3.935781000	1.655963000	0.632006000
H	-4.856740000	0.175142000	0.887473000
C	-0.436547000	-3.063956000	1.296054000
H	0.570334000	-2.980931000	1.718246000
H	-0.356453000	-3.561025000	0.324608000
H	-0.988178000	-3.746590000	1.955243000
C	0.076778000	-0.675204000	3.274092000
H	-0.322124000	-1.220966000	4.139449000
H	0.314587000	0.334877000	3.622309000
H	1.019269000	-1.160557000	3.000032000
C	-2.142225000	1.563387000	2.727848000
H	-2.945605000	1.388204000	3.455463000
H	-1.255249000	1.851015000	3.301566000
H	-2.436575000	2.424555000	2.120508000
C	6.289723000	-0.161871000	-1.119863000
C	5.834001000	-0.395754000	0.174903000
C	4.516629000	-0.796585000	0.377433000
C	3.621115000	-0.967505000	-0.698430000
C	4.119999000	-0.730978000	-1.994847000

C	5.431554000	-0.330754000	-2.207888000
H	6.493921000	-0.273096000	1.027392000
H	3.470518000	-0.907609000	-2.847430000
H	5.791383000	-0.169892000	-3.219524000
C	2.252073000	-1.439696000	-0.491670000
C	1.217739000	-1.299671000	-1.352467000
H	2.077285000	-1.985376000	0.433064000
H	0.300995000	-1.873390000	-1.197109000
H	1.318851000	-0.798429000	-2.311681000
Si	-3.093418000	-2.624576000	-0.839993000
C	-3.632314000	-4.153539000	0.141506000
H	-4.176513000	-4.841543000	-0.516303000
H	-2.786527000	-4.702819000	0.566426000
H	-4.302765000	-3.876554000	0.962743000
C	-1.903582000	-3.146585000	-2.230045000
H	-1.015751000	-3.686188000	-1.882228000
H	-2.438578000	-3.825417000	-2.905542000
H	-1.580570000	-2.286035000	-2.828372000
C	-4.622933000	-1.905537000	-1.692598000
H	-5.400500000	-1.599875000	-0.986449000
H	-4.389661000	-1.057185000	-2.344684000
H	-5.047912000	-2.694173000	-2.325887000
Cl	3.994232000	-1.062803000	2.021774000
H	7.320791000	0.141567000	-1.276325000

***o*TS1^b**, $E_{(\text{SCF Done})} = -1979.678445$ a.u. $\text{IF} = i294.62$ cm^{-1}

Sc	0.225687000	-0.037039000	0.162443000
N	1.002842000	2.137338000	0.630494000
C	0.091119000	1.101256000	-1.995506000
H	1.076377000	1.514831000	-2.215136000
H	-0.443329000	0.972386000	-2.934700000
C	-0.709029000	2.041298000	-1.143897000
C	-0.250679000	2.615869000	0.071150000
C	-0.999208000	3.617791000	0.706695000
H	-0.634077000	4.072545000	1.620561000
C	-2.199054000	4.058769000	0.169845000
H	-2.752235000	4.851371000	0.664919000
C	-2.686369000	3.481337000	-1.006173000
H	-3.622839000	3.822169000	-1.438055000
C	-1.958983000	2.483739000	-1.632720000
H	-2.324551000	2.060537000	-2.564169000
C	1.134227000	2.372867000	2.083019000
H	1.275169000	3.437629000	2.309019000
H	2.011086000	1.832817000	2.443450000

H	0.247991000	2.010269000	2.607056000
C	2.192720000	2.726916000	-0.033738000
H	2.126864000	2.634923000	-1.116204000
H	3.089349000	2.205754000	0.309330000
H	2.269966000	3.792401000	0.218756000
C	-0.802231000	-0.902276000	2.254400000
C	-1.830266000	-0.328260000	1.454942000
C	-1.982306000	-1.119715000	0.257588000
C	-1.043862000	-2.205742000	0.374698000
C	-0.319131000	-2.067767000	1.581822000
C	-2.713270000	0.804021000	1.896777000
H	-3.047653000	1.421079000	1.061903000
H	-2.214804000	1.460918000	2.616360000
H	-3.609116000	0.413302000	2.397436000
C	-0.949367000	-3.415581000	-0.510611000
H	0.076941000	-3.784707000	-0.618723000
H	-1.347395000	-3.239485000	-1.512946000
H	-1.526418000	-4.242650000	-0.076861000
C	0.626301000	-3.085657000	2.147742000
H	0.064207000	-3.954316000	2.516436000
H	1.201374000	-2.693353000	2.990609000
H	1.341204000	-3.461575000	1.407074000
C	-0.421411000	-0.506954000	3.654478000
H	-0.824358000	-1.232521000	4.373072000
H	0.662823000	-0.476507000	3.815819000
H	-0.829304000	0.468018000	3.935199000
C	5.805706000	-0.130427000	-1.021892000
C	5.070647000	-0.233831000	0.157980000
C	3.726182000	-0.569744000	0.067513000
C	3.060583000	-0.842264000	-1.134749000
C	3.838027000	-0.717265000	-2.299759000
C	5.183564000	-0.363607000	-2.248325000
H	5.529917000	-0.049543000	1.124033000
H	3.381262000	-0.940341000	-3.260537000
H	5.754745000	-0.289656000	-3.169257000
C	1.639892000	-1.266840000	-1.148758000
C	0.759478000	-0.817214000	-2.167598000
H	1.431060000	-2.229424000	-0.687333000
H	-0.162202000	-1.377624000	-2.311987000
H	1.166383000	-0.451121000	-3.106612000
Si	-3.513859000	-1.225015000	-0.894448000
C	-4.406693000	-2.843733000	-0.470115000
H	-5.349111000	-2.902185000	-1.027803000
H	-3.820018000	-3.733018000	-0.718955000

H	-4.648863000	-2.886427000	0.597776000
C	-3.064699000	-1.241085000	-2.743305000
H	-2.473164000	-2.114080000	-3.039815000
H	-3.992392000	-1.273876000	-3.327604000
H	-2.520503000	-0.340782000	-3.047496000
C	-4.767184000	0.169817000	-0.622276000
H	-5.164704000	0.169994000	0.397286000
H	-4.371881000	1.165697000	-0.839089000
H	-5.611159000	-0.007578000	-1.300492000
Cl	2.765373000	-0.628543000	1.552183000
H	6.858496000	0.131743000	-0.977297000

oP1^b, $E_{(\text{SCF Done})} = -1979.716676$ a.u.

Sc	0.200567000	-0.425614000	0.340887000
N	0.819712000	1.442343000	1.590695000
C	0.967775000	2.442882000	-1.370626000
H	1.973389000	2.510668000	-0.948660000
H	0.918853000	3.252050000	-2.106406000
C	-0.113052000	2.757111000	-0.342114000
C	-0.190967000	2.332307000	1.014372000
C	-1.253747000	2.773181000	1.821995000
H	-1.304596000	2.480702000	2.863714000
C	-2.241066000	3.619806000	1.332757000
H	-3.037321000	3.953960000	1.991349000
C	-2.183463000	4.042191000	0.009258000
H	-2.938757000	4.710224000	-0.393830000
C	-1.134825000	3.611371000	-0.793167000
H	-1.083634000	3.961932000	-1.820953000
C	0.478768000	0.897232000	2.923555000
H	0.461702000	1.675368000	3.697890000
H	1.248531000	0.170422000	3.198402000
H	-0.497295000	0.400998000	2.915997000
C	2.152254000	2.083831000	1.721306000
H	2.488527000	2.497048000	0.775823000
H	2.878049000	1.337133000	2.049649000
H	2.098738000	2.891229000	2.463007000
C	-0.768768000	-2.509850000	1.243098000
C	-1.807244000	-1.540419000	1.159098000
C	-2.022686000	-1.207141000	-0.226701000
C	-1.117090000	-2.037748000	-0.985566000
C	-0.353440000	-2.825661000	-0.090989000
C	-2.611363000	-1.059295000	2.336831000
H	-2.855127000	0.005705000	2.280727000
H	-2.097054000	-1.246395000	3.285605000

H	-3.565118000	-1.599546000	2.394716000
C	-1.063182000	-2.178108000	-2.479392000
H	-0.121982000	-2.628686000	-2.808681000
H	-1.174873000	-1.223110000	-2.999504000
H	-1.867009000	-2.836382000	-2.833587000
C	0.628342000	-3.889198000	-0.488055000
H	0.098048000	-4.769090000	-0.874715000
H	1.236783000	-4.225390000	0.355428000
H	1.314182000	-3.555411000	-1.274686000
C	-0.292062000	-3.193859000	2.494792000
H	-0.923983000	-4.062191000	2.723124000
H	0.732894000	-3.566585000	2.400254000
H	-0.326104000	-2.540527000	3.373481000
C	5.759804000	0.150846000	-0.605896000
C	4.924428000	-0.581483000	0.234554000
C	3.567392000	-0.604995000	-0.057218000
C	2.956779000	0.027467000	-1.145688000
C	3.846035000	0.759272000	-1.956434000
C	5.212716000	0.824615000	-1.696901000
H	5.317585000	-1.112650000	1.095645000
H	3.451596000	1.274810000	-2.827807000
H	5.856618000	1.396789000	-2.358967000
C	1.483800000	-0.104380000	-1.425583000
C	0.853997000	1.103198000	-2.136484000
H	1.348449000	-0.987873000	-2.066371000
H	-0.206868000	0.897670000	-2.342809000
H	1.297827000	1.258453000	-3.132617000
Si	-3.599950000	-0.413736000	-0.983172000
C	-4.688328000	-1.857890000	-1.552665000
H	-5.636805000	-1.477309000	-1.950222000
H	-4.214532000	-2.453609000	-2.339672000
H	-4.919961000	-2.527965000	-0.717288000
C	-3.234574000	0.726218000	-2.454491000
H	-2.777299000	0.213245000	-3.305599000
H	-4.184857000	1.147111000	-2.805469000
H	-2.593487000	1.565117000	-2.163954000
C	-4.594201000	0.610058000	0.264291000
H	-4.993022000	0.010555000	1.087819000
H	-4.022327000	1.445277000	0.681357000
H	-5.452383000	1.036479000	-0.270011000
H	6.825663000	0.192333000	-0.403157000
Cl	2.513187000	-1.521654000	1.064369000

oC2^b_{syn}, $E_{(\text{SCF Done})} = -2748.79036$ a.u.

N	5. 755138000	-0. 157324000	-1. 838748000
C	3. 901431000	1. 895765000	-0. 932841000
H	4. 402617000	2. 094595000	-1. 883925000
H	3. 668225000	2. 871517000	-0. 488823000
C	4. 798384000	1. 131869000	0. 011949000
C	5. 651587000	0. 095864000	-0. 437453000
C	6. 361711000	-0. 659514000	0. 504613000
H	7. 020573000	-1. 454563000	0. 168298000
C	6. 256337000	-0. 398308000	1. 870329000
H	6. 824857000	-0. 996245000	2. 578051000
C	5. 450882000	0. 644885000	2. 315703000
H	5. 381423000	0. 876774000	3. 375154000
C	4. 735320000	1. 397290000	1. 383848000
H	4. 104815000	2. 215631000	1. 727779000
C	6. 068455000	-1. 524943000	-2. 218884000
H	7. 118648000	-1. 813138000	-2. 032763000
H	5. 885645000	-1. 641331000	-3. 293339000
H	5. 420780000	-2. 224052000	-1. 681228000
C	6. 637518000	0. 777884000	-2. 536092000
H	6. 420493000	1. 807338000	-2. 242189000
H	6. 485982000	0. 686801000	-3. 617795000
H	7. 702381000	0. 584779000	-2. 318275000
C	1. 148805000	-2. 247775000	0. 083734000
C	0. 085798000	-2. 408182000	1. 022051000
C	-1. 167029000	-2. 459670000	0. 314101000
C	-0. 844825000	-2. 319485000	-1. 078116000
C	0. 570199000	-2. 176259000	-1. 214286000
C	0. 298161000	-2. 649329000	2. 491938000
H	-0. 557891000	-2. 341231000	3. 099073000
H	1. 183046000	-2. 128307000	2. 871283000
H	0. 457055000	-3. 718855000	2. 679456000
C	-1. 752845000	-2. 482929000	-2. 265232000
H	-1. 498591000	-1. 799687000	-3. 084411000
H	-2. 805236000	-2. 347865000	-2. 015802000
H	-1. 650311000	-3. 498157000	-2. 672144000
C	1. 304807000	-2. 134015000	-2. 523125000
H	1. 233721000	-3. 107290000	-3. 026679000
H	2. 366376000	-1. 915532000	-2. 389201000
H	0. 898889000	-1. 390523000	-3. 219566000
C	2. 611311000	-2. 295453000	0. 404867000
H	2. 964895000	-3. 335189000	0. 387794000
H	3. 215655000	-1. 731554000	-0. 309248000
H	2. 834411000	-1. 898946000	1. 399642000
C	0. 100773000	2. 165052000	1. 554285000

C	0.927044000	2.175267000	0.405196000
C	0.904935000	3.414899000	-0.292131000
C	0.187752000	4.513289000	0.154777000
C	-0.578600000	4.447992000	1.326050000
C	-0.626293000	3.254204000	2.033501000
H	1.504898000	3.509152000	-1.190980000
H	0.237555000	5.443056000	-0.405417000
H	-1.206723000	3.160827000	2.946151000
C	1.629334000	0.974707000	-0.078086000
C	2.586779000	1.138065000	-1.249568000
H	2.127231000	0.463587000	0.760400000
H	2.082757000	1.642734000	-2.086856000
H	2.865335000	0.152403000	-1.633734000
C	-5.291369000	1.098388000	-1.227566000
C	-3.955640000	1.469636000	-0.955220000
C	-3.751617000	2.554441000	-0.079425000
C	-4.814029000	3.227015000	0.503524000
C	-6.123693000	2.834368000	0.217945000
C	-6.363390000	1.773610000	-0.649981000
H	-2.736585000	2.864727000	0.151223000
H	-4.626771000	4.056961000	1.177938000
H	-7.376945000	1.469075000	-0.888594000
C	-2.841680000	0.764298000	-1.576797000
C	-1.548218000	1.171542000	-1.654031000
H	-3.098876000	-0.172495000	-2.063040000
H	-0.863407000	0.621659000	-2.307253000
H	-1.222074000	2.157771000	-1.332272000
Sc	-0.249449000	-0.229876000	0.037471000
Si	-2.830472000	-2.915245000	1.157149000
C	-2.587265000	-4.521836000	2.131321000
H	-1.925590000	-4.416550000	2.995538000
H	-3.560234000	-4.866591000	2.501686000
H	-2.180949000	-5.308887000	1.486059000
C	-4.232575000	-3.232236000	-0.074463000
H	-3.988373000	-4.022478000	-0.791832000
H	-5.101440000	-3.574389000	0.501540000
H	-4.547005000	-2.341657000	-0.627229000
C	-3.388020000	-1.514840000	2.316834000
H	-2.659024000	-1.287201000	3.102064000
H	-3.595868000	-0.589943000	1.764050000
H	-4.320317000	-1.806889000	2.815365000
H	-6.963403000	3.356225000	0.667741000
H	-1.121520000	5.316375000	1.686001000
Cl	-5.660873000	-0.190993000	-2.338554000

Cl -0.005213000 0.646658000 2.492963000

***o*TS2^b_{syn}, $E_{(\text{SCF Done})} = -2748.777151$ a.u. $\text{IF} = i213.06$ cm⁻¹**

N	-5.484623000	-0.602161000	1.698981000
C	-3.866740000	1.491221000	0.498450000
H	-4.603013000	1.738016000	1.266209000
H	-3.837402000	2.341183000	-0.193389000
C	-4.286049000	0.252774000	-0.257804000
C	-5.041796000	-0.774621000	0.354666000
C	-5.329267000	-1.935953000	-0.375613000
H	-5.911454000	-2.727878000	0.086033000
C	-4.900347000	-2.088232000	-1.693249000
H	-5.146501000	-2.995733000	-2.238500000
C	-4.191653000	-1.063286000	-2.314104000
H	-3.884722000	-1.153638000	-3.352756000
C	-3.895856000	0.093918000	-1.592030000
H	-3.356736000	0.904741000	-2.079302000
C	-5.618364000	-1.816858000	2.487631000
H	-6.497027000	-2.430647000	2.220445000
H	-5.724182000	-1.539428000	3.542453000
H	-4.721438000	-2.434172000	2.383206000
C	-6.692288000	0.216316000	1.811910000
H	-6.600733000	1.126576000	1.214011000
H	-6.842152000	0.503101000	2.858863000
H	-7.592951000	-0.320984000	1.467803000
C	-0.319553000	-2.108023000	0.629397000
C	0.345710000	-2.187205000	-0.627847000
C	1.764918000	-2.088567000	-0.410335000
C	1.950848000	-1.986011000	1.014628000
C	0.673875000	-1.983239000	1.645869000
C	-0.354367000	-2.509473000	-1.917665000
H	0.235801000	-2.235610000	-2.794929000
H	-1.329435000	-2.018702000	-1.997173000
H	-0.538078000	-3.590559000	-1.976719000
C	3.255325000	-2.046277000	1.753102000
H	3.159039000	-1.693085000	2.781873000
H	4.042738000	-1.463018000	1.273100000
H	3.605161000	-3.085728000	1.804251000
C	0.392807000	-2.005579000	3.119972000
H	0.194238000	-3.032581000	3.453840000
H	-0.489417000	-1.411141000	3.383109000
H	1.234630000	-1.635941000	3.711647000
C	-1.782886000	-2.334817000	0.862528000
H	-1.980128000	-3.411794000	0.953497000

H	-2.130524000	-1.868741000	1.789173000
H	-2.407680000	-1.964327000	0.045215000
C	-0.464685000	2.326349000	-1.862892000
C	-1.106105000	2.442163000	-0.616570000
C	-1.570965000	3.740481000	-0.315018000
C	-1.440459000	4.802204000	-1.203902000
C	-0.836457000	4.616623000	-2.446631000
C	-0.335031000	3.361169000	-2.780576000
H	-2.069376000	3.910959000	0.634071000
H	-1.823920000	5.779661000	-0.926315000
H	0.156549000	3.188416000	-3.732760000
C	-1.264482000	1.314200000	0.339702000
C	-2.506832000	1.377537000	1.229684000
H	-1.326520000	0.350928000	-0.219718000
H	-2.430191000	2.236801000	1.908601000
H	-2.531351000	0.490537000	1.872299000
C	3.934924000	1.375980000	1.807236000
C	2.600967000	1.584175000	1.367620000
C	2.446057000	2.095356000	0.053500000
C	3.541783000	2.348342000	-0.782384000
C	4.826942000	2.097448000	-0.325573000
C	5.019214000	1.628937000	0.980753000
H	1.462765000	2.454070000	-0.261807000
H	3.377569000	2.765922000	-1.771316000
H	6.022882000	1.478745000	1.366441000
C	1.432174000	1.210206000	2.143126000
C	0.166397000	1.805073000	1.966363000
H	1.577458000	0.559197000	2.998671000
H	-0.571289000	1.570503000	2.726264000
H	0.100872000	2.815936000	1.567797000
Sc	0.802530000	0.029776000	0.247714000
Si	3.085855000	-2.462832000	-1.756610000
C	2.828980000	-4.263633000	-2.284608000
H	1.846865000	-4.427994000	-2.739467000
H	3.589801000	-4.550103000	-3.020255000
H	2.920877000	-4.939724000	-1.427315000
C	4.860999000	-2.255926000	-1.131173000
H	5.114070000	-2.942566000	-0.318328000
H	5.534061000	-2.478184000	-1.968636000
H	5.073956000	-1.232220000	-0.804154000
C	2.934755000	-1.318975000	-3.267656000
H	1.975238000	-1.382168000	-3.790733000
H	3.115707000	-0.271626000	-2.999746000
H	3.709948000	-1.606272000	-3.988931000

Cl	0.272469000	0.771948000	-2.291693000
Cl	4.236641000	0.903678000	3.452573000
H	-0.744619000	5.438924000	-3.149322000
H	5.688031000	2.291406000	-0.957640000

oP2_{syn}, $E_{(\text{SCF Done})} = -2748.808851$ a.u.

N	-5.345346000	-0.368208000	1.781207000
C	-4.434268000	1.204539000	-0.502738000
H	-5.399312000	1.609481000	-0.180294000
H	-4.293979000	1.555464000	-1.532738000
C	-4.457005000	-0.308475000	-0.502411000
C	-4.860957000	-1.056686000	0.630241000
C	-4.771092000	-2.454505000	0.592420000
H	-5.081810000	-3.033809000	1.456828000
C	-4.319955000	-3.121912000	-0.546014000
H	-4.279408000	-4.208307000	-0.552892000
C	-3.963119000	-2.394647000	-1.677626000
H	-3.643487000	-2.902418000	-2.583937000
C	-4.035508000	-1.001551000	-1.641484000
H	-3.760050000	-0.429563000	-2.525925000
C	-5.111796000	-1.017338000	3.060593000
H	-5.760779000	-1.891999000	3.244787000
H	-5.304875000	-0.294601000	3.861347000
H	-4.068448000	-1.339101000	3.132428000
C	-6.739251000	0.059297000	1.668028000
H	-6.922889000	0.530897000	0.700266000
H	-6.963762000	0.787443000	2.455525000
H	-7.441770000	-0.786272000	1.767268000
C	0.578446000	-2.181195000	1.181524000
C	1.275800000	-2.479885000	-0.025342000
C	2.615036000	-1.961576000	0.070931000
C	2.730203000	-1.373943000	1.380252000
C	1.479381000	-1.510014000	2.058968000
C	0.716057000	-3.339327000	-1.125347000
H	1.147905000	-3.116439000	-2.105012000
H	-0.372371000	-3.252870000	-1.206358000
H	0.930796000	-4.394887000	-0.913594000
C	3.978060000	-0.825104000	2.014632000
H	3.749310000	-0.224962000	2.898613000
H	4.565925000	-0.206070000	1.333183000
H	4.624781000	-1.648472000	2.344358000
C	1.200650000	-1.174617000	3.493832000
H	1.448099000	-2.031431000	4.134811000
H	0.145226000	-0.940256000	3.661581000

H	1.788075000	-0.323921000	3.847244000
C	-0.825878000	-2.591618000	1.515503000
H	-0.837882000	-3.607683000	1.932678000
H	-1.273568000	-1.932566000	2.265186000
H	-1.486422000	-2.596509000	0.642936000
C	-0.941438000	1.237646000	-2.369657000
C	-1.590017000	2.003759000	-1.398298000
C	-1.947744000	3.298419000	-1.818734000
C	-1.696006000	3.764270000	-3.104034000
C	-1.064201000	2.944534000	-4.039617000
C	-0.674252000	1.662305000	-3.669460000
H	-2.447379000	3.952622000	-1.109972000
H	-1.999213000	4.770320000	-3.378770000
H	-0.176936000	1.001357000	-4.372136000
C	-1.891704000	1.549076000	0.020854000
C	-3.361555000	1.820075000	0.410403000
H	-1.755061000	0.460474000	0.082941000
H	-3.525279000	2.904700000	0.471070000
H	-3.515834000	1.431750000	1.423003000
C	2.770673000	2.486716000	1.808112000
C	1.646672000	2.192842000	0.986951000
C	1.887314000	2.299737000	-0.416633000
C	3.123603000	2.682848000	-0.955643000
C	4.186765000	2.955089000	-0.105289000
C	3.998067000	2.866751000	1.278046000
H	1.027444000	2.227833000	-1.091092000
H	3.233334000	2.788215000	-2.031368000
H	4.810406000	3.110756000	1.955931000
C	0.398015000	1.589323000	1.450619000
C	-0.951792000	2.236641000	1.060498000
H	0.427609000	1.395004000	2.521313000
H	-1.528186000	2.304870000	1.990104000
H	-0.788862000	3.274492000	0.740065000
Sc	1.171497000	-0.056665000	0.120214000
Si	3.958285000	-2.210647000	-1.275623000
C	4.171851000	-4.066419000	-1.578702000
H	3.266478000	-4.541116000	-1.968359000
H	4.974217000	-4.229808000	-2.307893000
H	4.452415000	-4.580882000	-0.652871000
C	5.638153000	-1.486252000	-0.789981000
H	6.032764000	-1.915394000	0.135870000
H	6.348995000	-1.725038000	-1.590757000
H	5.618813000	-0.395968000	-0.687505000
C	3.422153000	-1.334986000	-2.880135000

H	2.468930000	-1.697900000	-3.278714000
H	3.344189000	-0.248883000	-2.738780000
H	4.181847000	-1.500902000	-3.653766000
Cl	2.609416000	2.470221000	3.540447000
Cl	-0.369115000	-0.410725000	-1.971862000
H	5.151753000	3.258486000	-0.499374000
H	-0.873055000	3.296030000	-5.048981000

oC2_{iso}, $E_{(\text{SCF Done})} = -2748.793232$ a.u.

Sc	0.989120000	0.105533000	0.234051000
C	-1.895708000	-2.735320000	0.805775000
C	1.798431000	0.326903000	3.674612000
C	2.085866000	0.837704000	2.293795000
C	1.470983000	1.987400000	1.707678000
C	2.120739000	2.249983000	0.467351000
C	3.115245000	1.232823000	0.241838000
C	3.106957000	0.390026000	1.408182000
C	0.424734000	2.830612000	2.380317000
C	1.963593000	3.509387000	-0.336853000
C	4.096218000	-0.686445000	1.739876000
C	-1.053831000	-1.484552000	1.161110000
C	0.433114000	-1.767207000	1.303675000
H	-1.436812000	-3.208948000	-0.063709000
H	-1.787644000	-3.442043000	1.637201000
H	0.734385000	0.394926000	3.925793000
H	2.340722000	0.921981000	4.421657000
H	2.104758000	-0.714057000	3.804406000
H	-0.332691000	2.224797000	2.890811000
H	-0.094885000	3.490434000	1.680927000
H	0.884719000	3.469067000	3.146154000
H	1.058158000	4.061282000	-0.074075000
H	1.961258000	3.339250000	-1.418183000
H	2.804747000	4.181228000	-0.125788000
H	4.351252000	-1.311304000	0.882542000
H	3.734001000	-1.342137000	2.533722000
H	5.027949000	-0.229866000	2.099507000
H	-1.422204000	-1.042017000	2.094324000
H	-1.282367000	-0.722200000	0.380343000
H	0.739323000	-2.066233000	2.301162000
C	0.843750000	-2.036065000	-1.131731000
C	1.139395000	-2.405968000	0.217541000
C	2.268235000	-3.261713000	0.380200000
C	3.043123000	-3.669336000	-0.692435000
C	2.747817000	-3.246155000	-1.998035000

C	1. 636740000	-2. 450106000	-2. 217124000
H	-0. 142749000	-1. 622805000	-1. 353467000
C	-2. 722414000	3. 851748000	-0. 115356000
C	-2. 385806000	2. 515485000	-0. 431863000
C	-3. 331797000	1. 522631000	-0. 107524000
C	-4. 535627000	1. 831667000	0. 506561000
C	-4. 835164000	3. 161414000	0. 809418000
C	-3. 931771000	4. 172307000	0. 494681000
H	-3. 119180000	0. 483864000	-0. 340007000
H	-4. 159357000	5. 209795000	0. 715700000
C	-1. 120867000	2. 193849000	-1. 080600000
C	-0. 720423000	1. 001192000	-1. 596095000
H	-0. 437985000	3. 030120000	-1. 192740000
H	0. 184796000	0. 977072000	-2. 208287000
H	-1. 390592000	0. 148082000	-1. 684453000
Si	4. 348356000	1. 254619000	-1. 229243000
C	5. 534592000	-0. 219179000	-1. 234337000
H	6. 177018000	-0. 250940000	-0. 349300000
H	5. 015523000	-1. 179128000	-1. 324959000
H	6. 187699000	-0. 115761000	-2. 109807000
C	5. 378328000	2. 841551000	-1. 133482000
H	6. 169456000	2. 808232000	-1. 892036000
H	4. 788993000	3. 745899000	-1. 312406000
H	5. 859970000	2. 937089000	-0. 154012000
C	3. 391777000	1. 191517000	-2. 874004000
H	4. 103995000	1. 222971000	-3. 707550000
H	2. 830918000	0. 253052000	-2. 967928000
H	2. 699860000	2. 028939000	-3. 013946000
H	3. 875428000	-4. 343610000	-0. 513994000
C	-3. 359056000	-2. 445391000	0. 575833000
C	-3. 890438000	-2. 163481000	-0. 705079000
C	-4. 217704000	-2. 415704000	1. 679730000
C	-5. 250142000	-1. 843654000	-0. 821221000
C	-5. 568830000	-2. 099240000	1. 556174000
H	-3. 811365000	-2. 650235000	2. 662041000
C	-6. 083044000	-1. 805522000	0. 296550000
H	-5. 675020000	-1. 638698000	-1. 798701000
H	-6. 211004000	-2. 091161000	2. 432368000
H	-7. 136740000	-1. 569140000	0. 172611000
N	-3. 029748000	-2. 211361000	-1. 852540000
C	-3. 462711000	-1. 406001000	-2. 990145000
H	-2. 644688000	-1. 356637000	-3. 717549000
H	-4. 339497000	-1. 820850000	-3. 515692000
H	-3. 705379000	-0. 388226000	-2. 669834000

C	-2.771945000	-3.584455000	-2.306330000
H	-3.662611000	-4.030557000	-2.778936000
H	-1.957962000	-3.580554000	-3.039635000
H	-2.482816000	-4.224502000	-1.470979000
H	-5.235109000	1.036530000	0.743446000
H	1.345004000	-2.178017000	-3.228005000
Cl	-1.651239000	5.173588000	-0.498796000
Cl	2.632757000	-3.909837000	1.953411000
H	-5.776268000	3.417112000	1.287896000
H	3.364768000	-3.583411000	-2.825061000

***o*TS2^b_{iso}, $E_{(\text{SCF Done})} = -2748.765699$ a.u. $\text{IF} = i168.99$ cm⁻¹**

Sc	1.087449000	-0.175887000	0.341414000
C	-3.289549000	-1.154406000	-0.725013000
C	2.390033000	-1.067886000	3.491972000
C	2.720280000	-0.617094000	2.096549000
C	2.922597000	0.743238000	1.699703000
C	3.350025000	0.748372000	0.344668000
C	3.395687000	-0.614269000	-0.131254000
C	3.041802000	-1.450573000	0.986152000
C	2.862909000	1.930338000	2.615372000
C	3.856176000	1.964443000	-0.370978000
C	3.106030000	-2.948996000	1.048183000
C	-2.557185000	-0.777352000	0.572699000
C	-1.027339000	-0.827889000	0.517199000
H	-2.892182000	-0.574557000	-1.562491000
H	-3.106772000	-2.210978000	-0.955757000
H	1.748282000	-0.352168000	4.016399000
H	3.308058000	-1.165303000	4.086625000
H	1.887460000	-2.038433000	3.512153000
H	2.113882000	1.811201000	3.403983000
H	2.636938000	2.856510000	2.081629000
H	3.833162000	2.064881000	3.112552000
H	3.370318000	2.876394000	-0.018325000
H	3.716910000	1.912708000	-1.453403000
H	4.931909000	2.082777000	-0.186284000
H	2.748897000	-3.426797000	0.134298000
H	2.524798000	-3.344375000	1.885290000
H	4.144483000	-3.271620000	1.199240000
H	-2.903886000	-1.451037000	1.368427000
H	-2.867213000	0.230392000	0.874367000
H	-0.692127000	-0.609078000	1.567914000
C	-0.124669000	-2.418130000	-1.242265000
C	-0.475246000	-2.176004000	0.102019000

C	-0.397473000	-3.283442000	0.981307000
C	-0.033578000	-4.550703000	0.535948000
C	0.292520000	-4.748565000	-0.805328000
C	0.258107000	-3.679634000	-1.696807000
H	-0.215731000	-1.608210000	-1.962433000
C	0.896847000	4.156093000	-0.073122000
C	0.317270000	2.901905000	0.203978000
C	-0.344701000	2.774319000	1.440816000
C	-0.397882000	3.813952000	2.364209000
C	0.218714000	5.028914000	2.073258000
C	0.858425000	5.201019000	0.847311000
H	-0.852271000	1.838661000	1.675182000
H	1.311136000	6.152740000	0.587636000
C	0.340629000	1.783973000	-0.758851000
C	-0.782540000	0.966655000	-0.912174000
H	1.057184000	1.836598000	-1.577351000
H	-0.860329000	0.372825000	-1.819510000
H	-1.742646000	1.254781000	-0.494009000
Si	4.097251000	-1.103565000	-1.850774000
C	4.209196000	-2.977406000	-2.100399000
H	4.850947000	-3.459459000	-1.356358000
H	3.233795000	-3.473919000	-2.090165000
H	4.658880000	-3.156176000	-3.084918000
C	5.845211000	-0.396925000	-2.015122000
H	6.291219000	-0.744335000	-2.954717000
H	5.865681000	0.696428000	-2.022450000
H	6.484096000	-0.743745000	-1.195278000
C	2.975033000	-0.409458000	-3.223241000
H	3.401794000	-0.653339000	-4.203682000
H	1.973762000	-0.858140000	-3.192185000
H	2.864689000	0.679506000	-3.182318000
H	-0.011894000	-5.378176000	1.238089000
C	-4.775570000	-0.926151000	-0.577428000
C	-5.326096000	0.370220000	-0.657613000
C	-5.617851000	-2.000820000	-0.281488000
C	-6.692779000	0.548867000	-0.418557000
C	-6.978991000	-1.816332000	-0.046750000
H	-5.194212000	-3.001820000	-0.222553000
C	-7.514472000	-0.533361000	-0.107670000
H	-7.125159000	1.543232000	-0.481168000
H	-7.612525000	-2.667575000	0.186230000
H	-8.573341000	-0.370883000	0.075009000
N	-4.460194000	1.467648000	-0.987802000
C	-4.790853000	2.731433000	-0.340601000

H	-3.956432000	3.428811000	-0.478351000
H	-5.694698000	3.217789000	-0.746059000
H	-4.936421000	2.572443000	0.731834000
C	-4.323672000	1.649682000	-2.433015000
H	-5.253884000	2.014948000	-2.901113000
H	-3.529697000	2.377861000	-2.637533000
H	-4.060655000	0.702568000	-2.913340000
H	-0.921674000	3.675392000	3.305700000
H	0.499451000	-3.827612000	-2.744971000
H	0.569546000	-5.741574000	-1.147249000
H	0.188385000	5.849134000	2.784156000
Cl	1.608078000	4.475099000	-1.636534000
Cl	-0.821653000	-3.103184000	2.659535000

oP2_{iso}, $E_{(\text{SCF Done})} = -2748.806754$ a.u.

Sc	1.809379000	0.015899000	0.420969000
C	-3.635338000	-0.712465000	0.010470000
C	4.932598000	0.408263000	2.014679000
C	4.222031000	-0.186767000	0.831920000
C	4.077848000	0.436012000	-0.444896000
C	3.414879000	-0.477862000	-1.309923000
C	3.158185000	-1.699580000	-0.582005000
C	3.689350000	-1.503030000	0.742739000
C	4.687752000	1.749606000	-0.828266000
C	3.186028000	-0.241371000	-2.776190000
C	3.800474000	-2.509620000	1.853165000
C	-3.170123000	0.640371000	0.568440000
C	-1.637124000	0.886433000	0.593730000
H	-3.270358000	-0.833361000	-1.014194000
H	-3.207446000	-1.531607000	0.604189000
H	4.849523000	1.499490000	2.035567000
H	6.003945000	0.169072000	1.980257000
H	4.554970000	0.024257000	2.968591000
H	4.568676000	2.509580000	-0.050222000
H	4.267050000	2.145794000	-1.755069000
H	5.766250000	1.619219000	-0.990387000
H	2.973465000	0.808966000	-2.993642000
H	2.352009000	-0.830459000	-3.166268000
H	4.079786000	-0.515703000	-3.351132000
H	3.069486000	-3.313679000	1.768624000
H	3.688655000	-2.049276000	2.841328000
H	4.794863000	-2.975528000	1.837972000
H	-3.562139000	0.760027000	1.585401000
H	-3.618717000	1.435285000	-0.038300000

H	-1. 510037000	1. 873674000	1. 055791000
C	-0. 349826000	-1. 282505000	0. 948106000
C	-0. 929456000	-0. 111789000	1. 485043000
C	-0. 810191000	0. 054329000	2. 880428000
C	-0. 128253000	-0. 867328000	3. 682534000
C	0. 443890000	-2. 003201000	3. 116200000
C	0. 322761000	-2. 219629000	1. 741344000
H	-0. 477932000	-1. 481997000	-0. 115059000
C	1. 746724000	3. 409644000	-1. 050600000
C	1. 115900000	2. 357968000	-0. 332225000
C	1. 282981000	2. 421748000	1. 081134000
C	1. 989954000	3. 446472000	1. 728206000
C	2. 570067000	4. 454658000	0. 975109000
C	2. 433370000	4. 436561000	-0. 417935000
H	0. 692157000	1. 755453000	1. 717454000
H	2. 860681000	5. 234126000	-1. 018066000
C	0. 487914000	1. 178108000	-0. 954743000
C	-1. 035090000	0. 958190000	-0. 817740000
H	0. 731876000	1. 142181000	-2. 018426000
H	-1. 279343000	0. 047231000	-1. 378142000
H	-1. 569382000	1. 763448000	-1. 342487000
Si	2. 630475000	-3. 329955000	-1. 453136000
C	2. 708812000	-4. 848188000	-0. 317130000
H	3. 704219000	-4. 994111000	0. 114123000
H	1. 975790000	-4. 851255000	0. 497060000
H	2. 492657000	-5. 726351000	-0. 938349000
C	3. 854921000	-3. 648295000	-2. 862744000
H	3. 658355000	-4. 636868000	-3. 294745000
H	3. 783455000	-2. 914423000	-3. 670479000
H	4. 885926000	-3. 645925000	-2. 491625000
C	0. 860653000	-3. 224601000	-2. 143443000
H	0. 705434000	-4. 046325000	-2. 853071000
H	0. 106794000	-3. 343291000	-1. 355888000
H	0. 656079000	-2. 291222000	-2. 678974000
H	-0. 059190000	-0. 688980000	4. 751292000
C	-5. 143055000	-0. 824112000	0. 051734000
C	-5. 954634000	-0. 182857000	-0. 907900000
C	-5. 757324000	-1. 510897000	1. 102180000
C	-7. 346249000	-0. 230372000	-0. 768112000
C	-7. 143989000	-1. 557498000	1. 233694000
H	-5. 132429000	-2. 008598000	1. 842128000
C	-7. 939967000	-0. 904882000	0. 297364000
H	-7. 976092000	0. 262031000	-1. 503451000
H	-7. 595782000	-2. 093715000	2. 063724000

H	-9.022995000	-0.927087000	0.385619000
N	-5.322604000	0.503057000	-1.994244000
C	-5.998482000	1.708002000	-2.450993000
H	-5.318569000	2.268680000	-3.103197000
H	-6.920535000	1.514683000	-3.027689000
H	-6.252812000	2.338845000	-1.594394000
C	-5.011506000	-0.377277000	-3.116991000
H	-5.914729000	-0.704187000	-3.662194000
H	-4.357737000	0.147525000	-3.823986000
H	-4.493379000	-1.274720000	-2.766335000
H	2.044301000	3.462187000	2.813017000
H	0.719228000	-3.121242000	1.286914000
H	0.959551000	-2.720839000	3.746744000
H	3.108991000	5.266978000	1.453135000
Cl	1.609989000	3.480601000	-2.784949000
Cl	-1.495804000	1.443084000	3.665642000

mC1St, $E_{(\text{SCF Done})} = -769.0726812$ a.u.

C	0.073204000	-0.782110000	0.000025000
C	-1.189908000	-0.172172000	0.000061000
C	-1.251791000	1.230910000	0.000069000
C	-0.089295000	1.991046000	0.000027000
C	1.166659000	1.382106000	-0.000018000
C	1.227902000	-0.007235000	-0.000017000
H	0.153509000	-1.865292000	0.000024000
H	-2.214958000	1.732316000	0.000122000
H	2.077010000	1.972279000	-0.000048000
C	-2.380382000	-1.033572000	0.000093000
C	-3.661402000	-0.648437000	-0.000070000
H	-2.166516000	-2.102512000	0.000255000
H	-4.461719000	-1.382348000	-0.000027000
H	-3.967025000	0.394689000	-0.000261000
Cl	2.786089000	-0.799337000	-0.000066000
H	-0.153720000	3.076379000	0.000036000

mC1^a, $E_{(\text{SCF Done})} = -2255.828384$ a.u.

Sc	-0.633001000	-0.105347000	-0.247083000
Si	-0.812727000	3.640944000	-0.140604000
C	-1.254612000	1.873338000	0.403985000
C	-0.967024000	3.883862000	-2.019421000
C	0.962171000	4.068244000	0.406526000
C	-1.977451000	4.876170000	0.710142000
C	-1.218537000	-1.032892000	-3.693019000
C	-1.624947000	-1.212684000	-2.257180000

C	-2.639555000	-0.473874000	-1.583356000
C	-2.845633000	-1.055818000	-0.284585000
C	-1.952733000	-2.183107000	-0.196322000
C	-1.201612000	-2.273224000	-1.397181000
C	-3.413365000	0.649692000	-2.212371000
C	-1.924920000	-3.207357000	0.903500000
C	-0.253508000	-3.379924000	-1.763650000
C	1.239015000	0.777751000	-1.796120000
C	2.064272000	-0.280608000	-1.975474000
H	-2.356003000	1.833871000	0.422811000
H	-0.963151000	1.853241000	1.473887000
H	-0.252188000	3.277463000	-2.587996000
H	-0.780417000	4.932626000	-2.278952000
H	-1.976096000	3.636169000	-2.368371000
H	1.081943000	3.932877000	1.488599000
H	1.175144000	5.120905000	0.186481000
H	1.738882000	3.477793000	-0.094973000
H	-3.020849000	4.702049000	0.421913000
H	-1.725817000	5.908582000	0.439769000
H	-1.914471000	4.791297000	1.801416000
H	-1.264238000	0.011437000	-4.018498000
H	-1.894183000	-1.594865000	-4.351272000
H	-0.208226000	-1.402680000	-3.896111000
H	-2.855281000	1.121201000	-3.026734000
H	-3.675785000	1.431108000	-1.497664000
H	-4.349442000	0.273504000	-2.645774000
H	-2.733078000	-3.936057000	0.761626000
H	-2.061239000	-2.768785000	1.896308000
H	-0.992561000	-3.780542000	0.911076000
H	0.337610000	-3.731511000	-0.910849000
H	0.445059000	-3.084209000	-2.552872000
H	-0.805701000	-4.249283000	-2.144604000
H	1.503212000	1.638012000	-1.186330000
H	0.369565000	0.894291000	-2.445070000
H	1.746513000	-1.051464000	-2.676837000
C	1.481020000	-1.884835000	1.518325000
O	0.590613000	-0.723617000	1.456657000
C	0.589494000	-0.036422000	2.759619000
C	1.368785000	-0.949874000	3.692270000
C	2.345304000	-1.646915000	2.742974000
H	0.858314000	-2.777470000	1.624932000
H	2.036435000	-1.926286000	0.579425000
H	1.078424000	0.930807000	2.614457000
H	-0.449911000	0.115285000	3.054624000

H	1.869079000	-0.384068000	4.482640000
H	0.702267000	-1.679371000	4.165431000
H	3.188917000	-0.992521000	2.498822000
H	2.741804000	-2.582156000	3.147476000
C	3.971408000	0.402085000	-0.486470000
C	3.374726000	-0.514216000	-1.371106000
C	4.073037000	-1.683757000	-1.716426000
C	5.337683000	-1.933765000	-1.190640000
C	5.924675000	-1.028590000	-0.310496000
C	5.230355000	0.135333000	0.035533000
H	3.473046000	1.327358000	-0.216677000
H	3.627191000	-2.390114000	-2.412348000
H	5.875296000	-2.834653000	-1.471061000
Si	-4.231286000	-0.678429000	0.987857000
C	-5.352137000	-2.204505000	1.090298000
H	-4.849401000	-3.073927000	1.525737000
H	-6.221107000	-1.977548000	1.719512000
H	-5.723642000	-2.487821000	0.099245000
C	-5.316564000	0.794314000	0.501015000
H	-5.818586000	0.643078000	-0.459615000
H	-6.097653000	0.891786000	1.265348000
H	-4.778719000	1.747054000	0.464222000
C	-3.508447000	-0.306529000	2.707584000
H	-4.330855000	-0.141574000	3.414168000
H	-2.901178000	-1.125647000	3.108444000
H	-2.903948000	0.608041000	2.691924000
Cl	5.956581000	1.269329000	1.132197000
H	6.912029000	-1.211215000	0.101186000

***m*TS1^a, $E_{(\text{SCF Done})} = -2255.817303$ a.u. IF = *i*430.23 cm⁻¹**

Sc	-0.340754000	-0.439852000	-0.324517000
Si	-0.453321000	3.810164000	-0.201889000
C	-0.563611000	1.919966000	-0.133670000
C	-0.971878000	4.464220000	-1.909380000
C	1.303691000	4.408928000	0.214680000
C	-1.633264000	4.550016000	1.095579000
C	-1.030618000	-2.412744000	-3.297755000
C	-1.486245000	-2.045006000	-1.916240000
C	-2.402693000	-1.020244000	-1.571604000
C	-2.667674000	-1.087418000	-0.155045000
C	-1.881202000	-2.193953000	0.345438000
C	-1.150514000	-2.766696000	-0.734134000
C	-3.029666000	-0.080686000	-2.564684000
C	-1.928689000	-2.765784000	1.736450000

C	-0.319622000	-4.017997000	-0.697320000
C	0.590614000	1.390856000	-1.798388000
C	1.169520000	0.101516000	-2.025064000
H	-1.635853000	1.669708000	-0.184089000
H	-0.203191000	1.644594000	0.880147000
H	-0.259646000	4.183771000	-2.692547000
H	-1.035956000	5.558694000	-1.893460000
H	-1.957858000	4.078828000	-2.195514000
H	1.632848000	4.015040000	1.183888000
H	1.323055000	5.503400000	0.280916000
H	2.044857000	4.113364000	-0.536050000
H	-2.672020000	4.256292000	0.904851000
H	-1.588050000	5.646290000	1.083407000
H	-1.373007000	4.217160000	2.107479000
H	-1.024641000	-1.556097000	-3.980831000
H	-1.693934000	-3.168648000	-3.741995000
H	-0.020515000	-2.837497000	-3.293734000
H	-2.436319000	-0.015590000	-3.483046000
H	-3.137228000	0.934511000	-2.172584000
H	-4.033095000	-0.418704000	-2.859403000
H	-2.707322000	-3.537037000	1.827225000
H	-2.144990000	-2.006165000	2.494172000
H	-0.983301000	-3.243993000	2.018975000
H	-0.014277000	-4.276826000	0.321843000
H	0.592206000	-3.928864000	-1.299095000
H	-0.881120000	-4.881115000	-1.084837000
H	1.279203000	2.199923000	-1.567811000
H	-0.172341000	1.695562000	-2.511574000
H	0.746223000	-0.498105000	-2.828030000
C	1.947874000	-1.893211000	1.562903000
O	0.964885000	-0.822150000	1.492043000
C	0.897420000	-0.124877000	2.760743000
C	1.674061000	-0.991744000	3.742218000
C	2.733808000	-1.625323000	2.837148000
H	1.402157000	-2.841900000	1.610808000
H	2.543419000	-1.858578000	0.649990000
H	1.365600000	0.858258000	2.633479000
H	-0.156014000	0.006803000	3.023207000
H	2.097784000	-0.403096000	4.561055000
H	1.022806000	-1.761307000	4.173036000
H	3.548850000	-0.920335000	2.641429000
H	3.163516000	-2.540905000	3.254181000
C	3.248681000	0.504604000	-0.664209000
C	2.495239000	-0.277318000	-1.575088000

C	3.109194000	-1.465079000	-2.049692000
C	4.376777000	-1.845968000	-1.639229000
C	5.110276000	-1.075027000	-0.726842000
C	4.515278000	0.093643000	-0.263480000
H	2.847672000	1.433095000	-0.270584000
H	2.567170000	-2.081134000	-2.763927000
H	4.817059000	-2.758046000	-2.036437000
Si	-4.015955000	-0.217158000	0.842304000
C	-5.345749000	-1.482264000	1.345312000
H	-4.935449000	-2.275825000	1.979100000
H	-6.156842000	-0.994691000	1.900100000
H	-5.780176000	-1.956917000	0.457911000
C	-4.898936000	1.167128000	-0.117942000
H	-5.383703000	0.801614000	-1.028567000
H	-5.679539000	1.590570000	0.526661000
H	-4.224131000	1.984625000	-0.395223000
C	-3.346809000	0.606097000	2.428551000
H	-4.162607000	1.125758000	2.946615000
H	-2.917453000	-0.109993000	3.137790000
H	-2.581161000	1.353078000	2.187247000
Cl	5.398170000	1.097805000	0.880740000
H	6.103429000	-1.364042000	-0.401579000

mP1^a, $E_{(\text{SCF Done})} = -2255.858856$ a.u.

Sc	-0.136497000	-0.562040000	-0.376612000
Si	-0.494488000	3.885440000	-0.079477000
C	-0.168265000	1.990570000	-0.389424000
C	-1.551428000	4.548004000	-1.497717000
C	1.180921000	4.756232000	-0.005239000
C	-1.395448000	4.055608000	1.574232000
C	-0.944371000	-2.245622000	-3.432863000
C	-1.351446000	-1.949400000	-2.021067000
C	-2.224862000	-0.917193000	-1.589555000
C	-2.488962000	-1.086116000	-0.181050000
C	-1.763102000	-2.260602000	0.227776000
C	-1.050405000	-2.771971000	-0.891071000
C	-2.804072000	0.117785000	-2.512320000
C	-1.819279000	-2.926880000	1.573277000
C	-0.238084000	-4.035621000	-0.938971000
C	0.500755000	1.717373000	-1.775687000
C	0.947727000	0.279495000	-2.063411000
H	-1.174042000	1.529326000	-0.285485000
H	0.459311000	1.687139000	0.470219000
H	-1.027793000	4.496051000	-2.458208000

H	-1.795874000	5.600896000	-1.314911000
H	-2.497786000	4.003659000	-1.593180000
H	1.812337000	4.359702000	0.798300000
H	1.028570000	5.823240000	0.195652000
H	1.735574000	4.679069000	-0.946510000
H	-2.380351000	3.576004000	1.560164000
H	-1.553180000	5.116240000	1.802524000
H	-0.816375000	3.629126000	2.401832000
H	-0.944965000	-1.352849000	-4.064553000
H	-1.645222000	-2.959580000	-3.886074000
H	0.051201000	-2.696987000	-3.492128000
H	-2.130042000	0.330587000	-3.348057000
H	-3.018147000	1.061411000	-2.006693000
H	-3.748450000	-0.234395000	-2.948121000
H	-2.601418000	-3.697020000	1.587263000
H	-2.045944000	-2.223327000	2.377928000
H	-0.881167000	-3.430791000	1.827557000
H	0.089737000	-4.357211000	0.054108000
H	0.651896000	-3.937369000	-1.570307000
H	-0.834317000	-4.857538000	-1.356958000
H	1.348151000	2.411956000	-1.873561000
H	-0.225561000	2.011256000	-2.539828000
H	0.722308000	-0.047320000	-3.077463000
C	2.005809000	-1.974854000	1.628435000
O	0.959695000	-0.955824000	1.491858000
C	0.747331000	-0.287650000	2.774354000
C	1.481652000	-1.144163000	3.792934000
C	2.652983000	-1.691227000	2.973060000
H	1.514465000	-2.952914000	1.605749000
H	2.678946000	-1.875375000	0.775134000
H	1.180239000	0.716315000	2.701594000
H	-0.329860000	-0.215263000	2.941538000
H	1.800898000	-0.559038000	4.659500000
H	0.839632000	-1.958434000	4.146714000
H	3.441545000	-0.938501000	2.868066000
H	3.094401000	-2.591969000	3.408070000
C	3.039777000	0.601017000	-0.671388000
C	2.292277000	-0.127416000	-1.623471000
C	2.865179000	-1.331306000	-2.105297000
C	4.119215000	-1.756456000	-1.685273000
C	4.852653000	-1.023685000	-0.746784000
C	4.291310000	0.149912000	-0.252523000
H	2.680500000	1.552043000	-0.291298000
H	2.329096000	-1.902273000	-2.859566000

H	4.546278000	-2.665688000	-2.100319000
Si	-3.867848000	-0.275178000	0.876809000
C	-5.186242000	-1.597073000	1.191101000
H	-4.804065000	-2.437892000	1.778920000
H	-6.029957000	-1.163247000	1.740746000
H	-5.570660000	-1.994293000	0.245175000
C	-4.695206000	1.194487000	0.012781000
H	-5.168861000	0.915907000	-0.933237000
H	-5.486092000	1.566400000	0.675908000
H	-4.012775000	2.031031000	-0.174680000
C	-3.215286000	0.378636000	2.541203000
H	-4.040986000	0.870309000	3.070211000
H	-2.840680000	-0.409078000	3.203313000
H	-2.428095000	1.130710000	2.410780000
Cl	5.174539000	1.096546000	0.918202000
H	5.835207000	-1.346843000	-0.420184000

$mC2^a_{syn}$, $E_{(SCF\ Done)} = -3024.926501$ a.u.

Sc	0.558676000	-0.962532000	0.164337000
Si	1.473731000	4.534802000	-1.872740000
C	0.907431000	3.182318000	-0.635633000
C	1.881970000	3.739457000	-3.549122000
C	3.000528000	5.432741000	-1.197392000
C	0.040641000	5.757991000	-2.078699000
C	2.715859000	-1.946019000	-0.439942000
C	1.834439000	-2.215952000	-1.539718000
C	0.812687000	-3.113032000	-1.106437000
C	1.039268000	-3.404310000	0.267580000
C	2.189976000	-2.678555000	0.685115000
C	2.019017000	-1.743448000	-2.956255000
C	-0.212706000	-3.805469000	-1.959429000
C	0.267865000	-4.416379000	1.063056000
C	2.810689000	-2.767807000	2.053105000
C	1.937313000	2.082858000	-0.361951000
C	1.594488000	0.950947000	0.652657000
H	-0.034067000	2.770988000	-1.028278000
H	0.647412000	3.697627000	0.298461000
H	2.715732000	3.031617000	-3.472880000
H	2.170937000	4.506496000	-4.276922000
H	1.016772000	3.206050000	-3.961744000
H	2.795449000	5.882775000	-0.219141000
H	3.301864000	6.238866000	-1.876290000
H	3.857476000	4.758738000	-1.085661000
H	-0.855156000	5.266208000	-2.475934000

H	0.312211000	6.561987000	-2.772324000
H	-0.226124000	6.221278000	-1.121817000
H	2.352015000	-0.703514000	-3.006981000
H	1.100011000	-1.830284000	-3.544231000
H	2.776359000	-2.347637000	-3.472426000
H	-0.244632000	-3.401893000	-2.975020000
H	-1.227797000	-3.756355000	-1.546360000
H	0.035187000	-4.870835000	-2.053672000
H	0.663726000	-5.424384000	0.879454000
H	-0.792470000	-4.441546000	0.789357000
H	0.332150000	-4.246234000	2.141591000
H	2.147979000	-3.263866000	2.768243000
H	3.068991000	-1.786894000	2.464080000
H	3.737194000	-3.355393000	2.022201000
H	2.854797000	2.577406000	-0.006593000
H	2.221586000	1.611043000	-1.313970000
H	2.562844000	0.498212000	0.912263000
C	-0.962248000	-1.421013000	3.036656000
O	-1.064849000	-1.392806000	1.571824000
C	-2.403597000	-1.820848000	1.164007000
C	-3.055460000	-2.362256000	2.426218000
C	-2.397503000	-1.518086000	3.519874000
H	-0.375668000	-2.304485000	3.308365000
H	-0.441290000	-0.515718000	3.346777000
H	-2.928064000	-0.942845000	0.777133000
H	-2.293521000	-2.558792000	0.365341000
H	-4.142999000	-2.254458000	2.395608000
H	-2.819694000	-3.423723000	2.560727000
H	-2.851090000	-0.522617000	3.571881000
H	-2.461281000	-1.977297000	4.510071000
C	-0.335856000	1.897830000	2.018452000
C	0.966363000	1.356956000	1.945797000
C	1.643510000	1.168875000	3.170964000
C	1.065021000	1.515659000	4.390225000
C	-0.217867000	2.060705000	4.443941000
C	-0.901608000	2.242762000	3.242682000
H	-0.908133000	2.071562000	1.113142000
H	2.658840000	0.778949000	3.155941000
H	1.623789000	1.376284000	5.312142000
C	-3.641672000	-1.877042000	-3.032100000
C	-3.084550000	-0.800309000	-2.321750000
C	-3.938313000	0.073493000	-1.624255000
C	-5.308719000	-0.153176000	-1.627011000
C	-5.859113000	-1.235154000	-2.321385000

C	-5.016573000	-2.092337000	-3.024724000
H	-2.992549000	-2.543159000	-3.594495000
H	-3.548476000	0.946575000	-1.110597000
H	-5.440051000	-2.925743000	-3.577315000
C	-1.638305000	-0.606382000	-2.363892000
C	-0.887001000	0.229463000	-1.607296000
H	-1.123321000	-1.199573000	-3.117703000
H	0.148027000	0.430162000	-1.895222000
H	-1.331392000	0.919561000	-0.892378000
Si	4.537700000	-1.355200000	-0.583154000
C	5.528721000	-2.948020000	-0.867838000
H	6.595592000	-2.719204000	-0.974935000
H	5.419453000	-3.647748000	-0.031851000
H	5.202379000	-3.462599000	-1.778576000
C	5.215049000	-0.503174000	0.972356000
H	4.704435000	0.436204000	1.208615000
H	5.199030000	-1.142849000	1.859440000
H	6.265410000	-0.255350000	0.773625000
C	4.851656000	-0.181508000	-2.038962000
H	5.900041000	0.137372000	-1.987069000
H	4.708003000	-0.661600000	-3.011285000
H	4.236034000	0.722876000	-2.000238000
Cl	-2.517940000	2.905165000	3.268349000
Cl	-6.354332000	0.931991000	-0.765826000
H	-6.933532000	-1.387917000	-2.318601000
H	-0.673625000	2.344535000	5.386652000

***m*TS2^a_{syn}, $E_{(\text{SCF Done})} = -3024.914405$ a.u., IF = *i*141.48 cm⁻¹**

Sc	0.209951000	-1.193261000	-0.092219000
Si	2.035043000	4.977551000	-1.015623000
C	1.030465000	3.495373000	-0.312847000
C	2.466231000	4.639449000	-2.831988000
C	3.619766000	5.204477000	-0.000239000
C	0.940394000	6.516192000	-0.883045000
C	2.492424000	-2.190859000	-0.179431000
C	1.888085000	-2.439018000	-1.456649000
C	0.786092000	-3.331938000	-1.284297000
C	0.692257000	-3.642903000	0.100800000
C	1.716876000	-2.930860000	0.783220000
C	2.404436000	-1.997675000	-2.797829000
C	0.019163000	-4.010503000	-2.383118000
C	-0.182611000	-4.687534000	0.727928000
C	2.027725000	-3.148071000	2.239055000
C	1.798543000	2.171090000	-0.277489000

C	1. 075126000	0. 897105000	0. 200061000
H	0. 113341000	3. 422298000	-0. 915225000
H	0. 712160000	3. 777503000	0. 699209000
H	3. 114261000	3. 762768000	-2. 947880000
H	2. 998267000	5. 495702000	-3. 262446000
H	1. 563869000	4. 477414000	-3. 433291000
H	3. 396265000	5. 353685000	1. 062503000
H	4. 171016000	6. 085562000	-0. 348434000
H	4. 290935000	4. 342520000	-0. 088854000
H	0. 014624000	6. 399866000	-1. 458284000
H	1. 463304000	7. 397505000	-1. 271696000
H	0. 667021000	6. 724860000	0. 157613000
H	2. 890473000	-1. 021341000	-2. 759172000
H	1. 614383000	-1. 948097000	-3. 554149000
H	3. 148180000	-2. 711817000	-3. 175807000
H	0. 000062000	-3. 424487000	-3. 307061000
H	-1. 018664000	-4. 228197000	-2. 108904000
H	0. 488717000	-4. 971150000	-2. 633625000
H	0. 403699000	-5. 592963000	0. 934460000
H	-1. 006555000	-4. 989593000	0. 075333000
H	-0. 606924000	-4. 363777000	1. 684556000
H	1. 122961000	-3. 188938000	2. 856430000
H	2. 675240000	-2. 371869000	2. 650579000
H	2. 545688000	-4. 106584000	2. 379530000
H	2. 666309000	2. 309980000	0. 384821000
H	2. 226591000	1. 965320000	-1. 268130000
H	1. 881193000	0. 138742000	0. 332209000
C	-2. 087392000	-1. 583892000	2. 241919000
O	-1. 727191000	-1. 740891000	0. 830298000
C	-2. 785588000	-2. 494164000	0. 146468000
C	-3. 603845000	-3. 127910000	1. 255209000
C	-3. 526270000	-2. 062345000	2. 349238000
H	-1. 403798000	-2. 204726000	2. 830065000
H	-1. 949643000	-0. 536703000	2. 501597000
H	-3. 371939000	-1. 780920000	-0. 434844000
H	-2. 300099000	-3. 201427000	-0. 526777000
H	-4. 627491000	-3. 333207000	0. 930167000
H	-3. 154973000	-4. 068630000	1. 592037000
H	-4. 220971000	-1. 241844000	2. 139421000
H	-3. 749136000	-2. 451269000	3. 346565000
C	-0. 803977000	1. 818830000	1. 649404000
C	0. 332534000	0. 991639000	1. 486257000
C	0. 794614000	0. 285644000	2. 618984000
C	0. 188039000	0. 442459000	3. 869655000

C	-0.892248000	1.300596000	4.027578000
C	-1.383378000	1.976946000	2.901959000
H	-1.207612000	2.368769000	0.807774000
H	1.701145000	-0.307197000	2.541005000
H	0.586902000	-0.083759000	4.732751000
C	-2.939669000	-1.270034000	-3.118325000
C	-2.214493000	-0.386334000	-2.299421000
C	-2.925102000	0.593142000	-1.585957000
C	-4.309986000	0.675415000	-1.698994000
C	-5.027255000	-0.200021000	-2.514134000
C	-4.323539000	-1.171549000	-3.225273000
H	-2.407942000	-2.024169000	-3.693128000
H	-2.408643000	1.290884000	-0.935213000
H	-4.864792000	-1.852966000	-3.875949000
C	-0.747319000	-0.490892000	-2.252694000
C	0.101038000	0.560896000	-1.937708000
H	-0.325917000	-1.316219000	-2.820179000
H	1.129658000	0.519730000	-2.280706000
H	-0.290414000	1.558619000	-1.778028000
Si	4.280805000	-1.557466000	0.143546000
C	5.331472000	-3.113726000	0.393546000
H	6.383853000	-2.842769000	0.538318000
H	5.009643000	-3.684985000	1.270709000
H	5.270547000	-3.773726000	-0.478736000
C	4.454771000	-0.442645000	1.675607000
H	3.858156000	0.473643000	1.609523000
H	4.222412000	-0.940407000	2.622248000
H	5.506127000	-0.133894000	1.733252000
C	4.997137000	-0.558523000	-1.300493000
H	5.987173000	-0.199257000	-0.993563000
H	5.135654000	-1.155091000	-2.206718000
H	4.397930000	0.323778000	-1.551180000
Cl	-2.746281000	3.037616000	3.081050000
Cl	-5.160993000	1.897668000	-0.796780000
H	-6.105797000	-0.114522000	-2.593501000
H	-1.353185000	1.454803000	4.997765000

mP2^a_{syn}, $E_{(\text{SCF Done})} = -3024.957533$ a.u.

Sc	-1.176956000	-0.716652000	-0.099137000
Si	5.928174000	0.859789000	-0.718958000
C	4.026763000	1.052171000	-0.509024000
C	6.303365000	0.085637000	-2.409018000
C	6.604903000	-0.246715000	0.665369000
C	6.691882000	2.588450000	-0.603592000

C	-0.822028000	-3.150745000	-0.150740000
C	-1.128358000	-2.749759000	-1.500016000
C	-2.464426000	-2.268469000	-1.544297000
C	-3.015820000	-2.379213000	-0.229950000
C	-2.013572000	-2.910708000	0.622568000
C	-0.242628000	-2.927917000	-2.700122000
C	-3.228368000	-1.868235000	-2.772177000
C	-4.454576000	-2.153752000	0.135515000
C	-2.237432000	-3.256419000	2.068962000
C	3.242578000	-0.256722000	-0.584868000
C	1.690020000	-0.150025000	-0.499387000
H	3.686720000	1.753717000	-1.283549000
H	3.865867000	1.548008000	0.458470000
H	5.888012000	-0.924928000	-2.497444000
H	7.386152000	0.008553000	-2.561180000
H	5.897489000	0.692166000	-3.226967000
H	6.373919000	0.163420000	1.655526000
H	7.695260000	-0.329067000	0.588825000
H	6.196212000	-1.262641000	0.615058000
H	6.306439000	3.249947000	-1.387886000
H	7.780868000	2.538422000	-0.716966000
H	6.480001000	3.054716000	0.365443000
H	0.799300000	-2.667590000	-2.495469000
H	-0.573690000	-2.320521000	-3.546927000
H	-0.255945000	-3.972766000	-3.037764000
H	-2.566040000	-1.575113000	-3.590599000
H	-3.916021000	-1.035263000	-2.591987000
H	-3.832931000	-2.710436000	-3.134322000
H	-4.986993000	-3.112906000	0.179433000
H	-4.976486000	-1.540905000	-0.605246000
H	-4.578410000	-1.678647000	1.114292000
H	-3.126058000	-2.757603000	2.468125000
H	-1.388541000	-2.991776000	2.706562000
H	-2.404231000	-4.334683000	2.191604000
H	3.580965000	-0.936718000	0.208173000
H	3.457836000	-0.761223000	-1.536634000
H	1.338185000	-1.191142000	-0.640145000
C	-2.786946000	0.727485000	2.357154000
O	-2.617375000	0.572102000	0.910901000
C	-3.727542000	1.246251000	0.212486000
C	-4.739752000	1.565273000	1.297513000
C	-3.847625000	1.803828000	2.516803000
H	-3.113663000	-0.236946000	2.761274000
H	-1.816544000	0.992790000	2.776969000

H	-3.315586000	2.141920000	-0.253902000
H	-4.092046000	0.564939000	-0.557342000
H	-5.343568000	2.437894000	1.034277000
H	-5.415546000	0.720303000	1.469704000
H	-3.392658000	2.799314000	2.475403000
H	-4.381617000	1.708740000	3.466210000
C	1.302721000	1.609074000	1.321398000
C	1.248801000	0.271633000	0.892622000
C	0.867364000	-0.708168000	1.830362000
C	0.600902000	-0.370255000	3.164631000
C	0.698666000	0.949329000	3.587989000
C	1.041433000	1.931927000	2.652121000
H	1.597391000	2.396746000	0.637224000
H	0.888972000	-1.758036000	1.541827000
H	0.348628000	-1.147724000	3.880721000
C	-2.262761000	1.744871000	-3.041838000
C	-1.251868000	1.701400000	-2.059111000
C	-1.077466000	2.859883000	-1.275546000
C	-1.869673000	3.987611000	-1.477209000
C	-2.870153000	4.017162000	-2.446013000
C	-3.052864000	2.875371000	-3.227134000
H	-2.403847000	0.886614000	-3.693493000
H	-0.319689000	2.893014000	-0.500254000
H	-3.809757000	2.880607000	-4.007426000
C	-0.432255000	0.473788000	-1.861170000
C	1.081845000	0.693733000	-1.637630000
H	-0.568343000	-0.168572000	-2.736827000
H	1.628231000	0.437081000	-2.555663000
H	1.296331000	1.753956000	-1.464420000
Si	0.519229000	-4.452589000	0.297075000
C	-0.207655000	-6.111318000	-0.260618000
H	0.490892000	-6.927639000	-0.042314000
H	-1.148958000	-6.327027000	0.256965000
H	-0.408474000	-6.120885000	-1.337458000
C	0.888931000	-4.569719000	2.157466000
H	1.275802000	-3.646403000	2.602473000
H	0.026931000	-4.901731000	2.742703000
H	1.671655000	-5.328797000	2.279874000
C	2.182453000	-4.180679000	-0.572842000
H	2.881852000	-4.936786000	-0.195009000
H	2.123184000	-4.310725000	-1.657195000
H	2.626227000	-3.201017000	-0.365532000
Cl	1.160862000	3.582170000	3.162790000
Cl	-1.604830000	5.393012000	-0.475132000

H	-3.470660000	4.908274000	-2.593847000
H	0.522702000	1.222707000	4.623547000

$mC2^a_{iso}$, $E_{(SCF Done)} = -3024.936039$ a.u.

Sc	0.837860000	-0.629161000	-0.017208000
Si	-2.949497000	4.146470000	-1.328012000
C	-1.184579000	3.408002000	-1.248092000
C	-3.646912000	4.334144000	0.428238000
C	-4.078582000	3.003948000	-2.342237000
C	-2.841646000	5.843918000	-2.162997000
C	0.167010000	-0.095083000	-3.464922000
C	0.624965000	-1.070550000	-2.421418000
C	-0.248562000	-1.986337000	-1.777162000
C	0.544672000	-2.894294000	-1.006585000
C	1.903507000	-2.519137000	-1.157317000
C	1.977363000	-1.362902000	-2.017293000
C	-1.727860000	-2.091285000	-2.007723000
C	0.030346000	-4.126794000	-0.320298000
C	3.066438000	-3.291385000	-0.600276000
C	-1.055533000	2.014599000	-0.610029000
C	0.392459000	1.494533000	-0.549501000
H	-0.546755000	4.117044000	-0.700971000
H	-0.785232000	3.374998000	-2.272538000
H	-3.746401000	3.368077000	0.937798000
H	-4.642594000	4.791568000	0.399158000
H	-3.006218000	4.975668000	1.044448000
H	-3.684701000	2.852572000	-3.354244000
H	-5.078988000	3.441148000	-2.440622000
H	-4.197671000	2.019366000	-1.874468000
H	-2.199630000	6.526632000	-1.594571000
H	-3.832466000	6.306310000	-2.240481000
H	-2.431899000	5.763753000	-3.176489000
H	-0.849082000	0.260935000	-3.270345000
H	0.152153000	-0.578180000	-4.451444000
H	0.814859000	0.778205000	-3.542337000
H	-2.202306000	-1.111500000	-2.122671000
H	-2.238082000	-2.615112000	-1.195386000
H	-1.930947000	-2.651034000	-2.930692000
H	-0.985479000	-3.995125000	0.062606000
H	0.667068000	-4.448535000	0.510910000
H	-0.003772000	-4.966146000	-1.027920000
H	3.455497000	-3.994437000	-1.348114000
H	2.783136000	-3.893009000	0.269389000
H	3.897654000	-2.645811000	-0.303966000

H	-1. 676924000	1. 302942000	-1. 173817000
H	-1. 489845000	2. 051937000	0. 399032000
H	0. 840040000	1. 609019000	-1. 544819000
C	3. 385212000	-0. 359877000	2. 090840000
O	2. 125505000	-1. 037325000	1. 745735000
C	1. 898599000	-2. 140415000	2. 672708000
C	3. 230723000	-2. 361852000	3. 367138000
C	3. 788978000	-0. 938651000	3. 436034000
H	4. 105995000	-0. 600079000	1. 304586000
H	3. 189828000	0. 711829000	2. 102349000
H	1. 125909000	-1. 828398000	3. 385019000
H	1. 542200000	-2. 996055000	2. 094974000
H	3. 105532000	-2. 823935000	4. 350135000
H	3. 878754000	-3. 006485000	2. 763201000
H	3. 323071000	-0. 377695000	4. 253595000
H	4. 872591000	-0. 911047000	3. 578544000
C	0. 900017000	2. 393896000	1. 771612000
C	1. 290425000	2. 149788000	0. 434723000
C	2. 606530000	2. 525694000	0. 077034000
C	3. 467429000	3. 131889000	0. 988188000
C	3. 066919000	3. 371413000	2. 303230000
C	1. 776846000	2. 990862000	2. 673982000
H	-0. 110117000	2. 170439000	2. 101996000
H	2. 927560000	2. 393727000	-0. 953309000
H	4. 459110000	3. 442196000	0. 668764000
C	-3. 292728000	-3. 734308000	1. 882746000
C	-2. 990465000	-2. 395060000	1. 581948000
C	-3. 952211000	-1. 609786000	0. 921773000
C	-5. 170717000	-2. 169947000	0. 562984000
C	-5. 464243000	-3. 506356000	0. 852649000
C	-4. 517835000	-4. 282733000	1. 516007000
H	-2. 564192000	-4. 344010000	2. 411634000
H	-3. 765766000	-0. 564354000	0. 700418000
H	-4. 744071000	-5. 318085000	1. 752655000
C	-1. 700358000	-1. 859270000	2. 004001000
C	-1. 176289000	-0. 637020000	1. 743563000
H	-1. 124757000	-2. 534422000	2. 638186000
H	-0. 312558000	-0. 291438000	2. 313217000
H	-1. 727425000	0. 118956000	1. 189297000
Si	3. 603218000	-0. 748017000	-2. 833312000
C	4. 933391000	-0. 279630000	-1. 556903000
H	4. 581920000	0. 486294000	-0. 856760000
H	5. 307132000	-1. 134201000	-0. 983659000
H	5. 792604000	0. 141515000	-2. 093409000

C	3.370231000	0.770255000	-3.943276000
H	4.358789000	1.048776000	-4.329087000
H	2.731380000	0.566171000	-4.807650000
H	2.971006000	1.644068000	-3.416584000
C	4.245751000	-2.167100000	-3.911839000
H	5.153722000	-1.854532000	-4.441007000
H	4.493402000	-3.057501000	-3.325075000
H	3.501706000	-2.454096000	-4.663086000
H	3.725480000	3.854356000	3.017231000
H	-6.425600000	-3.921619000	0.568128000
Cl	1.239772000	3.276015000	4.308750000
Cl	-6.352805000	-1.192957000	-0.249743000

***m*TS2^a_{iso}, $E_{(\text{SCF Done})} = -3024.910673$ a.u. $\text{IF} = i 211.34 \text{ cm}^{-1}$**

Sc	0.822713000	-0.515933000	0.222839000
Si	-4.688094000	2.799731000	-0.965107000
C	-2.907729000	2.496395000	-0.299507000
C	-5.774203000	1.290247000	-0.598826000
C	-4.617459000	3.109761000	-2.834270000
C	-5.364558000	4.324714000	-0.070286000
C	0.700741000	-1.112975000	-3.273087000
C	1.262483000	-1.584534000	-1.958839000
C	0.654994000	-2.591544000	-1.164786000
C	1.536858000	-2.890698000	-0.079403000
C	2.692393000	-2.072213000	-0.223103000
C	2.541099000	-1.239736000	-1.385878000
C	-0.583856000	-3.354235000	-1.531395000
C	1.382626000	-4.029771000	0.885145000
C	3.925934000	-2.198812000	0.625985000
C	-2.147140000	1.369292000	-1.002683000
C	-0.718477000	1.018052000	-0.541017000
H	-2.997566000	2.320898000	0.782265000
H	-2.366372000	3.444110000	-0.415890000
H	-5.414258000	0.385940000	-1.102648000
H	-6.798267000	1.468723000	-0.947121000
H	-5.826223000	1.081695000	0.476177000
H	-3.951245000	3.944656000	-3.080986000
H	-5.614781000	3.361523000	-3.213092000
H	-4.273741000	2.225904000	-3.384090000
H	-5.397596000	4.173091000	1.014810000
H	-6.384585000	4.546339000	-0.404424000
H	-4.750877000	5.210859000	-0.269001000
H	-0.382687000	-1.260367000	-3.324425000
H	1.134532000	-1.686036000	-4.103295000

H	0.904160000	-0.057616000	-3.475476000
H	-1.381706000	-2.711887000	-1.917593000
H	-0.993300000	-3.910951000	-0.687124000
H	-0.347271000	-4.079530000	-2.321733000
H	0.334263000	-4.274104000	1.069078000
H	1.852160000	-3.830091000	1.854815000
H	1.863194000	-4.932038000	0.483510000
H	4.702094000	-2.764784000	0.095027000
H	3.726570000	-2.745359000	1.552396000
H	4.361142000	-1.231610000	0.890439000
H	-2.071460000	1.636521000	-2.067540000
H	-2.740665000	0.445231000	-0.983616000
H	-0.325889000	0.366393000	-1.360226000
C	2.891634000	1.242021000	2.077674000
O	1.977682000	0.094246000	2.031978000
C	2.097582000	-0.667037000	3.276848000
C	3.345927000	-0.134496000	3.957924000
C	3.343806000	1.332121000	3.524883000
H	3.722476000	1.029870000	1.399137000
H	2.341319000	2.113746000	1.727209000
H	1.199666000	-0.471388000	3.872847000
H	2.145535000	-1.726701000	3.018225000
H	3.300470000	-0.263742000	5.042675000
H	4.239547000	-0.648681000	3.587939000
H	2.628117000	1.911801000	4.118439000
H	4.324039000	1.808144000	3.613538000
C	0.048961000	3.098185000	0.685793000
C	0.254154000	2.105208000	-0.305899000
C	1.444847000	2.175702000	-1.060298000
C	2.364466000	3.215421000	-0.872485000
C	2.128879000	4.207190000	0.068076000
C	0.962980000	4.129454000	0.844431000
H	-0.841301000	3.083617000	1.302578000
H	1.599878000	1.475828000	-1.875115000
H	3.251476000	3.268121000	-1.497322000
C	-1.784398000	-3.556631000	2.335505000
C	-1.879367000	-2.401674000	1.539826000
C	-2.936253000	-2.320320000	0.619832000
C	-3.849555000	-3.363043000	0.504041000
C	-3.748635000	-4.511117000	1.287412000
C	-2.705929000	-4.592228000	2.208440000
H	-0.996669000	-3.630299000	3.081683000
H	-3.050559000	-1.452033000	-0.020277000
H	-2.619225000	-5.471713000	2.840551000

C	-0.936694000	-1.289822000	1.752244000
C	-1.264420000	0.040805000	1.490361000
H	-0.175684000	-1.480797000	2.508836000
H	-0.743066000	0.827219000	2.034829000
H	-2.275612000	0.293862000	1.195017000
Si	4.032453000	-0.494347000	-2.336656000
C	5.195024000	0.530457000	-1.238552000
H	4.673941000	1.341630000	-0.719199000
H	5.723027000	-0.076905000	-0.497049000
H	5.958586000	0.989925000	-1.878217000
C	3.550113000	0.593868000	-3.817176000
H	4.484031000	0.955524000	-4.265632000
H	3.020231000	0.031081000	-4.591232000
H	2.952994000	1.477375000	-3.567680000
C	4.984755000	-1.981625000	-3.026163000
H	5.851526000	-1.642290000	-3.605628000
H	5.352835000	-2.642700000	-2.234430000
H	4.349875000	-2.577767000	-3.691083000
H	2.817280000	5.035195000	0.201177000
H	-4.470760000	-5.313503000	1.181131000
Cl	0.662340000	5.354488000	2.039645000
Cl	-5.138373000	-3.230075000	-0.660737000

mP2^a_{iso}, $E_{(\text{SCF Done})} = -3024.956828$ a.u.

Sc	-1.061577000	-0.046524000	-0.032644000
Si	5.941371000	-0.891979000	-0.911565000
C	4.249842000	-0.514510000	-0.079079000
C	6.326883000	0.447841000	-2.196406000
C	5.867318000	-2.592371000	-1.749233000
C	7.254630000	-0.893624000	0.452316000
C	-0.321437000	-0.764897000	-3.459343000
C	-1.349506000	-0.275335000	-2.475060000
C	-1.538483000	1.102528000	-2.170854000
C	-2.694808000	1.215256000	-1.345831000
C	-3.229328000	-0.091376000	-1.162399000
C	-2.396037000	-1.042146000	-1.847838000
C	-0.786407000	2.248311000	-2.775774000
C	-3.306134000	2.500797000	-0.870224000
C	-4.545479000	-0.363716000	-0.489410000
C	3.058959000	-0.496858000	-1.035066000
C	1.669382000	-0.191222000	-0.394097000
H	4.354162000	0.452774000	0.431008000
H	4.102789000	-1.268325000	0.707384000
H	5.590364000	0.463374000	-3.008203000

H	7.308686000	0.269457000	-2.649965000
H	6.350181000	1.444589000	-1.740809000
H	5.617483000	-3.383394000	-1.032400000
H	6.840566000	-2.841119000	-2.187920000
H	5.128498000	-2.620520000	-2.558613000
H	7.301762000	0.074243000	0.964458000
H	8.247227000	-1.095584000	0.033688000
H	7.048647000	-1.663984000	1.204275000
H	0.500290000	-0.050662000	-3.572235000
H	-0.771856000	-0.879546000	-4.454001000
H	0.110563000	-1.733400000	-3.194455000
H	0.290638000	2.062599000	-2.847386000
H	-0.930368000	3.169097000	-2.207819000
H	-1.145065000	2.433450000	-3.797362000
H	-2.550445000	3.229695000	-0.562664000
H	-3.986923000	2.345229000	-0.027182000
H	-3.897610000	2.961007000	-1.673142000
H	-5.373688000	-0.042399000	-1.134309000
H	-4.657630000	0.180795000	0.455008000
H	-4.693574000	-1.425914000	-0.283832000
H	2.982382000	-1.462020000	-1.552329000
H	3.214964000	0.261030000	-1.814385000
H	0.974869000	-0.238403000	-1.261374000
C	-2.649215000	-1.833702000	2.247029000
O	-2.118498000	-0.531942000	1.830704000
C	-2.521025000	0.491414000	2.799456000
C	-3.600286000	-0.164565000	3.642023000
C	-3.141337000	-1.623804000	3.669331000
H	-3.461534000	-2.090971000	1.564049000
H	-1.842203000	-2.561523000	2.155533000
H	-1.637849000	0.743380000	3.394547000
H	-2.849668000	1.371440000	2.242035000
H	-3.664583000	0.284740000	4.636666000
H	-4.580465000	-0.073728000	3.161073000
H	-2.324764000	-1.759659000	4.386937000
H	-3.942992000	-2.321209000	3.926885000
C	1.581787000	-1.247167000	1.934548000
C	1.267563000	-1.301775000	0.565842000
C	0.657367000	-2.467218000	0.064514000
C	0.415989000	-3.565641000	0.897504000
C	0.755270000	-3.514892000	2.245157000
C	1.325638000	-2.343700000	2.754276000
H	2.050830000	-0.364480000	2.356208000
H	0.448167000	-2.547398000	-1.000776000

H	-0.016902000	-4.473045000	0.485799000
C	-0.722524000	3.564275000	2.039486000
C	-0.053219000	3.071270000	0.902483000
C	0.369500000	4.022109000	-0.044258000
C	0.095579000	5.376129000	0.130741000
C	-0.593308000	5.849100000	1.244268000
C	-0.991900000	4.919920000	2.202600000
H	-1.005405000	2.876076000	2.831399000
H	0.923390000	3.723226000	-0.926536000
H	-1.503282000	5.263626000	3.098143000
C	0.194302000	1.611920000	0.733750000
C	1.580839000	1.235208000	0.179580000
H	0.102452000	1.148270000	1.741476000
H	2.364972000	1.383114000	0.936709000
H	1.843817000	1.905781000	-0.644849000
Si	-2.931866000	-2.832141000	-2.280198000
C	-3.369209000	-3.889494000	-0.760761000
H	-2.544979000	-3.943144000	-0.041124000
H	-4.268130000	-3.553476000	-0.233759000
H	-3.568174000	-4.911897000	-1.104815000
C	-1.603900000	-3.803642000	-3.225419000
H	-2.010667000	-4.802591000	-3.426083000
H	-1.358395000	-3.354526000	-4.191951000
H	-0.672478000	-3.944951000	-2.665334000
C	-4.456778000	-2.681791000	-3.393256000
H	-4.804882000	-3.675250000	-3.699593000
H	-5.287129000	-2.177760000	-2.887677000
H	-4.223132000	-2.113594000	-4.300417000
H	0.589989000	-4.366586000	2.897394000
H	-0.791160000	6.908766000	1.363208000
Cl	1.734668000	-2.258620000	4.437812000
Cl	0.640810000	6.505662000	-1.081904000

mC1^b, $E_{(\text{SCF Done})} = -1979.703125$ a.u.

Sc	-0.552885000	0.087840000	0.009924000
N	0.900465000	1.879215000	0.145121000
C	-0.843128000	0.996136000	-1.975082000
H	0.143396000	0.904299000	-2.445644000
H	-1.614607000	0.770573000	-2.711709000
C	-1.087170000	2.262372000	-1.261436000
C	-0.283809000	2.678340000	-0.156879000
C	-0.610531000	3.825041000	0.586311000
H	0.022939000	4.144328000	1.407499000
C	-1.727004000	4.579326000	0.261087000

H	-1.961730000	5.472308000	0.832672000
C	-2.532504000	4.192826000	-0.817886000
H	-3.399400000	4.788878000	-1.089345000
C	-2.222654000	3.058570000	-1.545975000
H	-2.845032000	2.770998000	-2.389261000
C	1.431788000	2.043649000	1.511722000
H	1.888095000	3.032120000	1.655217000
H	2.206587000	1.289435000	1.674946000
H	0.637259000	1.915499000	2.251149000
C	1.995568000	2.134112000	-0.820313000
H	1.623818000	2.078404000	-1.843196000
H	2.786462000	1.393807000	-0.677503000
H	2.407256000	3.138732000	-0.657479000
C	-1.887763000	0.096148000	2.083891000
C	-2.784965000	0.033936000	0.975763000
C	-2.590572000	-1.212181000	0.289038000
C	-1.575565000	-1.925015000	1.024514000
C	-1.144428000	-1.119393000	2.117322000
C	-3.845553000	1.065957000	0.724755000
H	-4.090812000	1.172124000	-0.331307000
H	-3.548470000	2.049641000	1.098200000
H	-4.768124000	0.784887000	1.251078000
C	-1.196403000	-3.368611000	0.831075000
H	-0.167851000	-3.590395000	1.134093000
H	-1.315110000	-3.700774000	-0.202974000
H	-1.842667000	-4.008340000	1.445944000
C	-0.195955000	-1.521803000	3.211533000
H	-0.751296000	-1.782387000	4.122065000
H	0.500484000	-0.720944000	3.487642000
H	0.395039000	-2.403141000	2.944831000
C	-1.872959000	1.165489000	3.140024000
H	-2.739004000	1.055169000	3.805937000
H	-0.981677000	1.103547000	3.773141000
H	-1.922654000	2.175721000	2.719356000
C	6.016964000	-0.567574000	0.668746000
C	5.224055000	-1.007343000	1.725756000
C	3.905006000	-1.393157000	1.503394000
C	3.352427000	-1.332883000	0.213098000
C	4.158374000	-0.902611000	-0.855524000
C	5.474323000	-0.523081000	-0.618987000
H	5.645208000	-1.059343000	2.725424000
H	3.299412000	-1.753438000	2.331409000
H	3.779358000	-0.892385000	-1.872378000
C	1.966326000	-1.761712000	0.018146000

C	1.191611000	-1.590300000	-1.077943000
H	1.537767000	-2.302824000	0.861058000
H	0.233953000	-2.108221000	-1.158303000
H	1.551819000	-1.103675000	-1.980382000
Si	-3.605218000	-1.970130000	-1.151913000
C	-4.613066000	-3.414822000	-0.452970000
H	-5.243449000	-3.845723000	-1.239870000
H	-3.980782000	-4.217060000	-0.058977000
H	-5.271349000	-3.076527000	0.355010000
C	-2.463892000	-2.586833000	-2.543846000
H	-1.837564000	-3.439980000	-2.262482000
H	-3.084471000	-2.915125000	-3.386609000
H	-1.815198000	-1.783088000	-2.911313000
C	-4.804501000	-0.737794000	-1.944907000
H	-5.571257000	-0.385152000	-1.248619000
H	-4.297305000	0.130945000	-2.378339000
H	-5.319753000	-1.254809000	-2.763765000
H	7.049536000	-0.275327000	0.830250000
Cl	6.461026000	0.001717000	-1.945971000

***m*TS1^b**, $E_{(\text{SCF Done})} = -1979.683706$ a.u. $\text{IF} = i297.43$ cm^{-1}

Sc	-0.095249000	-0.186124000	0.181129000
N	1.087219000	1.589662000	1.133023000
C	0.354429000	1.262857000	-1.709776000
H	1.406439000	1.541176000	-1.750207000
H	-0.081881000	1.380080000	-2.700069000
C	-0.394925000	2.144086000	-0.755886000
C	-0.011202000	2.372097000	0.596255000
C	-0.683260000	3.328065000	1.373038000
H	-0.365470000	3.516422000	2.392863000
C	-1.736112000	4.057759000	0.843580000
H	-2.228776000	4.811277000	1.450920000
C	-2.157570000	3.819986000	-0.469149000
H	-2.979828000	4.389738000	-0.891938000
C	-1.509108000	2.869083000	-1.238083000
H	-1.818819000	2.710326000	-2.267368000
C	1.099059000	1.465293000	2.604674000
H	1.411134000	2.399814000	3.088899000
H	1.819059000	0.688510000	2.876477000
H	0.111887000	1.184411000	2.972170000
C	2.416515000	2.106851000	0.718666000
H	2.465561000	2.258581000	-0.356997000
H	3.185450000	1.388459000	1.007820000
H	2.604265000	3.068399000	1.213795000

C	-1.338354000	-1.185414000	2.105152000
C	-2.236468000	-0.369671000	1.360820000
C	-2.407254000	-0.950294000	0.049524000
C	-1.619793000	-2.155053000	0.035816000
C	-0.948863000	-2.283617000	1.278149000
C	-3.004072000	0.785386000	1.938267000
H	-3.197860000	1.570133000	1.205735000
H	-2.481364000	1.245436000	2.782681000
H	-3.975857000	0.442723000	2.317681000
C	-1.621133000	-3.212960000	-1.030737000
H	-0.665302000	-3.742497000	-1.108518000
H	-1.862669000	-2.818150000	-2.020824000
H	-2.374116000	-3.976748000	-0.797480000
C	-0.141676000	-3.462337000	1.736008000
H	-0.795506000	-4.214741000	2.197869000
H	0.603681000	-3.188049000	2.490102000
H	0.376997000	-3.963435000	0.912091000
C	-1.030946000	-1.093491000	3.574242000
H	-1.599661000	-1.858322000	4.119304000
H	0.026659000	-1.267770000	3.804398000
H	-1.317162000	-0.129902000	4.004958000
C	5.355547000	-0.970462000	0.382231000
C	4.467214000	-1.844267000	1.009325000
C	3.165167000	-1.994166000	0.542761000
C	2.704753000	-1.275173000	-0.580653000
C	3.608653000	-0.399542000	-1.210630000
C	4.908440000	-0.260799000	-0.731114000
H	4.803391000	-2.421827000	1.866307000
H	2.499913000	-2.702527000	1.029069000
H	3.327093000	0.148385000	-2.104187000
C	1.323887000	-1.465542000	-1.053887000
C	0.750231000	-0.690759000	-2.102527000
H	0.890083000	-2.441528000	-0.864501000
H	-0.195950000	-1.058860000	-2.500975000
H	1.380211000	-0.286507000	-2.891614000
Si	-3.800062000	-0.616480000	-1.228700000
C	-4.966699000	-2.109749000	-1.189477000
H	-5.833204000	-1.916604000	-1.833197000
H	-4.492669000	-3.030642000	-1.542106000
H	-5.339027000	-2.287643000	-0.174380000
C	-3.127496000	-0.392647000	-2.994144000
H	-2.627632000	-1.283011000	-3.390001000
H	-3.967244000	-0.175525000	-3.665545000
H	-2.430809000	0.449970000	-3.064037000

C	-4.841043000	0.914419000	-0.830851000
H	-5.343470000	0.837519000	0.138139000
H	-4.267907000	1.845796000	-0.852033000
H	-5.621812000	0.989596000	-1.597893000
H	6.373854000	-0.851019000	0.736501000
Cl	5.994197000	0.829446000	-1.545679000

mP1^b, $E_{(\text{SCF Done})} = -1979.705747$ a.u.

Sc	-0.285756000	-0.300865000	0.287016000
N	0.778597000	1.208412000	1.712228000
C	1.101332000	1.736046000	-1.323630000
H	2.104920000	1.786513000	-0.901161000
H	1.126346000	2.392465000	-2.197802000
C	0.069731000	2.367349000	-0.383104000
C	-0.033649000	2.205590000	1.031014000
C	-0.974769000	2.961605000	1.751703000
H	-1.037405000	2.859458000	2.828697000
C	-1.814206000	3.868963000	1.119519000
H	-2.515664000	4.452276000	1.708701000
C	-1.737947000	4.030734000	-0.261983000
H	-2.382739000	4.739275000	-0.773033000
C	-0.809544000	3.291976000	-0.981371000
H	-0.728235000	3.450078000	-2.053732000
C	0.338189000	0.872121000	3.082528000
H	0.526177000	1.694921000	3.784996000
H	0.912218000	0.004605000	3.416960000
H	-0.724851000	0.623366000	3.103207000
C	2.224140000	1.546782000	1.791540000
H	2.624661000	1.831964000	0.824541000
H	2.773640000	0.670374000	2.140360000
H	2.364584000	2.378573000	2.493435000
C	-1.458884000	-1.984388000	1.622943000
C	-2.409252000	-0.993311000	1.239975000
C	-2.547312000	-1.017601000	-0.195680000
C	-1.697606000	-2.081752000	-0.665562000
C	-1.021493000	-2.658601000	0.437951000
C	-3.214216000	-0.161803000	2.201964000
H	-3.285872000	0.888463000	1.906052000
H	-2.805938000	-0.200905000	3.216789000
H	-4.239296000	-0.546374000	2.270920000
C	-1.605144000	-2.611263000	-2.067692000
H	-0.596000000	-2.956608000	-2.317176000
H	-1.900981000	-1.873954000	-2.817461000
H	-2.268533000	-3.477933000	-2.187187000

C	-0.141569000	-3.872562000	0.397249000
H	-0.753047000	-4.784653000	0.373069000
H	0.501412000	-3.945879000	1.279717000
H	0.501513000	-3.894386000	-0.488419000
C	-1.084011000	-2.400649000	3.018987000
H	-1.592937000	-3.335963000	3.285205000
H	-0.009028000	-2.587541000	3.129212000
H	-1.371007000	-1.660738000	3.770984000
C	5.464318000	-1.025919000	0.340112000
C	4.482907000	-1.833982000	0.914237000
C	3.162297000	-1.768678000	0.479206000
C	2.773633000	-0.903140000	-0.561753000
C	3.774865000	-0.116094000	-1.155013000
C	5.091186000	-0.176392000	-0.697342000
H	4.757212000	-2.520394000	1.711224000
H	2.414665000	-2.414919000	0.934531000
H	3.554205000	0.520812000	-2.006032000
C	1.347884000	-0.882802000	-1.002572000
C	0.862633000	0.289584000	-1.866911000
H	1.096499000	-1.821822000	-1.506807000
H	-0.227865000	0.169791000	-2.071229000
H	1.287009000	0.252019000	-2.880009000
Si	-3.900685000	-0.192196000	-1.279337000
C	-5.065419000	-1.568411000	-1.857063000
H	-5.887470000	-1.143582000	-2.445084000
H	-4.555017000	-2.306900000	-2.483325000
H	-5.502598000	-2.095730000	-1.001935000
C	-3.162459000	0.703937000	-2.785139000
H	-2.581105000	0.057964000	-3.450864000
H	-3.982986000	1.121998000	-3.381289000
H	-2.528359000	1.542667000	-2.475499000
C	-4.911417000	1.100686000	-0.333273000
H	-5.456749000	0.679268000	0.516236000
H	-4.301748000	1.937707000	0.023724000
H	-5.656597000	1.512495000	-1.025205000
H	6.494613000	-1.062526000	0.677538000
Cl	6.293373000	0.829744000	-1.457652000

$mC2^b_{syn}, E_{(SCF Done)} = -2748.794703$ a.u.

N	-5.868299000	0.578071000	1.603505000
C	-3.790828000	2.124452000	0.284287000
H	-4.305062000	2.642138000	1.098359000
H	-3.418354000	2.898757000	-0.398569000
C	-4.724805000	1.207247000	-0.468486000

C	-5.687993000	0.413030000	0.197853000
C	-6.425262000	-0.523886000	-0.537811000
H	-7.167196000	-1.137321000	-0.035227000
C	-6.240603000	-0.672577000	-1.912056000
H	-6.832900000	-1.402176000	-2.458426000
C	-5.325616000	0.135146000	-2.579985000
H	-5.193972000	0.049926000	-3.655374000
C	-4.581316000	1.064734000	-1.852419000
H	-3.862819000	1.698704000	-2.369423000
C	-6.333121000	-0.592752000	2.328924000
H	-7.399737000	-0.827635000	2.163172000
H	-6.202751000	-0.415283000	3.402676000
H	-5.740768000	-1.469136000	2.049320000
C	-6.674668000	1.746613000	1.956754000
H	-6.349460000	2.625962000	1.396450000
H	-6.565373000	1.957022000	3.026834000
H	-7.746213000	1.590817000	1.742529000
C	-1.306851000	-2.378714000	0.397200000
C	-0.479825000	-2.526245000	-0.754419000
C	0.886811000	-2.706022000	-0.336106000
C	0.875192000	-2.680126000	1.100945000
C	-0.462745000	-2.449752000	1.545056000
C	-1.011453000	-2.602982000	-2.159480000
H	-0.246291000	-2.387080000	-2.910102000
H	-1.852018000	-1.920099000	-2.326783000
H	-1.385746000	-3.614278000	-2.365841000
C	2.014238000	-3.032710000	2.016615000
H	1.799101000	-2.757915000	3.053744000
H	2.961222000	-2.572178000	1.726725000
H	2.171106000	-4.118875000	2.012332000
C	-0.939356000	-2.412516000	2.969703000
H	-1.209457000	-3.419954000	3.312942000
H	-1.830731000	-1.787534000	3.087360000
H	-0.176721000	-2.036948000	3.659862000
C	-2.804666000	-2.342315000	0.411027000
H	-3.201049000	-3.365146000	0.468197000
H	-3.197749000	-1.795078000	1.272153000
H	-3.227816000	-1.884648000	-0.487532000
C	0.219406000	0.996344000	-1.740259000
C	-0.658884000	1.617700000	-0.797929000
C	-0.345948000	2.951336000	-0.423161000
C	0.735254000	3.609915000	-0.987859000
C	1.589809000	2.990777000	-1.918014000
C	1.313325000	1.687161000	-2.293525000

H	-0.080429000	0.046641000	-2.197213000
H	-0.981826000	3.481453000	0.277679000
H	1.929602000	1.201898000	-3.044810000
C	-1.627857000	0.779355000	-0.117333000
C	-2.589124000	1.361864000	0.899169000
H	-2.115114000	0.079486000	-0.806978000
H	-2.057553000	2.042118000	1.580698000
H	-2.998805000	0.564565000	1.530422000
C	4.633847000	-0.264182000	2.543309000
C	3.614822000	0.495055000	1.942588000
C	3.947147000	1.399140000	0.916943000
C	5.269843000	1.522248000	0.512814000
C	6.283267000	0.769520000	1.115313000
C	5.956308000	-0.120636000	2.134483000
H	4.387729000	-0.954692000	3.345695000
H	3.190038000	2.010861000	0.436351000
H	6.739794000	-0.702097000	2.611001000
C	2.250080000	0.327988000	2.434745000
C	1.140206000	1.032033000	2.092971000
H	2.135849000	-0.447059000	3.191224000
H	0.213870000	0.884129000	2.651560000
H	1.179064000	1.909812000	1.448991000
Sc	0.209274000	-0.463730000	0.276978000
Si	2.311063000	-3.212613000	-1.521918000
C	1.781625000	-4.796505000	-2.413252000
H	0.910434000	-4.649022000	-3.058964000
H	2.603857000	-5.157429000	-3.042423000
H	1.539539000	-5.587073000	-1.694248000
C	3.937915000	-3.553425000	-0.614183000
H	3.854541000	-4.360412000	0.119875000
H	4.673244000	-3.870025000	-1.364284000
H	4.344773000	-2.667077000	-0.115705000
C	2.671583000	-1.837432000	-2.783361000
H	1.797078000	-1.543841000	-3.373878000
H	3.076830000	-0.944822000	-2.291681000
H	3.433196000	-2.190340000	-3.489295000
H	2.422339000	3.538827000	-2.344709000
H	7.310851000	0.887860000	0.787080000
Cl	1.048607000	5.255900000	-0.537491000
Cl	5.677379000	2.632885000	-0.757943000

$mTS2^b_{syn}$, $E_{(SCF Done)} = -2748.783305$ a.u. IF = $i139.19$ cm^{-1}

N	5.555332000	-0.319000000	-1.488583000
C	3.865856000	1.772952000	-0.364682000

H	4. 601434000	2. 243855000	-1. 025374000
H	3. 499219000	2. 567616000	0. 296817000
C	4. 499499000	0. 690330000	0. 479127000
C	5. 283173000	-0. 343215000	-0. 087355000
C	5. 765944000	-1. 364590000	0. 741729000
H	6. 370455000	-2. 159822000	0. 315691000
C	5. 511467000	-1. 365765000	2. 112664000
H	5. 911950000	-2. 162966000	2. 733580000
C	4. 776060000	-0. 330423000	2. 681520000
H	4. 595850000	-0. 303603000	3. 752899000
C	4. 278451000	0. 681685000	1. 860214000
H	3. 702748000	1. 493642000	2. 301202000
C	5. 746978000	-1. 614195000	-2. 121882000
H	6. 712737000	-2. 092354000	-1. 880852000
H	5. 712241000	-1. 482325000	-3. 209238000
H	4. 943036000	-2. 297858000	-1. 831679000
C	6. 638799000	0. 593437000	-1. 857235000
H	6. 515494000	1. 560920000	-1. 365800000
H	6. 630629000	0. 752294000	-2. 941420000
H	7. 628576000	0. 197204000	-1. 572565000
C	0. 519227000	-2. 449086000	0. 574490000
C	-0. 633608000	-2. 194342000	1. 370370000
C	-1. 809243000	-2. 341677000	0. 551747000
C	-1. 345381000	-2. 725164000	-0. 755355000
C	0. 079561000	-2. 761885000	-0. 744956000
C	-0. 600611000	-2. 021445000	2. 863560000
H	-1. 423198000	-1. 406478000	3. 238055000
H	0. 338988000	-1. 581187000	3. 214476000
H	-0. 679391000	-3. 000143000	3. 353738000
C	-2. 183989000	-3. 214929000	-1. 898910000
H	-1. 655907000	-3. 147591000	-2. 855354000
H	-3. 127643000	-2. 676372000	-1. 989421000
H	-2. 425690000	-4. 276115000	-1. 753683000
C	0. 966871000	-3. 194585000	-1. 875886000
H	1. 124627000	-4. 280933000	-1. 847182000
H	1. 955434000	-2. 727290000	-1. 826305000
H	0. 540056000	-2. 963258000	-2. 856966000
C	1. 930788000	-2. 545146000	1. 076479000
H	2. 110968000	-3. 544543000	1. 494711000
H	2. 670710000	-2. 394809000	0. 285224000
H	2. 157695000	-1. 825358000	1. 869606000
C	0. 185146000	1. 078334000	1. 584604000
C	0. 804061000	1. 628882000	0. 429788000
C	0. 572878000	3. 000280000	0. 149216000

C	-0.232008000	3.756395000	0.986897000
C	-0.878511000	3.194457000	2.102652000
C	-0.659247000	1.859453000	2.393886000
H	0.528097000	0.116885000	1.958954000
H	1.052099000	3.476858000	-0.699719000
H	-1.102853000	1.424444000	3.284934000
C	1.517309000	0.750686000	-0.486663000
C	2.710382000	1.277693000	-1.262082000
H	1.768394000	-0.211658000	-0.012508000
H	2.411284000	2.105590000	-1.919846000
H	3.109789000	0.491553000	-1.911607000
C	-3.363151000	-0.149262000	-2.908499000
C	-2.217074000	0.392090000	-2.286217000
C	-2.399750000	1.396708000	-1.306048000
C	-3.692053000	1.854680000	-1.004075000
C	-4.808595000	1.324871000	-1.636277000
C	-4.627664000	0.324252000	-2.597846000
H	-3.239736000	-0.906034000	-3.676913000
H	-1.551338000	1.945248000	-0.886656000
H	-5.495075000	-0.077213000	-3.114467000
C	-0.886544000	-0.109131000	-2.623064000
C	0.282852000	0.630788000	-2.469236000
H	-0.840042000	-1.047555000	-3.167344000
H	1.182900000	0.262691000	-2.947405000
H	0.229739000	1.709686000	-2.344869000
Sc	-0.597207000	-0.427441000	-0.318122000
Si	-3.590823000	-2.386768000	1.269374000
C	-3.662343000	-3.786078000	2.545692000
H	-3.030465000	-3.601438000	3.419766000
H	-4.692841000	-3.901517000	2.902523000
H	-3.356009000	-4.739463000	2.100725000
C	-4.913710000	-2.738052000	-0.038202000
H	-4.780332000	-3.710078000	-0.522783000
H	-5.884169000	-2.758941000	0.473107000
H	-4.967536000	-1.963962000	-0.810060000
C	-4.028264000	-0.732934000	2.094580000
H	-3.394399000	-0.498996000	2.956081000
H	-3.970130000	0.103225000	1.388687000
H	-5.061503000	-0.778429000	2.459861000
H	-1.506453000	3.813335000	2.733756000
H	-5.798748000	1.697592000	-1.396836000
Cl	-0.456789000	5.439908000	0.651625000
Cl	-3.899533000	3.137931000	0.143281000

$mP2^b_{\text{syn}}, E_{(\text{SCF Done})} = -2748.818285 \text{ a.u.}$

N	6.030175000	-0.120248000	-1.182408000
C	4.357681000	1.572079000	0.525943000
H	5.263315000	2.163172000	0.350336000
H	3.874060000	2.025018000	1.401308000
C	4.693305000	0.133054000	0.856222000
C	5.458217000	-0.688066000	-0.008098000
C	5.621279000	-2.043915000	0.307903000
H	6.203374000	-2.680127000	-0.351987000
C	5.077820000	-2.589466000	1.469801000
H	5.236507000	-3.640807000	1.696052000
C	4.370506000	-1.776440000	2.350243000
H	3.975080000	-2.178854000	3.279444000
C	4.185533000	-0.430408000	2.031671000
H	3.629403000	0.208734000	2.715674000
C	6.222966000	-1.023354000	-2.304924000
H	7.066543000	-1.724497000	-2.175741000
H	6.428564000	-0.428753000	-3.202145000
H	5.312406000	-1.604688000	-2.479313000
C	7.239985000	0.662972000	-0.934909000
H	7.103098000	1.328990000	-0.080489000
H	7.467371000	1.273440000	-1.815957000
H	8.112568000	0.021108000	-0.723558000
C	-0.418738000	-2.757060000	-0.115257000
C	-1.269083000	-2.422516000	0.977738000
C	-2.563957000	-2.056370000	0.467197000
C	-2.496542000	-2.219574000	-0.962084000
C	-1.179980000	-2.642173000	-1.315623000
C	-0.892875000	-2.607452000	2.421636000
H	-1.559045000	-2.067345000	3.098261000
H	0.137341000	-2.303284000	2.639766000
H	-0.962761000	-3.670047000	2.688775000
C	-3.642927000	-2.131911000	-1.930478000
H	-3.292159000	-2.151502000	-2.964547000
H	-4.246321000	-1.229947000	-1.803735000
H	-4.310534000	-2.992926000	-1.799938000
C	-0.716471000	-3.076613000	-2.673743000
H	-0.961444000	-4.134807000	-2.835425000
H	0.366922000	-2.976256000	-2.787953000
H	-1.191008000	-2.511942000	-3.481392000
C	0.992440000	-3.261726000	-0.025239000
H	1.006798000	-4.359945000	-0.031485000
H	1.603797000	-2.930003000	-0.870641000
H	1.498648000	-2.944489000	0.891956000

C	0.651750000	0.471313000	1.370996000
C	1.240351000	1.430613000	0.523219000
C	0.931979000	2.779959000	0.746494000
C	0.059935000	3.150051000	1.770742000
C	-0.545974000	2.193356000	2.593212000
C	-0.232646000	0.852970000	2.396511000
H	1.001100000	-0.563018000	1.315019000
H	1.375936000	3.553650000	0.127718000
H	-0.643621000	0.103869000	3.065441000
C	2.107876000	1.006744000	-0.641944000
C	3.456299000	1.740622000	-0.710012000
H	2.319687000	-0.065355000	-0.525246000
H	3.291436000	2.812764000	-0.886954000
H	3.998308000	1.360503000	-1.582291000
C	-2.027933000	0.470641000	-3.550847000
C	-1.201086000	0.855243000	-2.467323000
C	-1.794667000	1.701384000	-1.482564000
C	-3.113501000	2.170210000	-1.625428000
C	-3.888188000	1.800834000	-2.713792000
C	-3.321511000	0.952406000	-3.676161000
H	-1.611472000	-0.170350000	-4.322769000
H	-1.168866000	2.156183000	-0.707636000
H	-3.914483000	0.674342000	-4.543563000
C	0.104336000	0.257373000	-2.195723000
C	1.307324000	1.194231000	-1.954110000
H	0.346139000	-0.516776000	-2.925688000
H	2.011675000	1.054833000	-2.784766000
H	0.983200000	2.242687000	-2.015489000
Sc	-1.027326000	-0.394800000	-0.345243000
Si	-4.113614000	-1.731903000	1.556852000
C	-4.466043000	-3.313358000	2.535653000
H	-3.636260000	-3.596740000	3.190809000
H	-5.354312000	-3.173857000	3.163012000
H	-4.662734000	-4.152780000	1.859492000
C	-5.646620000	-1.286768000	0.540119000
H	-5.948726000	-2.081131000	-0.148106000
H	-6.474322000	-1.128907000	1.242553000
H	-5.523870000	-0.359256000	-0.029638000
C	-3.827212000	-0.275887000	2.747894000
H	-3.049419000	-0.460573000	3.496012000
H	-3.584297000	0.649945000	2.211986000
H	-4.758854000	-0.090716000	3.296510000
H	-1.218213000	2.502073000	3.386604000
H	-4.899794000	2.176596000	-2.823049000

Cl	-0.283312000	4.824214000	2.026945000
Cl	-3.757236000	3.246548000	-0.424343000

$mC2^b_{iso}, E_{(SCF Done)} = -2748.799331 \text{ a.u.}$

Sc	1.171642000	0.087191000	0.427876000
C	-1.698849000	-2.515771000	1.681537000
C	1.077083000	1.209379000	3.814692000
C	1.690025000	1.388593000	2.457958000
C	1.235394000	2.310596000	1.468205000
C	2.167578000	2.292436000	0.390640000
C	3.194749000	1.322945000	0.684487000
C	2.897814000	0.798279000	1.990610000
C	0.065282000	3.237564000	1.633100000
C	2.194744000	3.298748000	-0.725016000
C	3.759642000	-0.106023000	2.820025000
C	-0.772856000	-1.273064000	1.708052000
C	0.705989000	-1.567759000	1.818821000
H	-1.316029000	-3.212784000	0.934681000
H	-1.592681000	-3.011511000	2.653873000
H	-0.009430000	1.345439000	3.800179000
H	1.479888000	1.952937000	4.515333000
H	1.286132000	0.223651000	4.239524000
H	-0.772711000	2.760183000	2.152768000
H	-0.309863000	3.611783000	0.677555000
H	0.354677000	4.110168000	2.233937000
H	1.208389000	3.733208000	-0.907386000
H	2.570040000	2.887365000	-1.666883000
H	2.859354000	4.129051000	-0.454019000
H	4.315946000	-0.825503000	2.218888000
H	3.175462000	-0.659038000	3.561611000
H	4.494720000	0.490421000	3.376944000
H	-1.070747000	-0.620424000	2.536969000
H	-1.027536000	-0.691497000	0.783449000
H	1.093138000	-1.647464000	2.831242000
C	0.893506000	-2.411060000	-0.514364000
C	1.378831000	-2.369187000	0.824504000
C	2.659495000	-2.944110000	1.064455000
C	3.378937000	-3.541964000	0.046908000
C	2.898402000	-3.575922000	-1.273945000
C	1.659708000	-3.016539000	-1.529064000
H	-0.148911000	-2.180759000	-0.728401000
H	3.048572000	-2.947042000	2.078198000
C	-1.477596000	3.842127000	-2.158178000
C	-1.535472000	2.528334000	-1.662310000

C	-2.662689000	2.124227000	-0.924759000
C	-3.692370000	3.028262000	-0.695340000
C	-3.635187000	4.333178000	-1.195137000
C	-2.523223000	4.731857000	-1.931068000
H	-0.615667000	4.158627000	-2.740217000
H	-2.745693000	1.117915000	-0.525481000
H	-2.474979000	5.741820000	-2.327085000
C	-0.421181000	1.634336000	-1.966405000
C	-0.332379000	0.294280000	-1.777963000
H	0.418959000	2.119796000	-2.460333000
H	0.488720000	-0.250987000	-2.245832000
H	-1.177295000	-0.307557000	-1.448316000
Si	4.713707000	1.020514000	-0.448949000
C	5.936255000	-0.240752000	0.254787000
H	6.346836000	0.064245000	1.222332000
H	5.503227000	-1.241197000	0.355887000
H	6.776180000	-0.318103000	-0.446719000
C	5.641148000	2.652829000	-0.694374000
H	6.568026000	2.462711000	-1.248688000
H	5.068010000	3.396875000	-1.255080000
H	5.916036000	3.092311000	0.271009000
C	4.095792000	0.342920000	-2.117498000
H	4.945127000	0.198980000	-2.796424000
H	3.617943000	-0.638604000	-1.998415000
H	3.391689000	1.012209000	-2.625046000
H	-4.454167000	5.019439000	-1.005752000
H	3.466592000	-4.050777000	-2.066258000
Cl	-5.074630000	2.533963000	0.229982000
Cl	0.997220000	-3.086148000	-3.138377000
H	4.335700000	-4.007072000	0.269668000
C	-3.146556000	-2.166233000	1.441308000
C	-3.712262000	-2.122853000	0.145873000
C	-3.942557000	-1.814160000	2.535873000
C	-5.041079000	-1.703977000	0.000139000
C	-5.263748000	-1.400654000	2.382476000
H	-3.509970000	-1.865479000	3.533798000
C	-5.809039000	-1.338549000	1.104379000
H	-5.493742000	-1.673106000	-0.985834000
H	-5.857908000	-1.133332000	3.251644000
H	-6.838623000	-1.022519000	0.959912000
N	-2.915044000	-2.513277000	-0.982014000
C	-3.331780000	-1.953618000	-2.263329000
H	-2.545843000	-2.144871000	-3.001992000
H	-4.264173000	-2.395011000	-2.654648000

H	-3.477134000	-0.872405000	-2.179320000
C	-2.798856000	-3.972295000	-1.111381000
H	-3.749590000	-4.428665000	-1.432837000
H	-2.030358000	-4.212299000	-1.854044000
H	-2.517583000	-4.427637000	-0.159882000

mTS2^b_{iso}, $E_{(\text{SCF Done})} = -2748.766641$ a.u. $\text{IF} = i194.05 \text{ cm}^{-1}$

Sc	1.170689000	0.287320000	0.336356000
C	-2.848624000	-1.952970000	-0.113942000
C	2.472967000	1.030264000	3.511288000
C	2.764003000	0.982281000	2.037209000
C	2.625538000	2.086858000	1.137255000
C	3.117108000	1.681451000	-0.134059000
C	3.540331000	0.303944000	-0.048750000
C	3.361378000	-0.096220000	1.321462000
C	2.185536000	3.467853000	1.527149000
C	3.344855000	2.607091000	-1.291316000
C	3.850740000	-1.365592000	1.956090000
C	-2.294015000	-0.920047000	0.880586000
C	-0.786276000	-0.661730000	0.833944000
H	-2.504374000	-1.721624000	-1.126361000
H	-2.462681000	-2.949078000	0.133450000
H	1.635683000	1.695949000	3.746010000
H	3.343107000	1.411402000	4.061877000
H	2.241720000	0.043681000	3.923985000
H	1.413595000	3.456545000	2.303369000
H	1.791566000	4.032150000	0.678810000
H	3.037172000	4.031018000	1.932073000
H	2.642213000	3.443479000	-1.287751000
H	3.268051000	2.102593000	-2.259112000
H	4.353864000	3.035213000	-1.231570000
H	3.621993000	-2.258155000	1.370206000
H	3.431403000	-1.504146000	2.955299000
H	4.941521000	-1.323368000	2.069852000
H	-2.556896000	-1.251654000	1.895888000
H	-2.820219000	0.029464000	0.725714000
H	-0.590900000	0.067778000	1.667491000
C	0.400285000	-2.736767000	-0.007373000
C	0.072170000	-1.880572000	1.064669000
C	0.496753000	-2.240051000	2.359013000
C	1.173154000	-3.437908000	2.580180000
C	1.473945000	-4.289337000	1.519402000
C	1.091209000	-3.925386000	0.227335000
H	0.064874000	-2.514369000	-1.015706000

H	0.239772000	-1.602092000	3.201372000
C	0.137071000	3.902640000	-1.731275000
C	-0.282887000	2.771551000	-1.009368000
C	-1.101402000	2.969050000	0.116768000
C	-1.462490000	4.256448000	0.508726000
C	-1.037562000	5.375297000	-0.202571000
C	-0.241153000	5.180758000	-1.331954000
H	0.732324000	3.773239000	-2.630978000
H	-1.483398000	2.124437000	0.684115000
H	0.078889000	6.042304000	-1.911538000
C	0.092618000	1.410929000	-1.439392000
C	-0.777946000	0.333951000	-1.244386000
H	0.864637000	1.323253000	-2.204298000
H	-0.589609000	-0.577391000	-1.809743000
H	-1.826676000	0.499068000	-1.011684000
Si	4.394848000	-0.636642000	-1.488752000
C	4.971551000	-2.372385000	-1.005107000
H	5.681750000	-2.366241000	-0.172772000
H	4.146459000	-3.047600000	-0.756807000
H	5.488649000	-2.801043000	-1.872524000
C	5.910268000	0.348014000	-2.053148000
H	6.454665000	-0.228379000	-2.810603000
H	5.653637000	1.315733000	-2.493712000
H	6.594276000	0.526247000	-1.215889000
C	3.165426000	-0.835773000	-2.929868000
H	3.659030000	-1.360232000	-3.757032000
H	2.299626000	-1.447515000	-2.643524000
H	2.800555000	0.117799000	-3.327062000
H	-1.331995000	6.370445000	0.113119000
H	1.996443000	-5.225755000	1.686394000
Cl	-2.463135000	4.458231000	1.919219000
Cl	1.450133000	-4.975856000	-1.104008000
H	1.467303000	-3.716911000	3.588032000
C	-4.358546000	-1.975921000	-0.057940000
C	-5.124987000	-0.956090000	-0.659170000
C	-5.013383000	-2.978658000	0.661681000
C	-6.514789000	-0.961665000	-0.502281000
C	-6.398808000	-2.980287000	0.811467000
H	-4.422745000	-3.768186000	1.122864000
C	-7.149587000	-1.961229000	0.233241000
H	-7.112150000	-0.180241000	-0.962980000
H	-6.884833000	-3.768760000	1.379207000
H	-8.230635000	-1.945502000	0.342858000
N	-4.447700000	0.056651000	-1.421723000

C	-5.027942000	1.391305000	-1.325313000
H	-4.324344000	2.114985000	-1.752520000
H	-5.982630000	1.502740000	-1.867286000
H	-5.194230000	1.649026000	-0.275486000
C	-4.277346000	-0.332115000	-2.821924000
H	-5.234143000	-0.357109000	-3.371145000
H	-3.614675000	0.383516000	-3.323340000
H	-3.830023000	-1.328269000	-2.888044000

mP2^b_{iso}, $E_{(\text{SCF Done})} = -2748.80643$ a.u.

Sc	1.643033000	0.208648000	0.256473000
C	-3.812335000	-0.598010000	0.114553000
C	4.385811000	0.442094000	2.429123000
C	3.934867000	-0.024214000	1.073427000
C	3.999668000	0.746767000	-0.126325000
C	3.546461000	-0.072636000	-1.200126000
C	3.207266000	-1.372650000	-0.680688000
C	3.476665000	-1.330309000	0.733118000
C	4.618628000	2.106305000	-0.245668000
C	3.586739000	0.330780000	-2.644927000
C	3.447629000	-2.478966000	1.700151000
C	-3.169369000	0.736379000	0.518167000
C	-1.634418000	0.880837000	0.348186000
H	-3.551928000	-0.834948000	-0.922332000
H	-3.424155000	-1.412659000	0.739597000
H	4.184029000	1.506684000	2.589411000
H	5.469129000	0.303454000	2.543703000
H	3.908126000	-0.114632000	3.241401000
H	4.485635000	2.706474000	0.658935000
H	4.215043000	2.673759000	-1.086906000
H	5.700062000	2.004841000	-0.409181000
H	3.433303000	1.406225000	-2.767559000
H	2.830211000	-0.185684000	-3.241768000
H	4.566321000	0.094454000	-3.079109000
H	2.697384000	-3.229159000	1.447628000
H	3.267428000	-2.145946000	2.727051000
H	4.421347000	-2.986458000	1.702510000
H	-3.424658000	0.950242000	1.564106000
H	-3.628918000	1.526373000	-0.087042000
H	-1.421320000	1.903762000	0.684738000
C	-0.701755000	-1.417043000	0.948399000
C	-0.863446000	-0.052244000	1.264717000
C	-0.321005000	0.405363000	2.482457000
C	0.311051000	-0.473604000	3.371422000

C	0.392549000	-1.834529000	3.085577000
C	-0.129118000	-2.296811000	1.874457000
H	-1.105957000	-1.814376000	0.023221000
H	-0.456610000	1.444832000	2.773730000
C	1.481108000	3.124591000	-2.099630000
C	0.919628000	2.301994000	-1.092404000
C	1.076598000	2.750892000	0.245609000
C	1.715376000	3.967999000	0.539401000
C	2.217174000	4.772773000	-0.466873000
C	2.085259000	4.333172000	-1.793301000
H	1.376764000	2.820152000	-3.137314000
H	0.551184000	2.271466000	1.071465000
H	2.459847000	4.964233000	-2.595136000
C	0.334720000	0.978323000	-1.381743000
C	-1.171507000	0.768005000	-1.113608000
H	0.549325000	0.696666000	-2.416707000
H	-1.436784000	-0.219232000	-1.510199000
H	-1.765674000	1.486110000	-1.698378000
Si	2.869361000	-2.894481000	-1.811788000
C	2.972114000	-4.538735000	-0.879089000
H	3.925485000	-4.659609000	-0.354671000
H	2.158067000	-4.694648000	-0.165914000
H	2.907709000	-5.340521000	-1.625175000
C	4.218820000	-2.953330000	-3.142294000
H	4.149468000	-3.912745000	-3.669001000
H	4.132579000	-2.160807000	-3.890362000
H	5.217410000	-2.894149000	-2.694805000
C	1.158212000	-2.766177000	-2.624255000
H	1.026891000	-3.588950000	-3.337193000
H	0.356539000	-2.849570000	-1.881128000
H	1.020666000	-1.828290000	-3.172878000
H	2.689405000	5.721021000	-0.233758000
H	0.832733000	-2.530902000	3.791166000
Cl	1.834565000	4.465206000	2.202396000
Cl	-0.125513000	-3.992988000	1.536186000
H	0.705107000	-0.097682000	4.311603000
C	-5.314447000	-0.541279000	0.288565000
C	-6.138160000	0.140681000	-0.632462000
C	-5.899380000	-1.107761000	1.424046000
C	-7.508070000	0.254113000	-0.370170000
C	-7.265249000	-0.994567000	1.677102000
H	-5.266181000	-1.638542000	2.133267000
C	-8.069623000	-0.300823000	0.778450000
H	-8.147481000	0.778346000	-1.074500000

H	-7.693368000	-1.439742000	2.570982000
H	-9.136219000	-0.198979000	0.960622000
N	-5.540332000	0.701533000	-1.806305000
C	-6.132680000	1.944411000	-2.277510000
H	-5.460000000	2.399252000	-3.014196000
H	-7.114768000	1.816424000	-2.766317000
H	-6.250268000	2.640320000	-1.441861000
C	-5.416834000	-0.261966000	-2.896905000
H	-6.392060000	-0.516719000	-3.348038000
H	-4.775501000	0.154469000	-3.682916000
H	-4.965327000	-1.190890000	-2.537151000

Styrene, $E_{(\text{SCF Done})} = -309.4773914$ a.u.

C	1.359938000	1.328099000	-0.000055000
C	-0.009506000	1.090869000	-0.000147000
C	-0.514707000	-0.220375000	-0.000085000
C	0.405967000	-1.279822000	0.000016000
C	1.778697000	-1.044692000	0.000119000
C	2.262203000	0.261906000	0.000078000
H	1.727962000	2.351212000	-0.000121000
H	-0.694900000	1.934088000	-0.000274000
H	0.034577000	-2.302805000	0.000048000
H	2.470325000	-1.883514000	0.000210000
H	3.332608000	0.450846000	0.000133000
C	-1.951155000	-0.529361000	-0.000204000
C	-2.973187000	0.334965000	0.000243000
H	-2.183770000	-1.594900000	-0.000675000
H	-4.000340000	-0.017820000	0.000123000
H	-2.835956000	1.413348000	0.000766000

SC1^a, $E_{(\text{SCF Done})} = -1796.236267$ a.u.

Sc	-0.326060000	0.003444000	-0.270585000
Si	-0.590598000	3.714264000	-0.173740000
C	-1.240352000	1.948315000	0.085516000
C	-0.264874000	4.056761000	-2.015636000
C	1.006362000	4.028226000	0.821831000
C	-1.879607000	4.970421000	0.432074000
C	-0.575663000	-1.074470000	-3.706514000
C	-1.033218000	-1.293068000	-2.291443000
C	-2.183370000	-0.696797000	-1.699953000
C	-2.375378000	-1.263072000	-0.392208000
C	-1.334399000	-2.245794000	-0.218954000
C	-0.514751000	-2.260155000	-1.375687000
C	-3.077679000	0.267387000	-2.425847000

C	-1.208508000	-3.239511000	0.902337000
C	0.594979000	-3.239902000	-1.638908000
C	1.632420000	0.907177000	-1.646026000
C	2.500900000	-0.130986000	-1.724708000
H	-2.218650000	1.943720000	-0.420559000
H	-1.490965000	1.884070000	1.163658000
H	0.565307000	3.472052000	-2.428236000
H	-0.020628000	5.115202000	-2.164032000
H	-1.158782000	3.842705000	-2.613945000
H	0.811320000	3.972548000	1.900041000
H	1.385159000	5.036553000	0.617208000
H	1.816580000	3.325771000	0.588884000
H	-2.817910000	4.871558000	-0.126108000
H	-1.521979000	5.999019000	0.303162000
H	-2.107427000	4.825905000	1.494742000
H	-0.753884000	-0.050221000	-4.050192000
H	-1.125346000	-1.733714000	-4.391337000
H	0.487984000	-1.291808000	-3.849105000
H	-2.513890000	0.935910000	-3.085197000
H	-3.660540000	0.889775000	-1.747003000
H	-3.788476000	-0.279100000	-3.060411000
H	-1.862854000	-4.101579000	0.718730000
H	-1.491520000	-2.827091000	1.874961000
H	-0.191503000	-3.636956000	0.983229000
H	1.347036000	-3.264539000	-0.840293000
H	1.112375000	-3.028615000	-2.579238000
H	0.194305000	-4.258103000	-1.724364000
H	1.826319000	1.791257000	-1.043765000
H	0.821208000	0.983947000	-2.373048000
H	2.253478000	-0.936986000	-2.414371000
C	1.706053000	-1.347745000	1.922829000
O	0.730578000	-0.301617000	1.612024000
C	0.564975000	0.578599000	2.782243000
C	1.378516000	-0.071920000	3.891423000
C	2.469965000	-0.818414000	3.121826000
H	1.152551000	-2.260618000	2.158086000
H	2.321874000	-1.500997000	1.034617000
H	0.946591000	1.562773000	2.500807000
H	-0.501957000	0.644717000	2.999373000
H	1.776516000	0.672732000	4.585960000
H	0.762104000	-0.773667000	4.463978000
H	3.263110000	-0.135656000	2.798817000
H	2.925963000	-1.625739000	3.701310000
C	4.338281000	0.703685000	-0.217094000

C	3.763354000	-0.305873000	-1.013151000
C	4.453399000	-1.522428000	-1.163877000
C	5.672646000	-1.734050000	-0.527185000
C	6.225432000	-0.727465000	0.263650000
C	5.557357000	0.492128000	0.413998000
H	3.846139000	1.667164000	-0.116872000
H	4.031503000	-2.301349000	-1.795147000
H	6.196233000	-2.676625000	-0.657601000
H	6.000926000	1.283961000	1.011067000
Si	-3.861252000	-1.070979000	0.807072000
C	-5.132415000	0.222013000	0.266398000
H	-5.574556000	0.001119000	-0.709961000
H	-5.945618000	0.209196000	1.002859000
H	-4.728360000	1.239729000	0.248691000
C	-4.740359000	-2.748242000	0.893792000
H	-4.115828000	-3.532992000	1.331453000
H	-5.642037000	-2.659756000	1.511348000
H	-5.050350000	-3.079064000	-0.103755000
C	-3.281177000	-0.563417000	2.547072000
H	-2.506302000	-1.215854000	2.963669000
H	-2.911056000	0.468441000	2.545134000
H	-4.136022000	-0.598218000	3.233284000
H	7.183070000	-0.884360000	0.752129000

STS1^a, $E_{(\text{SCF Done})} = -1796.225381$ a.u. IF = $i200.20$ cm⁻¹

Sc	0.152333000	-0.184812000	-0.329857000
Si	-1.086405000	3.637109000	0.361486000
C	-0.483907000	1.822830000	0.253393000
C	-1.964311000	4.173409000	-1.227553000
C	0.411304000	4.755539000	0.690908000
C	-2.279610000	3.782783000	1.827859000
C	-0.290248000	-0.973231000	-3.842699000
C	-0.699925000	-1.253090000	-2.425419000
C	-1.794756000	-0.655474000	-1.745265000
C	-1.982760000	-1.331023000	-0.486183000
C	-0.980542000	-2.363514000	-0.427068000
C	-0.184598000	-2.301863000	-1.603450000
C	-2.662857000	0.413008000	-2.347493000
C	-0.873193000	-3.439867000	0.616485000
C	0.905363000	-3.259251000	-1.993673000
C	0.941040000	1.908652000	-1.606437000
C	1.758766000	0.803759000	-1.794370000
H	-1.383224000	1.175245000	0.407223000
H	0.190324000	1.682930000	1.123148000

H	-1.309675000	4.127988000	-2.104580000
H	-2.298866000	5.212359000	-1.123653000
H	-2.850704000	3.563252000	-1.430735000
H	0.977380000	4.423669000	1.569601000
H	0.062197000	5.774192000	0.897461000
H	1.101641000	4.822372000	-0.157454000
H	-3.169434000	3.156773000	1.695902000
H	-2.619722000	4.819456000	1.937707000
H	-1.798035000	3.491959000	2.768732000
H	-0.302502000	0.093876000	-4.090845000
H	-0.982088000	-1.465096000	-4.538988000
H	0.708656000	-1.359337000	-4.069679000
H	-2.123759000	0.994457000	-3.102276000
H	-3.046437000	1.112683000	-1.603186000
H	-3.530008000	-0.032228000	-2.853162000
H	-1.526475000	-4.283327000	0.358649000
H	-1.169576000	-3.095869000	1.611127000
H	0.139362000	-3.848486000	0.690852000
H	1.379599000	-3.725956000	-1.124791000
H	1.694664000	-2.776319000	-2.579269000
H	0.502967000	-4.072838000	-2.611634000
H	1.301477000	2.783100000	-1.077856000
H	0.127645000	2.094102000	-2.300192000
H	1.570683000	0.174806000	-2.660746000
C	2.346576000	-1.756225000	1.523713000
O	1.203132000	-0.834923000	1.490790000
C	0.894529000	-0.388481000	2.849089000
C	1.590364000	-1.388156000	3.754268000
C	2.855409000	-1.712552000	2.956620000
H	1.970934000	-2.745583000	1.249193000
H	3.073162000	-1.412794000	0.785839000
H	1.300897000	0.622117000	2.970678000
H	-0.191376000	-0.364787000	2.953066000
H	1.800354000	-0.966119000	4.740797000
H	0.972120000	-2.282771000	3.887943000
H	3.600613000	-0.918526000	3.071993000
H	3.316299000	-2.659235000	3.250965000
C	3.452399000	1.351235000	0.004484000
C	3.042701000	0.588723000	-1.107003000
C	3.919763000	-0.406494000	-1.581142000
C	5.158054000	-0.621049000	-0.982146000
C	5.549982000	0.147097000	0.115511000
C	4.691228000	1.134129000	0.602816000
H	2.809674000	2.137520000	0.393494000

H	3.636584000	-0.993000000	-2.452573000
H	5.823832000	-1.381393000	-1.381461000
H	4.994606000	1.750139000	1.445545000
Si	-3.488412000	-1.234431000	0.697249000
C	-4.712715000	0.137798000	0.241850000
H	-5.123884000	0.022049000	-0.765423000
H	-5.551184000	0.076673000	0.946669000
H	-4.290506000	1.144710000	0.329785000
C	-4.407196000	-2.888059000	0.596712000
H	-3.807170000	-3.726819000	0.962538000
H	-5.318480000	-2.841865000	1.204568000
H	-4.703771000	-3.108766000	-0.434719000
C	-2.967670000	-0.907372000	2.497709000
H	-2.267592000	-1.651071000	2.892628000
H	-2.526551000	0.090122000	2.613714000
H	-3.860128000	-0.938418000	3.134636000
H	6.519737000	-0.012571000	0.578038000

SP1^a, $E_{(\text{SCF Done})} = -1796.261834$ a.u.

Sc	-0.937519000	-0.211406000	-0.377427000
Si	4.404663000	-0.349807000	-0.080687000
C	2.500473000	-0.504431000	-0.317703000
C	5.090370000	0.943754000	-1.282402000
C	5.204383000	-2.036886000	-0.405901000
C	4.730022000	0.185022000	1.709428000
C	-2.514281000	0.855180000	-3.407976000
C	-2.150046000	1.222019000	-1.997967000
C	-0.970067000	1.903359000	-1.595495000
C	-1.052712000	2.170341000	-0.181134000
C	-2.332968000	1.667690000	0.255530000
C	-2.991184000	1.066824000	-0.851421000
C	0.102152000	2.349374000	-2.547391000
C	-2.957422000	1.874849000	1.606768000
C	-4.377688000	0.487051000	-0.852919000
C	2.036622000	-0.863218000	-1.742072000
C	0.532546000	-1.020090000	-1.905581000
H	2.053661000	0.458102000	-0.010765000
H	2.154274000	-1.261459000	0.402794000
H	4.941099000	0.647477000	-2.326669000
H	6.168330000	1.069902000	-1.128750000
H	4.620982000	1.923711000	-1.137011000
H	4.816473000	-2.806008000	0.272567000
H	6.287873000	-1.978847000	-0.250271000
H	5.039946000	-2.376902000	-1.434567000

H	4.274678000	1.157335000	1.931318000
H	5.806825000	0.279353000	1.891670000
H	4.340683000	-0.545866000	2.428274000
H	-1.667141000	0.455157000	-3.975848000
H	-2.868486000	1.741087000	-3.950952000
H	-3.322103000	0.117667000	-3.449256000
H	0.101457000	1.749073000	-3.462107000
H	1.102130000	2.292067000	-2.113472000
H	-0.063541000	3.391307000	-2.851550000
H	-3.421751000	2.867762000	1.659506000
H	-2.231855000	1.816442000	2.423230000
H	-3.755150000	1.152985000	1.807098000
H	-4.658144000	0.074963000	0.121981000
H	-4.495871000	-0.309918000	-1.594357000
H	-5.119253000	1.259393000	-1.095924000
H	2.560182000	-1.771581000	-2.078991000
H	2.368999000	-0.072755000	-2.424293000
H	0.139246000	-0.595951000	-2.834353000
C	-2.292145000	-1.623054000	2.171875000
O	-1.029752000	-1.120277000	1.617615000
C	0.085184000	-1.553583000	2.466325000
C	-0.566122000	-2.059529000	3.741935000
C	-1.884302000	-2.639258000	3.224287000
H	-2.821676000	-0.770955000	2.605278000
H	-2.870807000	-2.049208000	1.348729000
H	0.611955000	-2.348888000	1.930413000
H	0.743682000	-0.695113000	2.610067000
H	0.058497000	-2.800393000	4.248179000
H	-0.749891000	-1.233773000	4.438210000
H	-1.723165000	-3.621041000	2.766827000
H	-2.643973000	-2.741813000	4.003908000
C	0.440931000	-3.311056000	-0.802621000
C	-0.148100000	-2.242977000	-1.533798000
C	-1.568788000	-2.292874000	-1.691551000
C	-2.331050000	-3.365174000	-1.197232000
C	-1.717271000	-4.399974000	-0.505546000
C	-0.324192000	-4.364961000	-0.325856000
H	1.519392000	-3.330451000	-0.672548000
H	-2.045777000	-1.578315000	-2.366380000
H	-3.399844000	-3.396541000	-1.395569000
H	0.169478000	-5.191315000	0.180703000
Si	0.056251000	3.313022000	0.889096000
C	1.591760000	3.935089000	-0.026430000
H	1.344138000	4.502552000	-0.928448000

H	2.128551000	4.612406000	0.649331000
H	2.284898000	3.132911000	-0.300060000
C	-0.972729000	4.823243000	1.387716000
H	-1.811153000	4.569963000	2.043320000
H	-0.337552000	5.538824000	1.923311000
H	-1.374279000	5.329818000	0.503143000
C	0.676614000	2.417925000	2.450248000
H	-0.123277000	1.965188000	3.045442000
H	1.409786000	1.640833000	2.202249000
H	1.187329000	3.143099000	3.095510000
H	-2.296657000	-5.243517000	-0.142302000

SC2^a_{syn}, $E_{(\text{SCF Done})} = -2105.735475$ a.u.

Sc	-0.230349000	-0.794219000	0.367450000
Si	5.140378000	0.275693000	-1.944774000
C	3.701305000	0.431502000	-0.686183000
C	4.525061000	-0.609236000	-3.509321000
C	6.577311000	-0.692340000	-1.175617000
C	5.709149000	2.028434000	-2.393263000
C	1.302431000	-3.753981000	-1.063285000
C	0.037977000	-3.054199000	-0.666084000
C	-0.816911000	-2.297269000	-1.513155000
C	-2.037857000	-2.002927000	-0.805046000
C	-1.903176000	-2.603644000	0.493621000
C	-0.627637000	-3.224992000	0.585199000
C	-0.510248000	-2.008936000	-2.958101000
C	-2.977819000	-2.744188000	1.534274000
C	-0.126926000	-4.060313000	1.728476000
C	3.143565000	-0.907599000	-0.193017000
C	1.950563000	-0.936254000	0.804430000
H	2.925787000	1.042606000	-1.171403000
H	4.081251000	1.022523000	0.157102000
H	4.218653000	-1.640997000	-3.301503000
H	5.317735000	-0.651275000	-4.265265000
H	3.673010000	-0.082458000	-3.956201000
H	6.933041000	-0.210359000	-0.257598000
H	7.422118000	-0.743225000	-1.872212000
H	6.292156000	-1.720826000	-0.926865000
H	4.894914000	2.614802000	-2.835281000
H	6.527912000	1.997501000	-3.121319000
H	6.072096000	2.567576000	-1.510521000
H	1.750861000	-3.327787000	-1.964223000
H	1.088680000	-4.808950000	-1.282051000
H	2.061320000	-3.738053000	-0.274479000

H	0.566011000	-1.916154000	-3.137417000
H	-0.989141000	-1.096756000	-3.320911000
H	-0.864234000	-2.828139000	-3.597730000
H	-3.591485000	-3.628928000	1.321777000
H	-3.652037000	-1.883970000	1.567659000
H	-2.563544000	-2.893004000	2.536076000
H	-0.482764000	-3.701360000	2.700359000
H	0.966418000	-4.093613000	1.765607000
H	-0.474714000	-5.097195000	1.626894000
H	3.979553000	-1.452007000	0.273747000
H	2.856640000	-1.512181000	-1.062797000
H	1.894839000	-1.986588000	1.143497000
C	-1.453075000	1.746847000	1.936568000
O	-1.256238000	0.297719000	1.981041000
C	-1.490015000	-0.186652000	3.345693000
C	-1.622109000	1.064293000	4.199009000
C	-2.206411000	2.076975000	3.212364000
H	-0.462034000	2.212113000	1.918675000
H	-1.997430000	1.979610000	1.020293000
H	-2.410753000	-0.772612000	3.325132000
H	-0.642045000	-0.816203000	3.624432000
H	-2.264192000	0.893098000	5.067465000
H	-0.637962000	1.388988000	4.550937000
H	-3.282428000	1.919161000	3.077661000
H	-2.047646000	3.114393000	3.518922000
C	2.176727000	1.296701000	2.041110000
C	2.068089000	-0.113374000	2.047475000
C	2.050178000	-0.732484000	3.318234000
C	2.152096000	-0.000462000	4.500101000
C	2.279744000	1.388778000	4.460156000
C	2.293825000	2.030040000	3.220903000
H	2.216979000	1.825341000	1.092738000
H	2.007948000	-1.819641000	3.370225000
H	2.162404000	-0.520861000	5.454973000
H	2.410716000	3.110346000	3.170901000
C	-2.753128000	3.294294000	-2.137413000
C	-1.494626000	2.984099000	-1.590012000
C	-0.793270000	3.990285000	-0.897257000
C	-1.345841000	5.254514000	-0.743488000
C	-2.604873000	5.541589000	-1.280517000
C	-3.306573000	4.560707000	-1.979959000
H	-3.295393000	2.533724000	-2.694024000
H	0.200111000	3.791571000	-0.504496000
H	-0.790679000	6.026971000	-0.218914000

H	-4.278465000	4.785058000	-2.409533000
C	-0.952861000	1.648261000	-1.805983000
C	0.172524000	1.107608000	-1.276069000
H	-1.523786000	1.031584000	-2.498583000
H	0.581895000	0.192120000	-1.714415000
H	0.844227000	1.674403000	-0.636404000
Si	-3.725330000	-1.431584000	-1.501051000
C	-3.676301000	-0.984481000	-3.345614000
H	-3.074179000	-0.104559000	-3.594758000
H	-3.323959000	-1.819394000	-3.959504000
H	-4.705901000	-0.766567000	-3.655742000
C	-4.422056000	0.063849000	-0.554416000
H	-4.584806000	-0.150261000	0.507176000
H	-3.769509000	0.941228000	-0.625967000
H	-5.393842000	0.341785000	-0.980518000
C	-4.939826000	-2.879836000	-1.350518000
H	-5.189324000	-3.121933000	-0.313369000
H	-5.875354000	-2.627245000	-1.863860000
H	-4.534553000	-3.782233000	-1.821739000
H	2.386973000	1.959773000	5.378279000
H	-3.029563000	6.534746000	-1.163944000

STS2^a_{syn}, $E_{(\text{SCF Done})} = -2105.723512$ a.u. $\text{IF} = i171.48\text{cm}^{-1}$

Sc	-0.561021000	-0.467740000	0.249467000
Si	5.880373000	-0.710125000	-0.843189000
C	4.172613000	-0.038669000	-0.270762000
C	5.694159000	-1.593839000	-2.510596000
C	6.558350000	-1.909823000	0.458717000
C	7.036460000	0.779920000	-1.021511000
C	0.550681000	-3.820631000	-0.520831000
C	-0.618270000	-2.956082000	-0.147416000
C	-1.551839000	-2.384575000	-1.052373000
C	-2.617760000	-1.775050000	-0.302704000
C	-2.324914000	-2.023761000	1.084885000
C	-1.094247000	-2.729170000	1.178951000
C	-1.481836000	-2.606852000	-2.537351000
C	-3.263337000	-1.853374000	2.247285000
C	-0.519447000	-3.329149000	2.430582000
C	3.109657000	-1.114245000	-0.033413000
C	1.711481000	-0.677587000	0.448436000
H	3.851957000	0.694018000	-1.025669000
H	4.347202000	0.530258000	0.652032000
H	5.052557000	-2.479704000	-2.437789000
H	6.672340000	-1.929666000	-2.873757000

H	5. 270765000	-0. 929281000	-3. 272858000
H	6. 636788000	-1. 431675000	1. 442050000
H	7. 561675000	-2. 248951000	0. 176104000
H	5. 930186000	-2. 801817000	0. 564612000
H	6. 656687000	1. 498033000	-1. 757609000
H	8. 031188000	0. 461271000	-1. 353646000
H	7. 159117000	1. 306451000	-0. 067968000
H	1. 026851000	-3. 505176000	-1. 455129000
H	0. 225169000	-4. 859134000	-0. 667979000
H	1. 323147000	-3. 838960000	0. 255009000
H	-0. 452948000	-2. 597814000	-2. 913313000
H	-2. 052136000	-1. 874837000	-3. 110064000
H	-1. 894667000	-3. 594210000	-2. 784441000
H	-3. 781339000	-2. 802479000	2. 439225000
H	-4. 035147000	-1. 103644000	2. 060787000
H	-2. 749362000	-1. 587697000	3. 177139000
H	-0. 766088000	-2. 747012000	3. 324681000
H	0. 570486000	-3. 433133000	2. 386474000
H	-0. 923687000	-4. 338149000	2. 589155000
H	3. 501686000	-1. 808281000	0. 725199000
H	2. 984478000	-1. 721544000	-0. 940306000
H	1. 228930000	-1. 608264000	0. 817967000
C	-1. 426151000	2. 679719000	0. 853513000
O	-1. 489341000	1. 272733000	1. 280222000
C	-2. 070215000	1. 206723000	2. 620029000
C	-2. 047127000	2. 630115000	3. 145893000
C	-2. 258419000	3. 442263000	1. 868765000
H	-0. 374467000	2. 975065000	0. 872231000
H	-1. 804845000	2. 735776000	-0. 165638000
H	-3. 089809000	0. 830489000	2. 519457000
H	-1. 470718000	0. 508518000	3. 207366000
H	-2. 824776000	2. 795102000	3. 897066000
H	-1. 075229000	2. 857602000	3. 595109000
H	-3. 315316000	3. 444259000	1. 579622000
H	-1. 928241000	4. 480791000	1. 959095000
C	2. 048200000	1. 677059000	1. 361758000
C	1. 663981000	0. 329489000	1. 546703000
C	1. 281140000	-0. 062657000	2. 848002000
C	1. 306288000	0. 836911000	3. 917108000
C	1. 719187000	2. 150681000	3. 713216000
C	2. 087672000	2. 565912000	2. 428998000
H	2. 341251000	2. 016245000	0. 374215000
H	1. 040413000	-1. 106192000	3. 038664000
H	1. 036767000	0. 496693000	4. 913830000

H	2.416393000	3.588775000	2.263991000
C	-1.710966000	2.293625000	-2.680983000
C	-0.454225000	1.872947000	-2.205695000
C	0.535491000	2.855520000	-2.027754000
C	0.272852000	4.196758000	-2.291784000
C	-0.984694000	4.597217000	-2.745614000
C	-1.973867000	3.634406000	-2.947991000
H	-2.486192000	1.551407000	-2.857739000
H	1.532089000	2.571838000	-1.701231000
H	1.060423000	4.933544000	-2.155391000
H	-2.950826000	3.926389000	-3.324267000
C	-0.225945000	0.435617000	-1.977374000
C	1.008211000	-0.147817000	-1.697808000
H	-0.994039000	-0.211921000	-2.392366000
H	1.161052000	-1.194384000	-1.944249000
H	1.914634000	0.445510000	-1.710265000
Si	-4.327781000	-1.177361000	-0.926903000
C	-4.469390000	-1.093107000	-2.816504000
H	-3.767879000	-0.396344000	-3.287577000
H	-4.353150000	-2.073173000	-3.289494000
H	-5.480715000	-0.738576000	-3.051958000
C	-4.754549000	0.555720000	-0.271659000
H	-4.797478000	0.607383000	0.821142000
H	-4.034223000	1.302980000	-0.622746000
H	-5.742728000	0.846104000	-0.648437000
C	-5.626412000	-2.425783000	-0.335128000
H	-5.703719000	-2.478734000	0.755063000
H	-6.612674000	-2.147113000	-0.725018000
H	-5.394278000	-3.430812000	-0.705254000
H	1.769846000	2.845353000	4.547206000
H	-1.184411000	5.643720000	-2.957159000

SP2^a_{syn}, $E_{(\text{SCF Done})} = -2105.771045\text{a.u.}$

Sc	-1.433961000	0.078651000	-0.048281000
Si	6.832639000	0.921514000	-0.551844000
C	4.998878000	0.552380000	-0.139108000
C	6.927368000	2.260786000	-1.893500000
C	7.684353000	-0.660104000	-1.161720000
C	7.674186000	1.540353000	1.031429000
C	-0.456892000	-2.256598000	-2.548305000
C	-1.565215000	-1.757789000	-1.670182000
C	-2.561997000	-0.816043000	-2.037356000
C	-3.533054000	-0.723865000	-0.978446000
C	-3.125568000	-1.673944000	0.027111000

C	-1.913406000	-2.290423000	-0.386857000
C	-2.603490000	-0.145342000	-3.381360000
C	-3.883685000	-2.013387000	1.281940000
C	-1.163833000	-3.391984000	0.307637000
C	4.168603000	0.026203000	-1.312027000
C	2.673384000	-0.281577000	-1.007357000
H	4.562147000	1.481845000	0.255388000
H	4.983155000	-0.170093000	0.689059000
H	6.454842000	1.935186000	-2.827556000
H	7.971514000	2.504333000	-2.121528000
H	6.435262000	3.186004000	-1.570990000
H	7.619083000	-1.461527000	-0.416616000
H	8.746782000	-0.474734000	-1.357816000
H	7.237665000	-1.027573000	-2.092655000
H	7.195074000	2.452022000	1.407208000
H	8.729636000	1.772141000	0.847920000
H	7.633369000	0.786183000	1.825964000
H	-0.052719000	-1.472689000	-3.196736000
H	-0.824772000	-3.056956000	-3.204992000
H	0.369526000	-2.668557000	-1.964073000
H	-1.599598000	0.043172000	-3.776821000
H	-3.145176000	0.801967000	-3.368471000
H	-3.110237000	-0.792179000	-4.110247000
H	-4.903533000	-2.335583000	1.045014000
H	-3.969586000	-1.169467000	1.975726000
H	-3.412011000	-2.840030000	1.820109000
H	-1.468613000	-3.510797000	1.351218000
H	-0.079941000	-3.235001000	0.293475000
H	-1.351251000	-4.351734000	-0.191616000
H	4.626582000	-0.891246000	-1.704154000
H	4.186612000	0.752591000	-2.136704000
H	2.236216000	-0.595140000	-1.967176000
C	-2.027189000	1.313933000	2.865829000
O	-1.434007000	0.197781000	2.112880000
C	-0.895208000	-0.795005000	3.043823000
C	-0.678530000	-0.017574000	4.327549000
C	-1.881403000	0.930252000	4.333745000
H	-1.461270000	2.208529000	2.597611000
H	-3.065286000	1.423147000	2.542708000
H	-1.643329000	-1.585247000	3.162413000
H	0.012850000	-1.206966000	2.597881000
H	-0.648983000	-0.673120000	5.202060000
H	0.262283000	0.542371000	4.283707000
H	-2.776931000	0.409165000	4.689169000

H	-1.729194000	1.809455000	4.965278000
C	2.483993000	-1.355897000	1.327339000
C	2.571491000	-1.472014000	-0.067440000
C	2.699996000	-2.765485000	-0.599313000
C	2.732566000	-3.894010000	0.217268000
C	2.638838000	-3.758430000	1.602947000
C	2.519323000	-2.484040000	2.153019000
H	2.434298000	-0.372636000	1.788998000
H	2.802722000	-2.885093000	-1.676561000
H	2.842228000	-4.879392000	-0.228313000
H	2.481592000	-2.361340000	3.233373000
C	-1.635194000	2.409876000	-0.907299000
C	-0.283143000	2.244593000	-0.478722000
C	0.179226000	3.171314000	0.497950000
C	-0.629704000	4.197601000	0.959481000
C	-1.958248000	4.339596000	0.521930000
C	-2.451407000	3.446001000	-0.414611000
H	-1.984437000	1.850372000	-1.779196000
H	1.205652000	3.109716000	0.845143000
H	-0.220733000	4.915881000	1.666490000
H	-3.457340000	3.564676000	-0.807705000
C	0.447101000	1.054958000	-0.891564000
C	1.933241000	0.990422000	-0.560654000
H	0.250454000	0.807523000	-1.945906000
H	2.432008000	1.844025000	-1.048189000
H	2.091429000	1.152280000	0.512043000
Si	-5.257741000	0.111773000	-1.008994000
C	-5.461992000	1.385000000	-2.400329000
H	-4.729512000	2.198985000	-2.370502000
H	-5.427619000	0.927349000	-3.393874000
H	-6.454165000	1.839927000	-2.289081000
C	-5.618709000	1.010059000	0.626870000
H	-5.651018000	0.335140000	1.487766000
H	-4.886577000	1.801574000	0.827980000
H	-6.601991000	1.491045000	0.557866000
C	-6.546239000	-1.249052000	-1.292072000
H	-6.558044000	-1.999915000	-0.495362000
H	-7.548652000	-0.807896000	-1.346002000
H	-6.357934000	-1.768463000	-2.238253000
H	2.677011000	-4.634003000	2.245168000
H	-2.573515000	5.156258000	0.887095000

SC2_{iso}, $E_{(\text{SCF Done})} = -2105.746205$ a.u.

Sc	-0.388654000	-0.460437000	-0.091088000
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Si	5.977526000	-0.098900000	-0.473321000
C	4.335544000	-1.082645000	-0.464004000
C	6.230477000	0.737821000	1.213576000
C	5.928363000	1.225984000	-1.833645000
C	7.394777000	-1.312207000	-0.804269000
C	1.020440000	-0.612282000	-3.412548000
C	-0.223948000	-0.509010000	-2.583935000
C	-0.871478000	0.704610000	-2.220205000
C	-2.126609000	0.381675000	-1.625900000
C	-2.261396000	-1.047942000	-1.582893000
C	-1.059325000	-1.583116000	-2.176932000
C	-0.398067000	2.077763000	-2.593622000
C	-3.149852000	1.427140000	-1.276978000
C	3.049386000	-0.260077000	-0.262759000
C	1.777876000	-1.097513000	-0.202597000
H	4.408062000	-1.854100000	0.316323000
H	4.265587000	-1.632724000	-1.413946000
H	5.434720000	1.457712000	1.439784000
H	7.180323000	1.284693000	1.232828000
H	6.260483000	-0.000647000	2.023572000
H	5.762261000	0.779124000	-2.820943000
H	6.877874000	1.772178000	-1.874172000
H	5.134606000	1.961439000	-1.656654000
H	7.435060000	-2.094647000	-0.037714000
H	8.361378000	-0.795455000	-0.803621000
H	7.280060000	-1.802588000	-1.777794000
H	0.778807000	-0.463002000	-4.473578000
H	1.494799000	-1.594603000	-3.330910000
H	1.767532000	0.141194000	-3.143651000
H	0.694890000	2.151659000	-2.591585000
H	-0.791560000	2.851727000	-1.929513000
H	-0.729104000	2.328725000	-3.610853000
H	-2.702818000	2.290946000	-0.771890000
H	-3.948940000	1.041187000	-0.644236000
H	-3.622926000	1.811145000	-2.190861000
H	2.959381000	0.461400000	-1.086685000
H	3.145708000	0.352658000	0.645009000
H	1.687820000	-1.716337000	-1.103520000
C	-1.003095000	-0.398682000	3.152673000
O	-1.553157000	-0.239886000	1.800775000
C	-2.961346000	0.124866000	1.895428000
C	-3.372786000	-0.245878000	3.308239000
C	-2.101181000	0.063798000	4.099150000
H	-0.757834000	-1.453987000	3.277186000

H	-0.087846000	0.193417000	3.218985000
H	-3.048113000	1.201211000	1.709821000
H	-3.489765000	-0.419492000	1.114951000
H	-4.241326000	0.326252000	3.645846000
H	-3.619070000	-1.311752000	3.369955000
H	-2.023622000	1.138945000	4.298557000
H	-2.052605000	-0.459658000	5.057794000
C	2.132076000	-1.749600000	2.242051000
C	1.500863000	-1.911301000	0.979584000
C	0.445218000	-2.861456000	0.917957000
C	0.090590000	-3.647110000	2.023383000
C	0.768549000	-3.504762000	3.228229000
C	1.790862000	-2.547974000	3.324342000
H	2.952114000	-1.043864000	2.341108000
H	0.007116000	-3.105611000	-0.051866000
H	-0.690186000	-4.396176000	1.918814000
H	2.338164000	-2.439780000	4.257872000
C	-1.820898000	4.600408000	1.257541000
C	-0.635064000	4.022189000	0.770896000
C	0.127370000	4.741244000	-0.168094000
C	-0.300289000	5.983263000	-0.620355000
C	-1.492760000	6.533579000	-0.143096000
C	-2.251891000	5.841128000	0.799729000
H	-2.405885000	4.069814000	2.006230000
H	1.071067000	4.338303000	-0.524349000
H	0.302495000	6.532679000	-1.337849000
H	-3.171673000	6.272443000	1.184170000
C	-0.223567000	2.722809000	1.295532000
C	0.744503000	1.898188000	0.834700000
H	-0.761057000	2.412762000	2.192222000
H	1.082551000	1.062436000	1.448570000
H	1.368979000	2.140927000	-0.020820000
C	-0.775963000	-3.025225000	-2.498861000
H	-1.337344000	-3.716232000	-1.863920000
H	-1.052208000	-3.246585000	-3.537843000
H	0.286999000	-3.273731000	-2.399504000
Si	-3.829594000	-2.117689000	-1.314956000
C	-5.389232000	-1.104542000	-0.923256000
H	-5.599154000	-0.364173000	-1.702047000
H	-6.231020000	-1.808307000	-0.911291000
H	-5.391167000	-0.593530000	0.045181000
C	-4.205838000	-3.020782000	-2.938177000
H	-3.441672000	-3.753657000	-3.211584000
H	-5.159207000	-3.554658000	-2.845928000

H	-4.302292000	-2.307415000	-3.764353000
C	-3.584138000	-3.387833000	0.079465000
H	-2.797077000	-4.113142000	-0.153865000
H	-3.329871000	-2.914778000	1.034949000
H	-4.511980000	-3.953714000	0.226487000
H	0.525601000	-4.136785000	4.077426000
H	-1.820205000	7.507516000	-0.495866000

STS2^a_{iso}, $E_{(\text{SCF}_{\text{Done}})} = -2105.725731$ a.u. **IF** = $i247.76$ cm⁻¹

Sc	-0.693800000	0.267547000	0.227835000
Si	5.596597000	-1.262626000	-0.820469000
C	3.693776000	-1.462361000	-0.651853000
C	6.399286000	-1.376855000	0.894499000
C	5.985936000	0.418212000	-1.610046000
C	6.224656000	-2.662737000	-1.930007000
C	0.882526000	1.602036000	-2.670287000
C	-0.421993000	1.146297000	-2.083521000
C	-1.394068000	1.982587000	-1.458933000
C	-2.533514000	1.181158000	-1.163562000
C	-2.299731000	-0.160528000	-1.630561000
C	-0.975976000	-0.156923000	-2.200630000
C	-1.370150000	3.479538000	-1.421632000
C	-3.806341000	1.766605000	-0.617347000
C	2.990301000	-0.394277000	0.197441000
C	1.483486000	-0.607241000	0.317348000
H	3.494095000	-2.459565000	-0.235367000
H	3.270780000	-1.468963000	-1.667720000
H	6.074071000	-0.566810000	1.557777000
H	7.490086000	-1.309994000	0.809752000
H	6.164269000	-2.330585000	1.381187000
H	5.506923000	0.517590000	-2.591257000
H	7.066170000	0.530101000	-1.758477000
H	5.654400000	1.254709000	-0.983699000
H	5.997493000	-3.645765000	-1.501791000
H	7.311410000	-2.598949000	-2.057180000
H	5.770884000	-2.616803000	-2.926728000
H	0.746624000	1.897062000	-3.719719000
H	1.642706000	0.812994000	-2.661494000
H	1.289062000	2.469339000	-2.142476000
H	-0.357854000	3.885505000	-1.379798000
H	-1.921025000	3.889375000	-0.572142000
H	-1.844799000	3.864558000	-2.335178000
H	-3.611148000	2.500902000	0.172216000
H	-4.480526000	1.009233000	-0.218075000

H	-4.352432000	2.298438000	-1.408315000
H	3.169668000	0.597593000	-0.237306000
H	3.439240000	-0.369339000	1.199188000
H	1.075524000	-0.572181000	-0.716521000
C	-1.554342000	-0.548840000	3.285721000
O	-2.025147000	-0.312625000	1.913829000
C	-3.418683000	-0.743335000	1.808425000
C	-3.652331000	-1.631576000	3.015325000
C	-2.789477000	-0.949739000	4.077278000
H	-0.814117000	-1.351509000	3.241692000
H	-1.087827000	0.371478000	3.644835000
H	-4.045516000	0.152875000	1.833345000
H	-3.530079000	-1.243785000	0.847570000
H	-4.710439000	-1.681098000	3.286586000
H	-3.295083000	-2.648599000	2.820731000
H	-3.297729000	-0.066690000	4.480399000
H	-2.535068000	-1.607068000	4.912962000
C	1.575064000	-2.263050000	2.219768000
C	1.009727000	-1.827402000	0.996791000
C	-0.075389000	-2.568714000	0.482466000
C	-0.587120000	-3.678262000	1.166885000
C	-0.011896000	-4.089181000	2.363382000
C	1.080942000	-3.379540000	2.879266000
H	2.431880000	-1.738079000	2.632815000
H	-0.462355000	-2.342639000	-0.510882000
H	-1.402894000	-4.246566000	0.729517000
H	1.554143000	-3.710221000	3.800296000
C	-0.389146000	4.451653000	1.633661000
C	0.449503000	3.405969000	1.213994000
C	1.605037000	3.743731000	0.489510000
C	1.903604000	5.071574000	0.193094000
C	1.056086000	6.097363000	0.612033000
C	-0.090907000	5.778950000	1.338397000
H	-1.279198000	4.219953000	2.216612000
H	2.283173000	2.963714000	0.150518000
H	2.805406000	5.305872000	-0.366869000
H	-0.753698000	6.567931000	1.684124000
C	0.129722000	2.022756000	1.613275000
C	1.123078000	1.040675000	1.774636000
H	-0.761728000	1.936829000	2.241397000
H	1.000898000	0.279580000	2.543678000
H	2.155041000	1.335129000	1.618543000
C	-0.322158000	-1.271820000	-2.972458000
H	-0.786373000	-2.243237000	-2.783732000

H	-0.402235000	-1.080726000	-4.050441000
H	0.747866000	-1.372411000	-2.755132000
Si	-3.617867000	-1.471160000	-2.112865000
C	-5.373569000	-1.042874000	-1.531153000
H	-5.717825000	-0.082578000	-1.927034000
H	-6.040413000	-1.816489000	-1.932127000
H	-5.508673000	-1.037070000	-0.444535000
C	-3.673434000	-1.510853000	-4.006748000
H	-2.746159000	-1.883330000	-4.452078000
H	-4.487504000	-2.166194000	-4.338564000
H	-3.864441000	-0.510091000	-4.409989000
C	-3.240493000	-3.217061000	-1.460041000
H	-2.274529000	-3.609640000	-1.794676000
H	-3.269995000	-3.264396000	-0.365629000
H	-4.012360000	-3.900329000	-1.834829000
H	-0.382610000	-4.971561000	2.877117000
H	1.291524000	7.132402000	0.381908000

SP2_{iso}^a, $E_{(\text{SCF Done})} = -2105.769367$ a.u.

Sc	-0.890547000	0.086182000	0.030062000
Si	6.147298000	-0.277925000	-0.237514000
C	4.241232000	-0.451763000	-0.080827000
C	6.835496000	0.552197000	1.322463000
C	6.563716000	0.764699000	-1.766082000
C	6.867549000	-2.020777000	-0.418673000
C	0.189656000	0.953825000	-3.260226000
C	-0.768574000	0.140262000	-2.442769000
C	-2.091956000	0.519458000	-2.076587000
C	-2.709164000	-0.600569000	-1.447080000
C	-1.778823000	-1.695897000	-1.417009000
C	-0.572513000	-1.210325000	-2.037027000
C	-2.784687000	1.799288000	-2.437395000
C	-4.154306000	-0.607387000	-1.032468000
C	3.479668000	0.864879000	0.062518000
C	1.935691000	0.747519000	0.173528000
H	4.042043000	-1.106744000	0.779137000
H	3.888707000	-0.996604000	-0.970071000
H	6.456472000	1.573415000	1.445040000
H	7.928680000	0.613867000	1.270865000
H	6.579251000	-0.015492000	2.224660000
H	6.155222000	0.317979000	-2.680180000
H	7.649820000	0.839881000	-1.892977000
H	6.172937000	1.785559000	-1.683825000
H	6.626089000	-2.645227000	0.449333000

H	7.959487000	-1.982575000	-0.505286000
H	6.482327000	-2.523233000	-1.313547000
H	0.069932000	0.720833000	-4.326982000
H	1.236220000	0.750031000	-3.008896000
H	0.016871000	2.025895000	-3.142230000
H	-2.078888000	2.596048000	-2.676169000
H	-3.426880000	2.176601000	-1.634746000
H	-3.424784000	1.642768000	-3.316272000
H	-4.491621000	0.389623000	-0.729161000
H	-4.359000000	-1.299931000	-0.213735000
H	-4.794326000	-0.906925000	-1.873067000
H	3.687065000	1.514318000	-0.798533000
H	3.829477000	1.413003000	0.948345000
H	1.612507000	0.165243000	-0.711746000
C	-3.105321000	0.911509000	2.228357000
O	-2.241918000	-0.161043000	1.730756000
C	-2.611319000	-1.427077000	2.367921000
C	-3.606916000	-1.052908000	3.455961000
C	-4.274520000	0.198969000	2.882602000
H	-2.522699000	1.495902000	2.947901000
H	-3.375273000	1.543438000	1.379715000
H	-3.053191000	-2.062281000	1.595720000
H	-1.694845000	-1.883811000	2.743539000
H	-4.313662000	-1.863074000	3.654640000
H	-3.085925000	-0.818167000	4.390724000
H	-5.029899000	-0.068383000	2.136039000
H	-4.751331000	0.818970000	3.646518000
C	1.586539000	0.532103000	2.691332000
C	1.539143000	-0.042978000	1.407652000
C	1.195034000	-1.403050000	1.305839000
C	0.950454000	-2.175549000	2.451689000
C	1.025242000	-1.592130000	3.711107000
C	1.335957000	-0.231802000	3.825489000
H	1.850792000	1.581003000	2.798385000
H	1.221800000	-1.890853000	0.330693000
H	0.736799000	-3.235568000	2.348828000
H	1.400843000	0.228002000	4.808133000
C	-1.887064000	4.016516000	0.793763000
C	-0.893829000	3.466517000	-0.038980000
C	-0.558331000	4.207173000	-1.188387000
C	-1.204715000	5.400142000	-1.503827000
C	-2.210422000	5.904133000	-0.680299000
C	-2.541504000	5.205202000	0.478825000
H	-2.123613000	3.522880000	1.734044000

H	0.227304000	3.855680000	-1.851798000
H	-0.913104000	5.943239000	-2.399510000
H	-3.297189000	5.597592000	1.155202000
C	-0.236250000	2.175592000	0.312257000
C	1.285004000	2.144926000	0.090570000
H	-0.410612000	2.006420000	1.401388000
H	1.795898000	2.820076000	0.796802000
H	1.521209000	2.532697000	-0.905241000
C	0.641290000	-2.023191000	-2.398197000
H	0.739577000	-2.923991000	-1.786209000
H	0.581201000	-2.350717000	-3.444316000
H	1.573924000	-1.454856000	-2.306840000
Si	-2.156574000	-3.560924000	-1.190325000
C	-3.946587000	-3.908761000	-0.663967000
H	-4.673211000	-3.495457000	-1.370110000
H	-4.078208000	-4.997993000	-0.662705000
H	-4.205092000	-3.556716000	0.340735000
C	-1.916287000	-4.387405000	-2.878319000
H	-0.877146000	-4.362466000	-3.219621000
H	-2.222364000	-5.438838000	-2.822300000
H	-2.534073000	-3.899761000	-3.640689000
C	-1.029414000	-4.397327000	0.092142000
H	0.035981000	-4.316447000	-0.148558000
H	-1.187967000	-3.987608000	1.095808000
H	-1.270382000	-5.466408000	0.133969000
H	0.859670000	-2.190475000	4.602865000
H	-2.711124000	6.835970000	-0.926696000

***di*CIS_t, $E_{(\text{SCF Done})} = -1228.666384$ a.u**

C	0.358590000	-1.430574000	0.000018000
C	-0.988898000	-1.042431000	0.000053000
C	-1.296653000	0.327467000	0.000060000
C	-0.273221000	1.264684000	0.000019000
C	1.070930000	0.892465000	-0.000025000
C	1.362927000	-0.467915000	-0.000023000
H	0.623099000	-2.483510000	0.000018000
H	-2.326349000	0.666649000	0.000111000
H	1.859096000	1.636083000	-0.000053000
C	-2.020062000	-2.089945000	0.000084000
C	-3.346962000	-1.919910000	-0.000075000
H	-1.630917000	-3.107827000	0.000241000
H	-4.015622000	-2.775389000	-0.000033000
H	-3.819914000	-0.941357000	-0.000261000
Cl	3.030934000	-0.974495000	-0.000071000

Cl	-0.671481000	2.962865000	0.000031000
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diTS2^a_{syn}, $E_{(\text{SCF Done})} = -3944.078188$ a.u. **IF** = $i122.30$ cm⁻¹

Sc	0.031748000	-1.139448000	-0.192515000
Si	3.115984000	4.348626000	-1.882370000
C	1.982749000	3.172490000	-0.863333000
C	3.060523000	3.852645000	-3.712506000
C	4.890671000	4.233360000	-1.227162000
C	2.442364000	6.103790000	-1.661589000
C	1.841837000	-2.708126000	-0.864446000
C	0.881333000	-2.700608000	-1.931046000
C	-0.340094000	-3.272849000	-1.460021000
C	-0.153211000	-3.632620000	-0.096229000
C	1.169818000	-3.270281000	0.279222000
C	1.129192000	-2.323704000	-3.365436000
C	-1.524807000	-3.650489000	-2.302671000
C	-1.088168000	-4.444734000	0.749327000
C	1.776841000	-3.654080000	1.600969000
C	2.344234000	1.689036000	-0.976248000
C	1.475639000	0.640041000	-0.254895000
H	0.950930000	3.370713000	-1.188057000
H	2.048205000	3.503872000	0.181023000
H	3.480089000	2.854263000	-3.882582000
H	3.647412000	4.557351000	-4.312896000
H	2.035872000	3.863832000	-4.102581000
H	4.939475000	4.487713000	-0.162084000
H	5.540409000	4.934299000	-1.763786000
H	5.314123000	3.230614000	-1.356573000
H	1.415411000	6.187909000	-2.035378000
H	3.055561000	6.825230000	-2.213603000
H	2.444431000	6.405138000	-0.607808000
H	1.870879000	-1.529617000	-3.467799000
H	0.216967000	-1.995551000	-3.874798000
H	1.503699000	-3.187783000	-3.930217000
H	-1.593591000	-3.058890000	-3.220484000
H	-2.477669000	-3.551545000	-1.771459000
H	-1.444945000	-4.700023000	-2.615781000
H	-0.779836000	-5.498985000	0.739588000
H	-2.118457000	-4.416946000	0.383317000
H	-1.087675000	-4.128028000	1.797502000
H	1.115273000	-3.440384000	2.448307000
H	2.725041000	-3.148462000	1.790571000
H	1.977788000	-4.733676000	1.626227000
H	3.368585000	1.566819000	-0.592701000

H	2.400821000	1.404293000	-2.035507000
H	2.044770000	-0.313815000	-0.340449000
C	-1.537788000	-0.997682000	2.696984000
O	-1.650586000	-1.181111000	1.245325000
C	-3.022219000	-1.590823000	0.923124000
C	-3.602645000	-2.092884000	2.230179000
C	-2.950503000	-1.149078000	3.241272000
H	-0.862920000	-1.771665000	3.074768000
H	-1.106628000	-0.013770000	2.871786000
H	-3.550560000	-0.708438000	0.558339000
H	-2.964432000	-2.335243000	0.128265000
H	-4.694467000	-2.033080000	2.233085000
H	-3.314553000	-3.132406000	2.419056000
H	-3.463654000	-0.181532000	3.250111000
H	-2.949098000	-1.543333000	4.261012000
C	0.436364000	1.982726000	1.640798000
C	1.184757000	0.872737000	1.182543000
C	1.701877000	-0.020223000	2.146840000
C	1.524609000	0.228879000	3.512988000
C	0.843692000	1.351542000	3.962092000
C	0.298480000	2.215909000	3.002550000
H	0.001645000	2.681405000	0.936889000
H	2.345177000	-0.838914000	1.842254000
C	-3.756487000	-0.217401000	-2.177166000
C	-2.620600000	0.408386000	-1.637066000
C	-2.799307000	1.517705000	-0.794807000
C	-4.082374000	1.977552000	-0.513516000
C	-5.216477000	1.364318000	-1.044381000
C	-5.027766000	0.264524000	-1.880411000
H	-3.649564000	-1.065065000	-2.846826000
H	-1.948943000	2.022581000	-0.349748000
C	-1.290367000	-0.100341000	-2.006674000
C	-0.134368000	0.666921000	-1.992658000
H	-1.292329000	-0.984337000	-2.638214000
H	0.698185000	0.361849000	-2.617865000
H	-0.176235000	1.725792000	-1.767652000
Si	3.756799000	-2.611916000	-1.032243000
C	4.353982000	-4.408773000	-0.994062000
H	5.441100000	-4.449045000	-1.129560000
H	4.117622000	-4.896963000	-0.042751000
H	3.892902000	-4.994677000	-1.796838000
C	4.624038000	-1.643468000	0.356111000
H	4.336563000	-0.586840000	0.389148000
H	4.494911000	-2.068442000	1.356359000

H	5.699814000	-1.670606000	0.141246000
C	4.334334000	-1.810541000	-2.649824000
H	5.430967000	-1.786441000	-2.627960000
H	4.040858000	-2.376761000	-3.538432000
H	3.993162000	-0.775700000	-2.766365000
H	-6.210172000	1.734506000	-0.820554000
H	0.733663000	1.556316000	5.021008000
Cl	2.201034000	-0.874816000	4.670177000
Cl	-0.576392000	3.611365000	3.544232000
Cl	-4.280141000	3.349398000	0.536277000
Cl	-6.416176000	-0.522259000	-2.566032000

diTS2_{iso}, $E_{(\text{SCF Done})} = -3944.073131$ a.u. $\text{IF} = i217.18\text{cm}^{-1}$

Sc	-0.199011000	-1.035601000	-0.078109000
Si	1.027718000	5.182028000	1.202111000
C	0.237896000	3.749982000	0.185131000
C	2.828364000	4.761508000	1.617526000
C	0.030641000	5.431669000	2.794959000
C	0.949909000	6.735164000	0.123453000
C	0.211297000	-0.534651000	3.390901000
C	0.158409000	-1.557730000	2.289246000
C	1.308399000	-2.070017000	1.636054000
C	0.890774000	-3.120986000	0.759530000
C	-0.519264000	-3.263392000	0.893074000
C	-1.002307000	-2.284291000	1.832421000
C	2.729621000	-1.742086000	1.982788000
C	1.825361000	-4.025926000	0.010822000
C	-1.340279000	-4.346257000	0.249858000
C	0.152836000	2.413325000	0.925027000
C	-0.569451000	1.222247000	0.249274000
H	0.804527000	3.669387000	-0.753536000
H	-0.767877000	4.092215000	-0.090987000
H	2.910623000	3.875040000	2.257092000
H	3.297139000	5.593807000	2.155336000
H	3.419613000	4.582643000	0.712028000
H	-1.027874000	5.620100000	2.581130000
H	0.413804000	6.296394000	3.348939000
H	0.094539000	4.564091000	3.461863000
H	1.511835000	6.604358000	-0.808518000
H	1.380673000	7.593370000	0.651701000
H	-0.083297000	6.991056000	-0.137780000
H	1.091281000	0.109873000	3.302513000
H	0.280452000	-1.028770000	4.369217000
H	-0.672609000	0.107545000	3.419154000

H	2. 876312000	-0. 684451000	2. 219039000
H	3. 423937000	-1. 999879000	1. 180763000
H	3. 027629000	-2. 313867000	2. 872306000
H	2. 671766000	-3. 478682000	-0. 413463000
H	1. 332071000	-4. 569030000	-0. 801589000
H	2. 241361000	-4. 784215000	0. 687409000
H	-1. 699036000	-5. 057662000	1. 003843000
H	-0. 755176000	-4. 927349000	-0. 468657000
H	-2. 222922000	-3. 958419000	-0. 267519000
H	-0. 376183000	2. 592733000	1. 872780000
H	1. 156960000	2. 076609000	1. 216200000
H	-0. 794343000	0. 541902000	1. 118936000
C	-2. 668074000	-1. 484277000	-2. 268460000
O	-1. 271581000	-1. 748582000	-1. 884353000
C	-0. 689368000	-2. 711606000	-2. 821066000
C	-1. 875807000	-3. 364597000	-3. 504332000
C	-2. 863167000	-2. 200066000	-3. 596878000
H	-3. 303646000	-1. 893333000	-1. 478371000
H	-2. 798811000	-0. 403558000	-2. 324368000
H	-0. 071895000	-2. 155005000	-3. 535184000
H	-0. 061923000	-3. 393833000	-2. 244503000
H	-1. 605631000	-3. 776085000	-4. 480623000
H	-2. 280147000	-4. 175299000	-2. 888917000
H	-2. 604351000	-1. 540887000	-4. 432703000
H	-3. 898428000	-2. 525150000	-3. 729706000
C	-1. 957212000	2. 266999000	-1. 597728000
C	-1. 871401000	1. 490707000	-0. 423066000
C	-3. 063487000	0. 970560000	0. 116607000
C	-4. 290704000	1. 229491000	-0. 497216000
C	-4. 377969000	1. 992126000	-1. 656635000
C	-3. 193220000	2. 504607000	-2. 190044000
H	-1. 073672000	2. 712207000	-2. 038045000
H	-3. 044625000	0. 411887000	1. 047147000
C	3. 889077000	-1. 462044000	-1. 643352000
C	3. 076194000	-0. 451129000	-1. 105067000
C	3. 675248000	0. 533144000	-0. 304463000
C	5. 042530000	0. 486895000	-0. 051309000
C	5. 856098000	-0. 518901000	-0. 569070000
C	5. 253819000	-1. 485621000	-1. 370834000
H	3. 467875000	-2. 213951000	-2. 303878000
H	3. 089184000	1. 336837000	0. 128553000
C	1. 647730000	-0. 423396000	-1. 462939000
C	0. 865464000	0. 740935000	-1. 452822000
H	1. 356017000	-1. 192627000	-2. 181288000

H	0.041691000	0.808205000	-2.159787000
H	1.324437000	1.692636000	-1.209945000
Si	-2.677930000	-2.441190000	2.755131000
C	-4.126431000	-2.792898000	1.580436000
H	-4.251478000	-2.016702000	0.817546000
H	-4.045789000	-3.764370000	1.084004000
H	-5.050585000	-2.808056000	2.170923000
C	-3.133590000	-0.915512000	3.786443000
H	-4.140647000	-1.081499000	4.188680000
H	-2.464337000	-0.780919000	4.641572000
H	-3.166658000	0.024967000	3.226274000
C	-2.471994000	-3.898428000	3.949224000
H	-3.392385000	-4.044765000	4.526806000
H	-2.253611000	-4.835646000	3.426459000
H	-1.657271000	-3.712496000	4.657767000
H	-5.335093000	2.198278000	-2.121938000
H	6.919327000	-0.543572000	-0.361705000
Cl	-5.748518000	0.602817000	0.209163000
Cl	-3.271931000	3.470454000	-3.629752000
Cl	6.232748000	-2.747354000	-2.056366000
Cl	5.759847000	1.713800000	0.950827000

3,5-diFSt, $E_{(\text{SCF Done})} = -507.9582172$ a.u.

C	0.009711000	-1.347677000	0.000013000
C	-0.982888000	-0.356083000	0.000044000
C	-0.593429000	0.993362000	0.000049000
C	0.754206000	1.309953000	0.000011000
C	1.756352000	0.345264000	-0.000028000
C	1.347995000	-0.980443000	-0.000025000
H	-0.252091000	-2.401151000	0.000012000
H	-1.320002000	1.798058000	0.000096000
H	2.805293000	0.617221000	-0.000054000
C	-2.391127000	-0.776246000	0.000074000
C	-3.471384000	0.012851000	-0.000075000
H	-2.541382000	-1.855597000	0.000222000
H	-4.470300000	-0.412981000	-0.000036000
H	-3.411810000	1.098148000	-0.000249000
F	1.116646000	2.602663000	0.000019000
F	2.284872000	-1.941505000	-0.000060000

diFTS2^a_{syn}, $E_{(\text{SCF Done})} = -2502.66011$ a.u. IF = $i141.94\text{cm}^{-1}$

Sc	-0.403545000	-1.006466000	-0.161239000
Si	4.121228000	3.774079000	-0.671134000
C	2.654681000	2.797107000	0.102389000

C	3.976715000	3.742298000	-2.561690000
C	5.758419000	2.988731000	-0.126737000
C	4.003545000	5.553981000	-0.037254000
C	1.156905000	-2.861490000	-0.744270000
C	0.478552000	-2.476184000	-1.951151000
C	-0.904668000	-2.812083000	-1.831826000
C	-1.099333000	-3.401977000	-0.550893000
C	0.151982000	-3.414718000	0.122235000
C	1.110939000	-1.980634000	-3.222190000
C	-1.921932000	-2.769239000	-2.937075000
C	-2.316139000	-4.135175000	-0.063237000
C	0.352110000	-4.121557000	1.434447000
C	2.661726000	1.296495000	-0.208340000
C	1.492442000	0.400169000	0.231887000
H	1.732900000	3.288119000	-0.242846000
H	2.709603000	2.959757000	1.185874000
H	4.057500000	2.727387000	-2.968034000
H	4.780454000	4.336455000	-3.011712000
H	3.024671000	4.169049000	-2.898478000
H	5.844671000	2.958967000	0.965729000
H	6.604384000	3.572255000	-0.507895000
H	5.871009000	1.965759000	-0.503840000
H	3.052555000	6.020307000	-0.319566000
H	4.809830000	6.167894000	-0.454615000
H	4.088012000	5.594656000	1.054777000
H	2.017278000	-1.400358000	-3.040199000
H	0.429933000	-1.359869000	-3.813924000
H	1.395884000	-2.825908000	-3.862803000
H	-1.616676000	-2.109981000	-3.754854000
H	-2.911644000	-2.442049000	-2.601080000
H	-2.046844000	-3.768628000	-3.374556000
H	-2.078404000	-5.200064000	0.058237000
H	-3.144730000	-4.081857000	-0.775529000
H	-2.674762000	-3.784298000	0.911809000
H	-0.417390000	-3.865693000	2.171121000
H	1.323503000	-3.910296000	1.885674000
H	0.298933000	-5.208987000	1.287815000
H	3.564630000	0.871619000	0.254763000
H	2.805048000	1.146404000	-1.287309000
H	1.829730000	-0.640325000	0.069556000
C	-2.707344000	-0.211396000	2.032996000
O	-2.414524000	-0.796189000	0.720992000
C	-3.682003000	-1.078262000	0.033927000
C	-4.742173000	-1.013441000	1.116315000

C	-4.196290000	0.087572000	2.025583000
H	-2.446569000	-0.958973000	2.786411000
H	-2.076430000	0.669944000	2.151180000
H	-3.825142000	-0.303718000	-0.722501000
H	-3.586351000	-2.051363000	-0.441900000
H	-5.726549000	-0.779193000	0.701907000
H	-4.813818000	-1.965805000	1.654237000
H	-4.391609000	1.075181000	1.595129000
H	-4.616247000	0.062662000	3.034821000
C	0.494854000	1.712405000	2.180169000
C	0.913888000	0.502224000	1.569858000
C	0.689035000	-0.706536000	2.284454000
C	0.144430000	-0.665591000	3.575057000
C	-0.196285000	0.512571000	4.204910000
C	-0.002402000	1.689247000	3.470211000
H	0.606421000	2.667025000	1.683892000
H	1.157565000	-1.632304000	1.963833000
C	-3.324317000	1.414720000	-2.488415000
C	-2.199480000	1.466699000	-1.646761000
C	-2.191414000	2.388887000	-0.587280000
C	-3.278435000	3.232735000	-0.406132000
C	-4.398155000	3.206202000	-1.228378000
C	-4.385651000	2.284109000	-2.268303000
H	-3.365054000	0.736734000	-3.335439000
H	-1.353937000	2.461119000	0.098891000
C	-1.048572000	0.594486000	-1.928812000
C	0.259996000	0.978713000	-1.659686000
H	-1.203642000	-0.167604000	-2.689310000
H	1.063633000	0.508841000	-2.216413000
H	0.464597000	1.984964000	-1.313582000
Si	3.040326000	-3.176581000	-0.502001000
C	3.275215000	-5.051698000	-0.628000000
H	4.339184000	-5.302280000	-0.542804000
H	2.742329000	-5.587609000	0.164354000
H	2.916782000	-5.430524000	-1.591450000
C	3.714083000	-2.579169000	1.175128000
H	3.620414000	-1.496830000	1.316724000
H	3.272374000	-3.077599000	2.043800000
H	4.786715000	-2.810101000	1.193137000
C	4.116566000	-2.341325000	-1.819590000
H	5.162546000	-2.573824000	-1.584220000
H	3.920992000	-2.713259000	-2.829513000
H	4.023226000	-1.249634000	-1.824735000
H	-5.234844000	3.877301000	-1.073646000

H	-0.581321000	0.534369000	5.217786000
F	-0.026834000	-1.822942000	4.223450000
F	-0.340577000	2.842904000	4.046318000
F	-5.440147000	2.228488000	-3.087550000
F	-3.253042000	4.097017000	0.616890000

diFTS2^a_{iso}, $E_{(\text{SCF Done})} = -2502.660582$ a.u. IF = $i247.28$ cm⁻¹

Sc	-0.707781000	0.339349000	0.119105000
Si	5.027390000	-2.515938000	-1.222642000
C	3.134351000	-2.332796000	-0.942218000
C	5.894355000	-2.766054000	0.445163000
C	5.689942000	-0.952640000	-2.068258000
C	5.294063000	-4.024323000	-2.334812000
C	1.240501000	1.435198000	-2.649335000
C	-0.152384000	1.270940000	-2.115048000
C	-0.915798000	2.273660000	-1.447598000
C	-2.222845000	1.751563000	-1.225629000
C	-2.302456000	0.426513000	-1.782216000
C	-0.997110000	0.147289000	-2.326961000
C	-0.540636000	3.716582000	-1.303888000
C	-3.331827000	2.587641000	-0.649894000
C	2.710042000	-1.177236000	-0.025368000
C	1.198264000	-1.065635000	0.155669000
H	2.758528000	-3.283643000	-0.539304000
H	2.665176000	-2.217841000	-1.930907000
H	5.780301000	-1.897338000	1.104065000
H	6.969027000	-2.918254000	0.292412000
H	5.509550000	-3.646992000	0.972109000
H	5.186707000	-0.770123000	-3.025073000
H	6.761064000	-1.057752000	-2.276060000
H	5.566839000	-0.060114000	-1.443614000
H	4.902832000	-4.937328000	-1.871561000
H	6.362056000	-4.180482000	-2.525303000
H	4.799444000	-3.899701000	-3.304963000
H	1.210848000	1.815073000	-3.679554000
H	1.790880000	0.488697000	-2.679482000
H	1.824365000	2.147838000	-2.060655000
H	0.539075000	3.867845000	-1.250739000
H	-0.983466000	4.184097000	-0.421148000
H	-0.906852000	4.266874000	-2.181833000
H	-2.997201000	3.167396000	0.218124000
H	-4.193623000	1.992479000	-0.349553000
H	-3.685843000	3.315701000	-1.392248000
H	3.081444000	-0.226646000	-0.429658000

H	3.191183000	-1.294949000	0.954297000
H	0.766573000	-0.902554000	-0.856400000
C	-1.824899000	-0.458416000	3.083399000
O	-2.187059000	-0.008511000	1.731285000
C	-3.643949000	-0.068159000	1.586714000
C	-4.104553000	-1.022401000	2.670179000
C	-3.143159000	-0.684826000	3.810935000
H	-1.250642000	-1.381596000	2.973089000
H	-1.203351000	0.314282000	3.542427000
H	-4.034531000	0.942721000	1.738768000
H	-3.853095000	-0.395537000	0.569308000
H	-5.153415000	-0.862009000	2.934378000
H	-3.985119000	-2.061234000	2.345240000
H	-3.463227000	0.227080000	4.326602000
H	-3.058691000	-1.482395000	4.553728000
C	1.020794000	-2.776617000	1.983786000
C	0.494253000	-2.175466000	0.820055000
C	-0.781683000	-2.581642000	0.370653000
C	-1.491362000	-3.536621000	1.101604000
C	-0.986967000	-4.142067000	2.238804000
C	0.288713000	-3.748699000	2.644450000
H	2.005723000	-2.522160000	2.359200000
H	-1.180526000	-2.261661000	-0.590760000
C	0.591871000	4.192752000	1.825587000
C	1.159945000	3.010889000	1.325737000
C	2.371841000	3.093194000	0.621212000
C	2.972318000	4.331207000	0.434982000
C	2.425923000	5.514991000	0.914222000
C	1.230842000	5.407323000	1.613455000
H	-0.329868000	4.178557000	2.399648000
H	2.864631000	2.215722000	0.216098000
C	0.506411000	1.724854000	1.624597000
C	1.231996000	0.522125000	1.714174000
H	-0.380810000	1.816332000	2.257033000
H	0.922999000	-0.229876000	2.438622000
H	2.306001000	0.567502000	1.569537000
C	-0.606410000	-1.044102000	-3.159904000
H	-1.249233000	-1.910309000	-2.984688000
H	-0.679220000	-0.797638000	-4.226976000
H	0.428507000	-1.360808000	-2.988551000
Si	-3.882863000	-0.469004000	-2.422706000
C	-5.506247000	0.288320000	-1.793096000
H	-5.612929000	1.339687000	-2.077340000
H	-6.318784000	-0.262205000	-2.283879000

H	-5.672755000	0.202170000	-0.714343000
C	-3.879755000	-0.231223000	-4.303257000
H	-3.041745000	-0.736351000	-4.793207000
H	-4.805140000	-0.639953000	-4.726312000
H	-3.834303000	0.832192000	-4.563279000
C	-3.939219000	-2.321369000	-2.021379000
H	-3.127117000	-2.892525000	-2.483268000
H	-3.928186000	-2.530334000	-0.948096000
H	-4.877179000	-2.725056000	-2.422425000
F	-2.711964000	-3.896450000	0.680044000
F	0.811878000	-4.326063000	3.726044000
F	4.125524000	4.384154000	-0.243303000
F	0.670747000	6.518939000	2.103220000
H	-1.538853000	-4.910575000	2.767568000
H	2.911785000	6.470933000	0.759180000

2,3,4,5,6-pentafluoro styrene, $E_{(\text{SCF Done})} = -805.6436917$ a.u.

C	-0.115116000	1.316254000	-0.000007000
C	-1.116164000	0.331449000	-0.000010000
C	-0.662931000	-0.996337000	-0.000005000
C	0.688029000	-1.323102000	0.000004000
C	1.647338000	-0.314860000	0.000009000
C	1.241237000	1.015187000	0.000003000
C	-2.519803000	0.750835000	-0.000029000
C	-3.615459000	-0.020356000	0.000027000
H	-2.651038000	1.829433000	-0.000092000
H	-4.596640000	0.445459000	0.000004000
H	-3.586799000	-1.102421000	0.000097000
F	1.068824000	-2.600154000	0.000007000
F	2.149630000	1.989809000	0.000007000
F	2.941145000	-0.621708000	0.000019000
F	-1.530164000	-2.014429000	-0.000014000
F	-0.457025000	2.610162000	-0.000013000

pantaTS2_{syn}, $E_{(\text{SCF Done})} = -3098.026967$ a.u. IF = $i126.60$ cm⁻¹

Sc	0.201667000	1.130954000	0.195176000
Si	-4.497844000	-2.109105000	-2.682540000
C	-2.858960000	-2.022830000	-1.680931000
C	-4.505468000	-0.747022000	-4.004795000
C	-5.978665000	-1.895371000	-1.517747000
C	-4.555571000	-3.809793000	-3.511247000
C	-1.577910000	2.834696000	0.393231000
C	-0.946127000	3.025946000	-0.882917000
C	0.396079000	3.465991000	-0.674250000

C	0.614714000	3.542639000	0.731391000
C	-0.575711000	3.127593000	1.386032000
C	-1.586596000	2.935445000	-2.239979000
C	1.327735000	4.003842000	-1.721492000
C	1.783135000	4.193571000	1.411468000
C	-0.753940000	3.161968000	2.878861000
C	-2.678990000	-0.744322000	-0.861116000
C	-1.384870000	-0.507489000	-0.042556000
H	-2.042023000	-2.167416000	-2.396865000
H	-2.848984000	-2.901289000	-1.023940000
H	-4.494818000	0.259215000	-3.569430000
H	-5.407662000	-0.822672000	-4.622681000
H	-3.641459000	-0.838032000	-4.673761000
H	-5.975291000	-2.651453000	-0.723924000
H	-6.917090000	-2.006525000	-2.073200000
H	-5.995429000	-0.906962000	-1.044097000
H	-3.703055000	-3.956844000	-4.184250000
H	-5.470114000	-3.920467000	-4.105013000
H	-4.541756000	-4.616603000	-2.769570000
H	-2.425146000	2.237179000	-2.257304000
H	-0.873984000	2.624976000	-3.012458000
H	-1.974616000	3.913866000	-2.552425000
H	1.086310000	3.642134000	-2.724857000
H	2.376714000	3.760804000	-1.527938000
H	1.251584000	5.098860000	-1.757731000
H	1.518061000	5.223796000	1.685575000
H	2.663187000	4.263093000	0.764592000
H	2.069561000	3.690308000	2.340882000
H	0.119274000	2.762590000	3.408862000
H	-1.625440000	2.592531000	3.206176000
H	-0.883766000	4.194556000	3.228893000
H	-3.514924000	-0.690838000	-0.147932000
H	-2.801122000	0.132016000	-1.511053000
H	-1.680769000	0.373245000	0.588985000
C	1.977685000	-0.243358000	2.630138000
O	1.957205000	0.634754000	1.449280000
C	3.301779000	1.179248000	1.249553000
C	3.929774000	1.149160000	2.626733000
C	3.400058000	-0.177016000	3.178583000
H	1.237669000	0.150744000	3.330495000
H	1.688272000	-1.243175000	2.304055000
H	3.830928000	0.526444000	0.550468000
H	3.191696000	2.169973000	0.810930000
H	5.021578000	1.183096000	2.577798000

H	3. 586579000	1. 995667000	3. 231695000
H	3. 996802000	-1. 013615000	2. 800737000
H	3. 411363000	-0. 221051000	4. 270701000
C	-0. 592626000	-2. 888982000	0. 556013000
C	-0. 992318000	-1. 589662000	0. 912954000
C	-1. 065258000	-1. 365982000	2. 297782000
C	-0. 816644000	-2. 333420000	3. 260925000
C	-0. 452544000	-3. 613809000	2. 855579000
C	-0. 332320000	-3. 883425000	1. 493930000
C	3. 629528000	0. 641813000	-2. 403117000
C	2. 563119000	-0. 049126000	-1. 805957000
C	2. 910476000	-1. 239124000	-1. 155221000
C	4. 211695000	-1. 722367000	-1. 098916000
C	5. 238985000	-1. 010461000	-1. 714697000
C	4. 942195000	0. 184876000	-2. 366466000
C	1. 195607000	0. 479848000	-1. 929579000
C	0. 036791000	-0. 292131000	-1. 941666000
H	1. 141996000	1. 452044000	-2. 409272000
H	-0. 839270000	0. 117235000	-2. 432792000
H	0. 073834000	-1. 369746000	-1. 871330000
Si	-3. 462689000	2. 911251000	0. 793544000
C	-3. 731192000	4. 633347000	1. 538419000
H	-4. 799945000	4. 794234000	1. 722947000
H	-3. 207248000	4. 761799000	2. 490799000
H	-3. 388088000	5. 416599000	0. 853378000
C	-4. 065148000	1. 603919000	2. 030475000
H	-3. 935289000	0. 579399000	1. 668295000
H	-3. 592242000	1. 677787000	3. 013848000
H	-5. 141005000	1. 761168000	2. 177382000
C	-4. 561203000	2. 782448000	-0. 744397000
H	-5. 597835000	2. 918607000	-0. 411685000
H	-4. 352157000	3. 565961000	-1. 478968000
H	-4. 509177000	1. 810686000	-1. 245035000
F	-0. 892959000	-2. 030814000	4. 554077000
F	0. 044078000	-5. 090577000	1. 092290000
F	5. 909027000	0. 879882000	-2. 952961000
F	4. 478084000	-2. 846317000	-0. 439637000
F	3. 390424000	1. 792716000	-3. 043545000
F	6. 485123000	-1. 458177000	-1. 667279000
F	1. 968062000	-1. 929985000	-0. 487739000
F	-0. 191250000	-4. 553007000	3. 751439000
F	-1. 352766000	-0. 121318000	2. 746146000
F	-0. 417229000	-3. 225288000	-0. 725802000

pantaTS2^a_{iso}, $E_{(\text{SCF Done})} = -3098.031006$ a.u. IF = $i221.20$ cm⁻¹

Sc	0.095544000	-0.877458000	0.112976000
Si	-1.213263000	5.203738000	1.797845000
C	-1.612517000	3.387458000	1.306506000
C	-0.988032000	6.236456000	0.224090000
C	0.371352000	5.249448000	2.838877000
C	-2.675637000	5.851121000	2.811460000
C	1.663164000	0.827382000	2.806750000
C	1.199794000	-0.504688000	2.293399000
C	2.016300000	-1.442227000	1.592540000
C	1.252547000	-2.629174000	1.393082000
C	-0.043888000	-2.456211000	1.989482000
C	-0.055214000	-1.122474000	2.543261000
C	3.500899000	-1.339430000	1.421063000
C	1.834025000	-3.866776000	0.767433000
C	-0.574932000	2.709571000	0.401193000
C	-0.939031000	1.272554000	0.011480000
H	-2.594391000	3.396444000	0.812604000
H	-1.746209000	2.810320000	2.233912000
H	-0.107018000	5.922444000	-0.347538000
H	-0.853164000	7.294354000	0.477031000
H	-1.862539000	6.161560000	-0.432374000
H	0.276228000	4.635215000	3.742109000
H	0.584017000	6.275363000	3.161004000
H	1.243397000	4.897304000	2.275936000
H	-3.603271000	5.841593000	2.227832000
H	-2.496224000	6.883848000	3.131713000
H	-2.837605000	5.248250000	3.712467000
H	2.252684000	0.694850000	3.723920000
H	0.828787000	1.488147000	3.058405000
H	2.300821000	1.351660000	2.088728000
H	3.841008000	-0.314633000	1.256276000
H	3.873386000	-1.961012000	0.603690000
H	3.987591000	-1.695317000	2.339792000
H	2.460835000	-3.628874000	-0.099070000
H	1.069108000	-4.574597000	0.448225000
H	2.477159000	-4.392147000	1.486249000
H	0.395241000	2.675897000	0.907742000
H	-0.430222000	3.315885000	-0.496846000
H	-1.033849000	0.734221000	0.984726000
C	-0.926876000	-1.807796000	-2.951668000
O	-0.656688000	-2.183697000	-1.557202000
C	-1.138881000	-3.551024000	-1.334101000
C	-2.099542000	-3.822185000	-2.475279000

C	-1.430731000	-3.073167000	-3.628429000
H	-1.687667000	-1.021361000	-2.936612000
H	-0.004314000	-1.419184000	-3.387572000
H	-0.270221000	-4.214930000	-1.363989000
H	-1.592087000	-3.578044000	-0.343800000
H	-2.210732000	-4.892732000	-2.667560000
H	-3.089268000	-3.407529000	-2.255745000
H	-0.594247000	-3.653854000	-4.032228000
H	-2.114495000	-2.844951000	-4.450371000
C	-2.763309000	1.924164000	-1.688464000
C	-2.211009000	1.062918000	-0.728518000
C	-2.936063000	-0.113334000	-0.523622000
C	-4.122537000	-0.440032000	-1.152687000
C	-4.650098000	0.458455000	-2.079903000
C	-3.962615000	1.640419000	-2.343581000
C	4.001903000	-0.621067000	-1.754158000
C	3.040548000	0.298602000	-1.310977000
C	3.551439000	1.484829000	-0.771426000
C	4.914513000	1.740301000	-0.667648000
C	5.833860000	0.800169000	-1.126075000
C	5.368908000	-0.394520000	-1.670501000
C	1.621382000	-0.014631000	-1.517355000
C	0.594826000	0.942487000	-1.602692000
H	1.486329000	-0.932311000	-2.088447000
H	-0.225865000	0.752443000	-2.290294000
H	0.833207000	1.989398000	-1.478951000
C	-1.143777000	-0.520974000	3.388966000
H	-2.133782000	-0.899806000	3.125460000
H	-0.972626000	-0.754517000	4.447384000
H	-1.175181000	0.570782000	3.314613000
Si	-1.245240000	-3.835333000	2.597179000
C	-0.826552000	-5.557324000	1.916367000
H	0.181030000	-5.879994000	2.195811000
H	-1.530475000	-6.259947000	2.379831000
H	-0.936272000	-5.666331000	0.832303000
C	-1.013109000	-3.927949000	4.475843000
H	-1.358405000	-3.026089000	4.990307000
H	-1.585497000	-4.774199000	4.874127000
H	0.039722000	-4.085123000	4.734907000
C	-3.079729000	-3.515609000	2.222302000
H	-3.456671000	-2.591074000	2.669949000
H	-3.316102000	-3.490570000	1.153799000
H	-3.652894000	-4.341756000	2.661254000
F	-4.727356000	-1.602251000	-0.912843000

F	-4.444780000	2.495854000	-3.233869000
F	5.337785000	2.882300000	-0.135940000
F	6.228453000	-1.312437000	-2.099513000
F	-5.774102000	0.174430000	-2.720395000
F	-2.157915000	3.070817000	-2.009763000
F	-2.395161000	-1.028863000	0.342112000
F	3.591815000	-1.795995000	-2.266391000
F	7.135581000	1.034509000	-1.033338000
F	2.714409000	2.426633000	-0.295391000

4-trifluoromethyl-2,3,5,6-tetrafluoro styrene, $E_{(\text{SCF Done})} = -1043.438848$ a.u.

C	1.101783000	1.329190000	0.000079000
C	1.917299000	0.189466000	0.000152000
C	1.239172000	-1.038225000	0.000127000
C	-0.145792000	-1.110231000	0.000046000
C	-0.943634000	0.037080000	0.000080000
C	-0.288680000	1.268437000	-0.000017000
C	3.371358000	0.360478000	0.000330000
C	4.313056000	-0.592817000	-0.000499000
H	3.688234000	1.399516000	0.001179000
H	5.361240000	-0.308117000	-0.000255000
H	4.093050000	-1.652710000	-0.001461000
F	-0.716908000	-2.315035000	-0.000062000
F	-0.954025000	2.421661000	-0.000260000
F	1.913761000	-2.192866000	0.000173000
F	1.663888000	2.543851000	0.000041000
C	-2.444033000	-0.131648000	-0.000020000
F	-2.843251000	-0.820982000	1.083011000
F	-3.093965000	1.037023000	0.001127000
F	-2.843466000	-0.819103000	-1.084155000

tetraTS2^a_{syn}, $E_{(\text{SCF Done})} = -3573.617342$ a.u. IF = $i98.26$ cm⁻¹

Sc	-0.575189000	-1.129290000	-0.800023000
Si	-4.247250000	0.507000000	4.153199000
C	-2.758490000	0.876435000	2.996324000
C	-4.459563000	-1.367898000	4.364549000
C	-5.829084000	1.261788000	3.429860000
C	-3.855101000	1.296806000	5.828578000
C	-2.662071000	-2.208533000	-1.524076000
C	-2.031573000	-3.091433000	-0.580366000
C	-0.820326000	-3.590815000	-1.152476000
C	-0.687484000	-3.022587000	-2.451428000
C	-1.791019000	-2.155726000	-2.668553000
C	-2.596244000	-3.582235000	0.723269000

C	0.026351000	-4.706283000	-0.608658000
C	0.276480000	-3.444353000	-3.521558000
C	-2.030981000	-1.454775000	-3.976301000
C	-2.927473000	0.361719000	1.562362000
C	-1.801653000	0.391123000	0.497234000
H	-1.868081000	0.466677000	3.487058000
H	-2.631386000	1.962361000	3.000875000
H	-4.734500000	-1.868118000	3.428592000
H	-5.257555000	-1.576507000	5.086602000
H	-3.543560000	-1.834555000	4.746270000
H	-5.716968000	2.340365000	3.269084000
H	-6.667627000	1.118087000	4.121058000
H	-6.112389000	0.805003000	2.474473000
H	-2.946009000	0.872338000	6.270021000
H	-4.675403000	1.132002000	6.536543000
H	-3.709659000	2.379164000	5.735953000
H	-3.261301000	-2.855153000	1.192153000
H	-1.812912000	-3.836876000	1.445332000
H	-3.181458000	-4.497980000	0.566262000
H	-0.119922000	-4.858467000	0.464404000
H	1.097874000	-4.556950000	-0.777568000
H	-0.246560000	-5.651524000	-1.096316000
H	-0.253426000	-4.050638000	-4.268300000
H	1.087433000	-4.068259000	-3.134589000
H	0.713830000	-2.598612000	-4.063312000
H	-1.110453000	-1.021044000	-4.383688000
H	-2.764839000	-0.651372000	-3.893914000
H	-2.401606000	-2.165109000	-4.726834000
H	-3.780914000	0.901731000	1.125174000
H	-3.249551000	-0.687189000	1.596261000
H	-2.343936000	-0.007731000	-0.391761000
C	1.782354000	0.688927000	-2.325151000
O	1.385109000	-0.614851000	-1.764225000
C	2.504835000	-1.543052000	-1.935436000
C	3.268625000	-1.005006000	-3.125731000
C	3.193034000	0.501827000	-2.872975000
H	1.064092000	0.931273000	-3.109500000
H	1.724529000	1.424498000	-1.521707000
H	3.113587000	-1.510466000	-1.029083000
H	2.086373000	-2.540116000	-2.058069000
H	4.294973000	-1.380964000	-3.155509000
H	2.774868000	-1.275724000	-4.065630000
H	3.941335000	0.803239000	-2.132648000
H	3.352606000	1.097893000	-3.775257000

C	-0.725535000	2.732706000	0.859152000
C	-1.195161000	1.670217000	0.067896000
C	-1.011080000	1.892132000	-1.303590000
C	-0.556445000	3.058443000	-1.888172000
C	-0.182804000	4.130372000	-1.076560000
C	-0.255256000	3.919392000	0.304003000
C	3.076977000	-2.462418000	1.475704000
C	2.109303000	-1.458847000	1.344352000
C	2.604607000	-0.151974000	1.274502000
C	3.959707000	0.132141000	1.319206000
C	4.913654000	-0.880749000	1.459063000
C	4.442775000	-2.192825000	1.535841000
C	0.688460000	-1.819176000	1.313531000
C	-0.325340000	-1.032330000	1.824853000
H	0.492653000	-2.880445000	1.197439000
H	-1.260656000	-1.503441000	2.104958000
H	-0.121108000	-0.073835000	2.282485000
Si	-4.515901000	-1.689264000	-1.633755000
C	-5.229225000	-2.664406000	-3.093530000
H	-6.310214000	-2.491220000	-3.154781000
H	-4.793483000	-2.372907000	-4.053949000
H	-5.071475000	-3.740603000	-2.961082000
C	-4.768949000	0.168953000	-1.933901000
H	-4.453406000	0.781521000	-1.082606000
H	-4.263163000	0.543692000	-2.829087000
H	-5.842759000	0.345013000	-2.073423000
C	-5.517374000	-2.166777000	-0.099001000
H	-6.566435000	-1.921951000	-0.307072000
H	-5.471225000	-3.238889000	0.115047000
H	-5.231061000	-1.616743000	0.802428000
F	-0.447970000	3.088968000	-3.215756000
F	0.152789000	4.867952000	1.137104000
F	5.262756000	-3.228231000	1.659819000
F	4.342793000	1.401085000	1.196882000
F	2.688889000	-3.742010000	1.535136000
F	1.751707000	0.873765000	1.082760000
F	-1.242789000	0.813766000	-2.137078000
F	-0.676269000	2.630519000	2.188708000
C	6.377948000	-0.494863000	1.477814000
F	7.178837000	-1.543083000	1.670655000
F	6.713859000	0.073160000	0.304359000
F	6.615528000	0.398027000	2.446757000
C	0.377324000	5.432767000	-1.605424000
F	-0.199070000	6.476848000	-1.000302000

F	0.182470000	5.557909000	-2.922301000
F	1.699563000	5.498214000	-1.374737000

tatraTS2^a_{iso}, $E_{(\text{SCF Done})} = -3573.622969$ a.u. $\text{IF} = i218.98$ cm⁻¹

Sc	-0.080562000	-0.958509000	0.307367000
Si	-0.532529000	5.195989000	2.194460000
C	-1.189333000	3.456269000	1.703522000
C	-0.368502000	6.262076000	0.635999000
C	1.152459000	5.020045000	3.046665000
C	-1.788467000	5.960588000	3.387196000
C	1.909144000	0.498058000	2.866826000
C	1.235989000	-0.755517000	2.390164000
C	1.864075000	-1.780038000	1.620883000
C	0.940517000	-2.858005000	1.484751000
C	-0.270781000	-2.527572000	2.182630000
C	-0.066119000	-1.208475000	2.736268000
C	3.328599000	-1.865716000	1.318253000
C	1.310216000	-4.155932000	0.822094000
C	-0.318669000	2.692032000	0.696027000
C	-0.874828000	1.315644000	0.318090000
H	-2.201735000	3.594147000	1.298261000
H	-1.310505000	2.869846000	2.626658000
H	0.384353000	5.867194000	-0.055998000
H	-0.064658000	7.281161000	0.901724000
H	-1.320810000	6.330748000	0.097690000
H	1.085994000	4.392977000	3.943661000
H	1.521059000	6.003145000	3.361505000
H	1.908429000	4.586629000	2.381712000
H	-2.772651000	6.069108000	2.917199000
H	-1.461514000	6.957262000	3.705009000
H	-1.910971000	5.349141000	4.288686000
H	2.558731000	0.273807000	3.723454000
H	1.192846000	1.253694000	3.200699000
H	2.539617000	0.952073000	2.096831000
H	3.787364000	-0.885050000	1.173962000
H	3.541440000	-2.480458000	0.440448000
H	3.839366000	-2.336758000	2.169554000
H	1.861778000	-3.998139000	-0.111668000
H	0.440096000	-4.774240000	0.604103000
H	1.966607000	-4.743731000	1.477780000
H	0.682728000	2.537801000	1.110922000
H	-0.187252000	3.302181000	-0.201372000
H	-0.952663000	0.763138000	1.283428000
C	-1.344942000	-1.739240000	-2.713477000

O	-1.053728000	-2.148325000	-1.331802000
C	-1.694488000	-3.445513000	-1.078255000
C	-2.699869000	-3.621240000	-2.200358000
C	-1.982469000	-2.951170000	-3.372262000
H	-2.035414000	-0.891424000	-2.667103000
H	-0.410031000	-1.428507000	-3.183521000
H	-0.909591000	-4.205799000	-1.107199000
H	-2.134942000	-3.402524000	-0.082726000
H	-2.923685000	-4.675921000	-2.381923000
H	-3.637879000	-3.106546000	-1.966592000
H	-1.214530000	-3.612982000	-3.787390000
H	-2.657078000	-2.660236000	-4.181838000
C	-2.733109000	2.186327000	-1.236095000
C	-2.201852000	1.255010000	-0.336007000
C	-3.018530000	0.140604000	-0.122122000
C	-4.256028000	-0.052874000	-0.694052000
C	-4.778766000	0.900610000	-1.574859000
C	-3.990321000	2.023150000	-1.828956000
C	3.714188000	-1.024168000	-1.826829000
C	2.878941000	-0.032064000	-1.299658000
C	3.541665000	1.083127000	-0.773736000
C	4.924776000	1.189067000	-0.768340000
C	5.740786000	0.189535000	-1.305291000
C	5.101340000	-0.932023000	-1.835473000
C	1.428731000	-0.203313000	-1.409486000
C	0.495963000	0.848294000	-1.416876000
H	1.166934000	-1.100140000	-1.969181000
H	-0.385199000	0.745611000	-2.045884000
H	0.840234000	1.866592000	-1.301657000
C	-1.001491000	-0.481181000	3.662787000
H	-2.051493000	-0.686914000	3.441855000
H	-0.818251000	-0.784864000	4.701120000
H	-0.860773000	0.603636000	3.628205000
Si	-1.594794000	-3.746079000	2.880327000
C	-1.488756000	-5.489463000	2.137777000
H	-0.524050000	-5.968249000	2.331301000
H	-2.254862000	-6.094282000	2.638894000
H	-1.694676000	-5.542283000	1.063804000
C	-1.209037000	-3.916983000	4.727620000
H	-1.376736000	-2.990386000	5.284920000
H	-1.856323000	-4.686088000	5.165689000
H	-0.169726000	-4.225802000	4.885054000
C	-3.389636000	-3.162953000	2.670553000
H	-3.595162000	-2.211013000	3.168854000

H	-3.703118000	-3.070770000	1.625905000
H	-4.036657000	-3.915663000	3.137927000
F	-4.925161000	-1.175833000	-0.429680000
F	-4.389645000	2.979032000	-2.654601000
F	5.468210000	2.279432000	-0.234857000
F	5.776843000	-1.950475000	-2.355728000
F	-2.049860000	3.286117000	-1.564733000
F	-2.508152000	-0.848865000	0.682835000
F	3.156775000	-2.140256000	-2.332067000
F	2.837238000	2.089416000	-0.221859000
C	7.241448000	0.379228000	-1.259968000
C	-6.123347000	0.628779000	-2.215257000
F	7.660181000	0.464948000	0.013870000
F	7.587741000	1.516367000	-1.880773000
F	7.898549000	-0.626074000	-1.842479000
F	-7.060184000	0.448372000	-1.274796000
F	-6.056854000	-0.500214000	-2.947121000
F	-6.517622000	1.616413000	-3.016295000

TS1^a_{right-o}, $E_{(\text{SCF Done})} = -2255.81641$ a.u. **IF = *i*203.39 cm⁻¹**

Sc	-0.128671000	-0.229501000	-0.304821000
Si	-0.947851000	3.726052000	0.171534000
C	-0.519940000	1.855931000	0.193799000
C	-1.504579000	4.302315000	-1.544801000
C	0.576530000	4.713923000	0.712553000
C	-2.346242000	4.025257000	1.416615000
C	-0.856744000	-0.538981000	-3.845052000
C	-1.185912000	-0.992912000	-2.451713000
C	-2.194475000	-0.433424000	-1.622995000
C	-2.322685000	-1.242613000	-0.437312000
C	-1.378767000	-2.320981000	-0.580756000
C	-0.673502000	-2.158740000	-1.804113000
C	-3.055389000	0.725432000	-2.037702000
C	-1.258629000	-3.529548000	0.304975000
C	0.305094000	-3.135961000	-2.389792000
C	1.046808000	1.710713000	-1.539388000
C	1.695226000	0.491927000	-1.705751000
H	-1.489271000	1.318491000	0.357779000
H	0.118186000	1.700235000	1.085550000
H	-0.717483000	4.199331000	-2.299677000
H	-1.766649000	5.365980000	-1.495056000
H	-2.391166000	3.763216000	-1.894113000
H	0.925162000	4.406280000	1.705245000
H	0.314607000	5.776903000	0.773946000

H	1.416881000	4.629080000	0.014892000
H	-3.263139000	3.494450000	1.135728000
H	-2.587643000	5.093755000	1.465462000
H	-2.062933000	3.703699000	2.425423000
H	-0.815374000	0.551570000	-3.940035000
H	-1.626328000	-0.885617000	-4.547106000
H	0.095981000	-0.940538000	-4.204233000
H	-2.536726000	1.377660000	-2.746677000
H	-3.377350000	1.338477000	-1.193736000
H	-3.963668000	0.367673000	-2.540786000
H	-2.010479000	-4.278274000	0.024495000
H	-1.413806000	-3.301027000	1.363784000
H	-0.285755000	-4.020182000	0.200185000
H	0.981362000	-3.559977000	-1.639537000
H	0.920659000	-2.682616000	-3.172282000
H	-0.224487000	-3.979030000	-2.852944000
H	1.493036000	2.529801000	-0.994137000
H	0.301432000	1.993785000	-2.274738000
H	1.381832000	-0.086179000	-2.572944000
C	1.825003000	-2.100468000	1.548325000
O	0.898601000	-0.962606000	1.493399000
C	0.808031000	-0.341338000	2.821935000
C	1.460904000	-1.334898000	3.766844000
C	2.539115000	-1.962713000	2.881779000
H	1.224686000	-3.012307000	1.497772000
H	2.484823000	-2.034084000	0.681084000
H	1.357489000	0.603785000	2.777818000
H	-0.246959000	-0.154908000	3.028117000
H	1.867209000	-0.840125000	4.653125000
H	0.739025000	-2.090059000	4.097247000
H	3.401697000	-1.295306000	2.786429000
H	2.890703000	-2.929098000	3.253343000
C	3.715461000	0.541271000	-0.065371000
C	2.971082000	0.010080000	-1.139947000
C	3.542956000	-1.116916000	-1.775165000
C	4.757679000	-1.667368000	-1.390429000
C	5.467319000	-1.104300000	-0.330379000
C	4.940216000	0.002170000	0.327710000
H	3.012153000	-1.547865000	-2.619966000
H	5.155260000	-2.523981000	-1.926859000
H	5.480111000	0.467688000	1.146474000
Si	-3.705149000	-1.211864000	0.890427000
C	-4.689525000	-2.825905000	0.762291000
H	-4.101262000	-3.708261000	1.031888000

H	-5.549198000	-2.781679000	1.441468000
H	-5.074264000	-2.971574000	-0.253232000
C	-4.919870000	0.223154000	0.663140000
H	-5.412248000	0.207893000	-0.313791000
H	-5.702310000	0.119918000	1.425240000
H	-4.459728000	1.206658000	0.805869000
C	-2.981541000	-1.041405000	2.641915000
H	-3.783926000	-1.162716000	3.379560000
H	-2.214621000	-1.789577000	2.870185000
H	-2.555284000	-0.041875000	2.793254000
Cl	3.159861000	1.924195000	0.857766000
H	6.425669000	-1.511274000	-0.022222000

TS1^a_{left-m}, $E_{(\text{SCF Done})} = -2255.815037$ a.u. **IF** = $i427.99$ cm⁻¹

Sc	-0.219093000	-0.301788000	-0.190110000
Si	-1.687474000	3.681573000	-0.197447000
C	-1.185996000	1.859037000	-0.085083000
C	-2.131349000	4.159681000	-1.982426000
C	-0.294226000	4.810174000	0.441099000
C	-3.217474000	3.988153000	0.891748000
C	0.245681000	-2.270543000	-3.209182000
C	-0.523197000	-2.121837000	-1.929067000
C	-1.760385000	-1.452034000	-1.757216000
C	-2.215979000	-1.652742000	-0.402693000
C	-1.210538000	-2.471418000	0.239298000
C	-0.170114000	-2.741816000	-0.695018000
C	-2.481562000	-0.716798000	-2.853829000
C	-1.290076000	-3.083718000	1.611249000
C	0.990938000	-3.673890000	-0.495770000
C	0.296075000	1.753477000	-1.562197000
C	1.309359000	0.744951000	-1.621405000
H	-2.102387000	1.269615000	-0.254550000
H	-0.872621000	1.703770000	0.968828000
H	-1.261711000	4.124914000	-2.647041000
H	-2.534406000	5.178964000	-2.014056000
H	-2.896079000	3.488969000	-2.392140000
H	-0.012425000	4.544639000	1.467486000
H	-0.630489000	5.853950000	0.452387000
H	0.608283000	4.763556000	-0.178506000
H	-4.066991000	3.376119000	0.567043000
H	-3.525807000	5.040028000	0.842751000
H	-3.016077000	3.748684000	1.942705000
H	0.076524000	-1.437236000	-3.899754000
H	-0.047654000	-3.187487000	-3.739838000

H	1.325106000	-2.336766000	-3.031658000
H	-1.796740000	-0.426936000	-3.658029000
H	-2.970882000	0.194568000	-2.498126000
H	-3.260762000	-1.341766000	-3.312362000
H	-1.707716000	-4.100606000	1.575438000
H	-1.924114000	-2.504854000	2.289594000
H	-0.302983000	-3.168870000	2.081825000
H	1.250734000	-3.787383000	0.562345000
H	1.891362000	-3.332480000	-1.018361000
H	0.761601000	-4.682314000	-0.871893000
H	0.619534000	2.754108000	-1.286955000
H	-0.408350000	1.764729000	-2.391280000
H	1.251251000	0.031292000	-2.440107000
C	2.118394000	-0.942345000	2.060725000
O	0.827959000	-0.310410000	1.824420000
C	0.269350000	0.161541000	3.075347000
C	1.150766000	-0.432118000	4.166562000
C	2.509656000	-0.520153000	3.467701000
H	1.979715000	-2.026258000	1.983130000
H	2.801113000	-0.604108000	1.280967000
H	0.310841000	1.257447000	3.073959000
H	-0.775243000	-0.157376000	3.129695000
H	1.162437000	0.189068000	5.067037000
H	0.795712000	-1.431193000	4.445040000
H	3.000620000	0.459054000	3.444925000
H	3.190834000	-1.235385000	3.937799000
C	2.874287000	1.853259000	0.018283000
C	2.592469000	0.861378000	-0.954415000
C	3.645378000	-0.033879000	-1.269727000
C	4.875138000	0.064680000	-0.640010000
C	5.146237000	1.038851000	0.325120000
C	4.120506000	1.932363000	0.633485000
H	2.106749000	2.572659000	0.290358000
H	3.488936000	-0.801069000	-2.022904000
Si	-3.923843000	-1.314794000	0.331087000
C	-4.820894000	-2.970198000	0.608161000
H	-4.271524000	-3.619611000	1.298296000
H	-5.822121000	-2.806200000	1.025435000
H	-4.932431000	-3.510206000	-0.339071000
C	-5.043722000	-0.253427000	-0.779968000
H	-5.210580000	-0.705242000	-1.762640000
H	-6.020103000	-0.156397000	-0.288590000
H	-4.651954000	0.758692000	-0.930511000
C	-3.854004000	-0.398648000	2.004699000

H	-4.875426000	-0.214230000	2.361086000
H	-3.337863000	-0.967516000	2.785868000
H	-3.359702000	0.574684000	1.903564000
H	6.120309000	1.097898000	0.797810000
H	4.302925000	2.714886000	1.367665000
Cl	6.142233000	-1.069810000	-1.074795000

pC3^a_{syn}, $E_{(\text{SCF Done})} = -3794.045039$ a.u.

Sc	0.958573000	-0.991181000	-0.540093000
Si	-4.700171000	4.983615000	-0.014193000
C	-4.093376000	3.177425000	-0.212252000
C	-3.334285000	6.033255000	0.788014000
C	-6.261768000	5.033750000	1.059370000
C	-5.083090000	5.660971000	-1.744012000
C	-1.517913000	-1.249199000	-3.102494000
C	-0.307394000	-1.894687000	-2.495168000
C	-0.303312000	-2.902487000	-1.495730000
C	1.053957000	-3.333551000	-1.272917000
C	1.868037000	-2.602882000	-2.209767000
C	1.037560000	-1.713925000	-2.943178000
C	-1.554283000	-3.500586000	-0.915472000
C	3.290117000	-2.911744000	-2.587593000
C	1.443409000	-0.931765000	-4.159415000
C	-3.730925000	2.464144000	1.093293000
C	-3.134048000	1.034902000	0.987016000
H	-3.230860000	3.203356000	-0.895245000
H	-4.885906000	2.627969000	-0.737645000
H	-3.086945000	5.679123000	1.795567000
H	-3.655552000	7.077464000	0.877649000
H	-2.416393000	6.020900000	0.187866000
H	-7.055282000	4.407789000	0.635040000
H	-6.648355000	6.057038000	1.130322000
H	-6.065988000	4.683608000	2.079112000
H	-4.196091000	5.641054000	-2.388135000
H	-5.429624000	6.699347000	-1.688184000
H	-5.868650000	5.075394000	-2.235501000
H	-2.326248000	-1.114358000	-2.378583000
H	-1.914566000	-1.869299000	-3.917859000
H	-1.292219000	-0.268512000	-3.536205000
H	-2.419131000	-2.843500000	-1.042401000
H	-1.475500000	-3.742726000	0.147270000
H	-1.792411000	-4.437424000	-1.436263000
H	3.300379000	-3.616476000	-3.429699000
H	3.850689000	-3.379429000	-1.775948000

H	3.846146000	-2.028033000	-2.917099000
H	2.512368000	-0.697149000	-4.167771000
H	0.885729000	0.004301000	-4.272633000
H	1.245552000	-1.521064000	-5.065016000
H	-4.620893000	2.404652000	1.733264000
H	-3.001021000	3.070896000	1.650595000
H	-2.901761000	0.740659000	2.020530000
C	3.108215000	0.233734000	1.580540000
O	2.929923000	-0.509337000	0.329228000
C	4.235313000	-0.687807000	-0.310644000
C	5.223799000	0.110206000	0.526847000
C	4.579883000	0.086929000	1.913206000
H	2.835159000	1.276713000	1.389654000
H	2.437735000	-0.202210000	2.317349000
H	4.454170000	-1.756920000	-0.299750000
H	4.154463000	-0.337600000	-1.341741000
H	6.220324000	-0.339617000	0.507594000
H	5.303744000	1.137390000	0.156762000
H	4.765739000	-0.867110000	2.418890000
H	4.931987000	0.892762000	2.562856000
C	-4.496331000	-0.077437000	-0.877556000
C	-4.126818000	0.009041000	0.472863000
C	-4.731742000	-0.884963000	1.365610000
C	-5.664264000	-1.830072000	0.942983000
C	-6.006579000	-1.890444000	-0.405574000
C	-5.427877000	-1.014657000	-1.321822000
H	-4.062206000	0.602654000	-1.605309000
H	-4.472056000	-0.841951000	2.421419000
H	-6.122105000	-2.512921000	1.651689000
H	-5.709539000	-1.062166000	-2.369211000
C	0.180414000	-1.803723000	1.963228000
C	-0.372927000	-0.521995000	1.704880000
C	-0.188160000	0.453226000	2.722324000
C	0.435077000	0.148807000	3.921298000
C	0.957035000	-1.135067000	4.143181000
C	0.836863000	-2.110378000	3.162424000
H	-0.031027000	-2.624833000	1.276931000
H	-0.596643000	1.450537000	2.589903000
H	0.516582000	0.900096000	4.701528000
H	1.212811000	-3.112829000	3.342472000
C	-0.987269000	-0.263819000	0.402325000
C	-1.791834000	1.014978000	0.215112000
H	-1.584249000	-1.130565000	0.096956000
H	-1.211562000	1.891839000	0.540322000

H	-1.980587000	1.177342000	-0.853658000
Si	1.660188000	-4.883353000	-0.318407000
C	0.341946000	-5.620220000	0.828672000
H	-0.000077000	-4.940438000	1.616559000
H	-0.534865000	-5.978890000	0.281523000
H	0.790725000	-6.488641000	1.326937000
C	3.181032000	-4.503774000	0.760772000
H	4.078243000	-4.269278000	0.178402000
H	2.997451000	-3.677536000	1.457035000
H	3.415513000	-5.391976000	1.360143000
C	2.106291000	-6.204489000	-1.601860000
H	2.932187000	-5.896842000	-2.251125000
H	2.406814000	-7.130523000	-1.097423000
H	1.245215000	-6.435661000	-2.238831000
Cl	1.738009000	-1.500749000	5.651589000
Cl	-7.164351000	-3.071001000	-0.953546000
C	5.152198000	4.490594000	-0.675268000
C	5.398593000	3.681384000	-1.784914000
C	4.407034000	2.809360000	-2.219335000
C	3.167676000	2.721534000	-1.561426000
C	2.942828000	3.561844000	-0.454811000
C	3.922184000	4.437455000	-0.010288000
H	6.349862000	3.744518000	-2.303032000
H	4.595120000	2.190123000	-3.093801000
H	1.982568000	3.552646000	0.053371000
H	3.738908000	5.090621000	0.836713000
C	2.165009000	1.794499000	-2.077691000
C	0.950288000	1.510508000	-1.554360000
H	2.440395000	1.306609000	-3.011709000
H	0.228199000	0.930031000	-2.130143000
H	0.567899000	2.008536000	-0.668545000
Cl	6.374142000	5.582521000	-0.121086000

***p*TS3^a_{syn}, $E_{(\text{SCF Done})} = -3794.031718$ a.u. **IF** = *i* -184.66 cm⁻¹**

Sc	1.368475000	-0.516021000	-0.628902000
Si	-6.244478000	3.777922000	-0.174975000
C	-5.001039000	2.337434000	-0.414348000
C	-5.323936000	5.293797000	0.505127000
C	-7.613683000	3.260728000	1.030151000
C	-6.989000000	4.188952000	-1.869025000
C	-0.826309000	-1.490266000	-3.306907000
C	0.351199000	-1.891796000	-2.466661000
C	0.303668000	-2.680076000	-1.283080000
C	1.647738000	-2.973025000	-0.863760000

C	2. 513623000	-2. 385931000	-1. 852977000
C	1. 721030000	-1. 719634000	-2. 824809000
C	-0. 968896000	-3. 259668000	-0. 729900000
C	3. 971979000	-2. 685515000	-2. 064010000
C	2. 230474000	-1. 182740000	-4. 130726000
C	-4. 321851000	1. 855220000	0. 869519000
C	-3. 242199000	0. 745122000	0. 736727000
H	-4. 256066000	2. 681508000	-1. 147341000
H	-5. 545820000	1. 511463000	-0. 890827000
H	-4. 886653000	5. 098203000	1. 491250000
H	-6. 008707000	6. 142864000	0. 613458000
H	-4. 516930000	5. 605417000	-0. 168732000
H	-8. 144532000	2. 370660000	0. 672977000
H	-8. 350681000	4. 064809000	1. 138676000
H	-7. 217962000	3. 039858000	2. 028092000
H	-6. 214435000	4. 486249000	-2. 585680000
H	-7. 703119000	5. 016679000	-1. 790090000
H	-7. 523422000	3. 328702000	-2. 288458000
H	-1. 711194000	-1. 255195000	-2. 706662000
H	-1. 111360000	-2. 309832000	-3. 980178000
H	-0. 606811000	-0. 624677000	-3. 940557000
H	-1. 848076000	-2. 665004000	-0. 993892000
H	-0. 965574000	-3. 379711000	0. 355398000
H	-1. 130451000	-4. 259725000	-1. 154075000
H	4. 069564000	-3. 497726000	-2. 796926000
H	4. 473933000	-3. 019619000	-1. 153958000
H	4. 529937000	-1. 834979000	-2. 468431000
H	3. 198193000	-0. 678791000	-4. 032733000
H	1. 531978000	-0. 483369000	-4. 601194000
H	2. 374542000	-2. 006676000	-4. 842723000
H	-5. 084590000	1. 484375000	1. 565948000
H	-3. 842136000	2. 706852000	1. 374138000
H	-2. 860090000	0. 592080000	1. 755983000
C	3. 328668000	0. 773081000	1. 682039000
O	3. 227662000	0. 018635000	0. 427914000
C	4. 566114000	-0. 104287000	-0. 160001000
C	5. 460019000	0. 811808000	0. 656803000
C	4. 803407000	0. 759404000	2. 035379000
H	2. 969933000	1. 786826000	1. 485202000
H	2. 690576000	0. 277699000	2. 410345000
H	4. 857482000	-1. 151038000	-0. 068850000
H	4. 497884000	0. 179397000	-1. 211546000
H	6. 496518000	0. 463098000	0. 659111000
H	5. 437792000	1. 829426000	0. 254423000

H	5.068118000	-0.164419000	2.561816000
H	5.072740000	1.606660000	2.671910000
C	-4.163343000	-0.851025000	-1.045257000
C	-3.822673000	-0.583350000	0.288916000
C	-4.085707000	-1.581323000	1.236435000
C	-4.660582000	-2.799600000	0.880987000
C	-4.983798000	-3.035177000	-0.453626000
C	-4.739970000	-2.063393000	-1.422122000
H	-3.996413000	-0.100701000	-1.813453000
H	-3.844313000	-1.401133000	2.282140000
H	-4.860653000	-3.558565000	1.630826000
H	-5.006970000	-2.251095000	-2.457514000
C	0.214256000	-0.957478000	1.893454000
C	-0.217209000	0.279683000	1.361835000
C	-0.095593000	1.415350000	2.205057000
C	0.364246000	1.306546000	3.504870000
C	0.766676000	0.057512000	4.007144000
C	0.709617000	-1.070371000	3.199645000
H	0.029516000	-1.873323000	1.337019000
H	-0.420432000	2.388449000	1.848348000
H	0.407903000	2.180587000	4.147632000
H	0.998949000	-2.038907000	3.594945000
C	-0.799112000	0.353865000	0.010118000
C	-2.049855000	1.219766000	-0.121666000
H	-1.025030000	-0.657490000	-0.360928000
H	-1.824558000	2.254802000	0.170153000
H	-2.350507000	1.273137000	-1.173471000
Si	2.237583000	-4.259409000	0.429499000
C	0.851608000	-4.892528000	1.561129000
H	0.365029000	-4.116666000	2.162134000
H	0.077317000	-5.433717000	1.008875000
H	1.304942000	-5.604343000	2.262304000
C	3.593859000	-3.550319000	1.558582000
H	4.528020000	-3.340253000	1.027252000
H	3.269672000	-2.629723000	2.056445000
H	3.828813000	-4.284747000	2.338536000
C	2.911490000	-5.757569000	-0.515293000
H	3.781771000	-5.511799000	-1.131728000
H	3.214760000	-6.538630000	0.192049000
H	2.142970000	-6.182018000	-1.170985000
Cl	1.322306000	-0.067961000	5.643515000
Cl	-5.695845000	-4.554579000	-0.916413000
C	4.488062000	4.382531000	-1.026245000
C	4.695226000	3.500636000	-2.087380000

C	3.736512000	2.533805000	-2.370979000
C	2.553210000	2.417563000	-1.617669000
C	2.377527000	3.321097000	-0.553737000
C	3.325970000	4.296162000	-0.259675000
H	5.590623000	3.584594000	-2.695339000
H	3.891243000	1.878448000	-3.225902000
H	1.474669000	3.282431000	0.051210000
H	3.163255000	4.994881000	0.555218000
C	1.538537000	1.429693000	-2.021743000
C	0.189740000	1.513699000	-1.652527000
H	1.758304000	0.904176000	-2.946433000
H	-0.549105000	1.079738000	-2.318868000
H	-0.154430000	2.392461000	-1.117015000
Cl	5.676075000	5.596966000	-0.662855000

pP3^a_{syn}, $E_{(\text{SCF Done})} = -3794.072635$ a.u.

Sc	-1.898689000	0.305619000	-0.466607000
Si	7.575375000	-2.546530000	0.051279000
C	5.899225000	-1.687313000	-0.299175000
C	7.270294000	-4.208064000	0.917980000
C	8.653645000	-1.435875000	1.146997000
C	8.432390000	-2.842212000	-1.614131000
C	0.038577000	1.428952000	-3.297819000
C	-1.088980000	1.731131000	-2.355920000
C	-1.001192000	2.521434000	-1.176498000
C	-2.325235000	2.724709000	-0.646561000
C	-3.224343000	2.058696000	-1.550867000
C	-2.466603000	1.443250000	-2.586658000
C	0.270113000	3.192863000	-0.734505000
C	-4.723773000	2.157314000	-1.565135000
C	-3.027054000	0.781770000	-3.811495000
C	5.074669000	-1.343777000	0.943728000
C	3.709462000	-0.637932000	0.705509000
H	5.335382000	-2.350590000	-0.971150000
H	6.113204000	-0.775126000	-0.873023000
H	6.783475000	-4.077781000	1.891630000
H	8.218072000	-4.730427000	1.092142000
H	6.637917000	-4.864628000	0.308643000
H	8.812084000	-0.454192000	0.685588000
H	9.638298000	-1.891263000	1.304250000
H	8.203851000	-1.276392000	2.133712000
H	7.825792000	-3.480444000	-2.267283000
H	9.400612000	-3.336558000	-1.473783000
H	8.614975000	-1.898406000	-2.140901000

H	1. 000931000	1. 341399000	-2. 784813000
H	0. 141967000	2. 237782000	-4. 033846000
H	-0. 124616000	0. 505113000	-3. 861327000
H	1. 160282000	2. 593752000	-0. 951875000
H	0. 278987000	3. 438405000	0. 328945000
H	0. 396926000	4. 139041000	-1. 277212000
H	-5. 031662000	3. 034438000	-2. 149154000
H	-5. 152606000	2. 271082000	-0. 566035000
H	-5. 192116000	1. 291334000	-2. 043740000
H	-3. 940556000	0. 214047000	-3. 607697000
H	-2. 306929000	0. 103782000	-4. 278794000
H	-3. 284017000	1. 540296000	-4. 563276000
H	5. 665206000	-0. 697627000	1. 606241000
H	4. 869681000	-2. 258885000	1. 517881000
H	3. 274327000	-0. 499736000	1. 706742000
C	-3. 709680000	-0. 584124000	2. 127836000
O	-3. 635567000	-0. 414131000	0. 674414000
C	-4. 854313000	-0. 968119000	0. 059542000
C	-5. 569303000	-1. 705194000	1. 178988000
C	-5. 164917000	-0. 902996000	2. 415925000
H	-3. 046910000	-1. 411175000	2. 399786000
H	-3. 359099000	0. 338788000	2. 589802000
H	-5. 438144000	-0. 122632000	-0. 309803000
H	-4. 545897000	-1. 608347000	-0. 768278000
H	-6. 650373000	-1. 728841000	1. 016979000
H	-5. 210118000	-2. 736374000	1. 248293000
H	-5. 752618000	0. 018149000	2. 497209000
H	-5. 277407000	-1. 463078000	3. 348204000
C	4. 026785000	0. 981206000	-1. 259256000
C	3. 885999000	0. 750337000	0. 116745000
C	3. 967984000	1. 859073000	0. 969870000
C	4. 181320000	3. 147432000	0. 484529000
C	4. 313783000	3. 342153000	-0. 888726000
C	4. 239182000	2. 262788000	-1. 766509000
H	3. 983885000	0. 151165000	-1. 959362000
H	3. 874415000	1. 712877000	2. 044437000
H	4. 249012000	3. 992255000	1. 162840000
H	4. 356945000	2. 422513000	-2. 833893000
C	0. 068777000	0. 470362000	1. 422688000
C	0. 622750000	-0. 778924000	1. 094522000
C	0. 521903000	-1. 798010000	2. 056432000
C	-0. 071522000	-1. 574432000	3. 294742000
C	-0. 598790000	-0. 315355000	3. 599837000
C	-0. 535718000	0. 713221000	2. 666615000

H	0.248650000	1.317772000	0.760954000
H	0.944221000	-2.778175000	1.850940000
H	-0.115558000	-2.368377000	4.034416000
H	-0.906299000	1.702661000	2.916992000
C	1.307850000	-1.000568000	-0.237475000
C	2.745855000	-1.532726000	-0.088882000
H	1.367886000	-0.025249000	-0.741095000
H	2.721755000	-2.523566000	0.386738000
H	3.136199000	-1.708676000	-1.098391000
Si	-2.906177000	4.000452000	0.662267000
C	-1.486577000	4.850934000	1.588424000
H	-0.859013000	4.165297000	2.168896000
H	-0.839286000	5.433683000	0.926106000
H	-1.937606000	5.552641000	2.301214000
C	-4.009770000	3.212844000	1.996814000
H	-4.828995000	2.608430000	1.594729000
H	-3.423389000	2.588477000	2.680961000
H	-4.458502000	4.010475000	2.601139000
C	-3.877829000	5.348070000	-0.247694000
H	-4.812700000	4.978516000	-0.680080000
H	-4.132518000	6.153040000	0.451900000
H	-3.279829000	5.784434000	-1.055483000
Cl	-1.329470000	-0.036735000	5.149183000
Cl	4.571353000	4.947773000	-1.513960000
C	-4.047491000	-4.442239000	-1.360971000
C	-3.898411000	-3.654592000	-2.501241000
C	-2.892191000	-2.691547000	-2.543601000
C	-2.009766000	-2.474029000	-1.464031000
C	-2.199873000	-3.290900000	-0.327651000
C	-3.190979000	-4.265381000	-0.273041000
H	-4.546451000	-3.812144000	-3.358121000
H	-2.759353000	-2.121686000	-3.459486000
H	-1.539221000	-3.178037000	0.529529000
H	-3.295490000	-4.897655000	0.603941000
C	-0.938266000	-1.436852000	-1.531175000
C	0.463599000	-1.942782000	-1.118289000
H	-0.884795000	-1.085559000	-2.567795000
H	1.048660000	-2.163183000	-2.022324000
H	0.371682000	-2.903682000	-0.595099000
Cl	-5.291559000	-5.655777000	-1.295656000

$pP3^a_{iso}, E_{(SCF Done)} = -3794.043522$ a.u.

Sc	1.517988000	-0.114324000	-0.013601000
Si	-6.554863000	1.048942000	1.457360000

C	-5.035186000	0.228741000	0.628321000
C	-5.999615000	1.997088000	3.007380000
C	-7.827503000	-0.271207000	1.939662000
C	-7.320478000	2.255667000	0.210113000
C	-0.483637000	0.091715000	-2.959526000
C	0.909122000	0.037853000	-2.409515000
C	1.701434000	-1.129170000	-2.252736000
C	3.033598000	-0.746376000	-1.850627000
C	3.028809000	0.689703000	-1.764664000
C	1.729758000	1.163955000	-2.106138000
C	1.229106000	-2.507664000	-2.623503000
C	4.186698000	1.608088000	-1.485423000
C	1.343897000	2.595529000	-2.325976000
C	-4.297321000	-0.793059000	1.497891000
C	-3.017262000	-1.443444000	0.908460000
H	-4.360180000	1.042236000	0.321618000
H	-5.386338000	-0.245664000	-0.297938000
H	-5.554889000	1.328318000	3.753717000
H	-6.854557000	2.493702000	3.480626000
H	-5.261799000	2.771126000	2.764000000
H	-8.139294000	-0.862015000	1.070580000
H	-8.724803000	0.195942000	2.362069000
H	-7.431317000	-0.962166000	2.692291000
H	-6.608634000	3.035562000	-0.085188000
H	-8.198851000	2.753226000	0.637107000
H	-7.643943000	1.733856000	-0.698004000
H	-1.063463000	-0.801805000	-2.712002000
H	-0.456500000	0.165434000	-4.055454000
H	-1.038394000	0.962788000	-2.595783000
H	0.208909000	-2.711336000	-2.278968000
H	1.877298000	-3.294814000	-2.229633000
H	1.214711000	-2.621264000	-3.715238000
H	4.633221000	1.964436000	-2.423401000
H	4.984543000	1.126368000	-0.917808000
H	3.873215000	2.498930000	-0.929738000
H	1.924831000	3.288564000	-1.712700000
H	0.285501000	2.779099000	-2.120519000
H	1.516601000	2.870740000	-3.375465000
H	-4.986849000	-1.605132000	1.763481000
H	-4.007768000	-0.322632000	2.449500000
H	-2.637174000	-2.105167000	1.700564000
C	2.850343000	0.802133000	2.936005000
O	3.031219000	0.201052000	1.611725000
C	4.315923000	-0.497389000	1.583650000

C	5. 124480000	0. 129594000	2. 701526000
C	4. 049092000	0. 360517000	3. 764660000
H	2. 832693000	1. 885613000	2. 794887000
H	1. 895356000	0. 457400000	3. 337733000
H	4. 121766000	-1. 557758000	1. 768643000
H	4. 731347000	-0. 367024000	0. 585488000
H	5. 927565000	-0. 528747000	3. 043602000
H	5. 569389000	1. 076936000	2. 375980000
H	3. 829458000	-0. 572105000	4. 294532000
H	4. 328550000	1. 116101000	4. 503889000
C	-3. 555458000	-1. 824465000	-1. 567392000
C	-3. 299258000	-2. 335099000	-0. 286576000
C	-3. 333014000	-3. 726315000	-0. 127793000
C	-3. 607398000	-4. 582343000	-1. 192346000
C	-3. 855623000	-4. 041902000	-2. 451583000
C	-3. 833371000	-2. 662473000	-2. 645983000
H	-3. 547183000	-0. 751486000	-1. 737548000
H	-3. 143546000	-4. 156125000	0. 853801000
H	-3. 629152000	-5. 657931000	-1. 047825000
C	1. 231439000	-2. 606762000	1. 065716000
C	0. 161253000	-1. 735407000	1. 409286000
C	-0. 026881000	-1. 493659000	2. 799480000
C	0. 756974000	-2. 111845000	3. 760852000
C	1. 794668000	-2. 974847000	3. 380006000
C	2. 028211000	-3. 228186000	2. 035493000
H	1. 349601000	-2. 916724000	0. 027618000
H	-0. 844768000	-0. 857014000	3. 125651000
H	2. 799209000	-3. 933048000	1. 739387000
C	-0. 543197000	-1. 026591000	0. 350491000
C	-1. 900570000	-0. 405536000	0. 638575000
H	-0. 584698000	-1. 639122000	-0. 556969000
H	-1. 854837000	0. 265323000	1. 508774000
H	-2. 189887000	0. 233032000	-0. 205728000
Si	4. 542652000	-1. 911924000	-2. 087891000
C	4. 529159000	-3. 428084000	-0. 942332000
H	4. 664935000	-3. 154005000	0. 109207000
H	3. 617071000	-4. 028188000	-1. 026260000
H	5. 367964000	-4. 079176000	-1. 217459000
C	6. 213735000	-1. 042239000	-1. 850348000
H	6. 328539000	-0. 177486000	-2. 511289000
H	6. 429404000	-0. 723861000	-0. 824927000
H	6. 990907000	-1. 765997000	-2. 126419000
C	4. 495682000	-2. 490420000	-3. 892015000
H	4. 475542000	-1. 633858000	-4. 575015000

H	5.396801000	-3.074237000	-4.114485000
H	3.629589000	-3.120521000	-4.114946000
C	0.113646000	6.977005000	-0.825011000
C	1.298705000	6.796861000	-0.110625000
C	1.515413000	5.591506000	0.544445000
C	0.575778000	4.547416000	0.484781000
C	-0.617647000	4.764814000	-0.228342000
C	-0.851481000	5.966136000	-0.879747000
H	2.031821000	7.595292000	-0.064304000
H	2.434353000	5.455626000	1.110547000
H	-1.386668000	3.997846000	-0.249985000
C	0.855869000	3.305734000	1.194097000
C	0.220598000	2.116291000	1.075874000
H	1.660467000	3.383771000	1.925303000
H	0.373543000	1.348532000	1.835816000
H	-0.626877000	1.972641000	0.411434000
H	-1.778110000	6.133791000	-1.418876000
H	0.560034000	-1.945550000	4.816305000
H	-4.037024000	-2.250454000	-3.629575000
Cl	-0.176443000	8.476485000	-1.638304000
Cl	2.770731000	-3.742001000	4.598638000
Cl	-4.192800000	-5.097241000	-3.796030000

***p*TS3^a_{iso}, $E_{(\text{SCF Done})} = -3794.025882$ a.u. $\text{IF} = i242.26$ cm⁻¹**

Sc	-1.597844000	0.407873000	-0.271410000
Si	7.009731000	-0.068319000	-1.448541000
C	5.244027000	-0.129091000	-0.702908000
C	6.903029000	0.123168000	-3.334414000
C	7.938428000	-1.663105000	-1.013947000
C	7.902271000	1.428563000	-0.702355000
C	0.112028000	1.560699000	2.638370000
C	-1.195990000	1.073520000	2.087656000
C	-1.657748000	-0.269023000	2.104119000
C	-3.022263000	-0.304585000	1.636840000
C	-3.371255000	1.057638000	1.328259000
C	-2.263514000	1.900219000	1.626813000
C	-0.881379000	-1.406580000	2.710405000
C	-4.708613000	1.609321000	0.917349000
C	-2.337348000	3.389346000	1.765783000
C	4.383289000	-1.297380000	-1.189322000
C	2.940405000	-1.411185000	-0.622040000
H	4.761782000	0.833486000	-0.929065000
H	5.360249000	-0.170363000	0.388544000
H	6.406395000	-0.733465000	-3.804696000

H	7. 906826000	0. 197799000	-3. 768467000
H	6. 354227000	1. 030030000	-3. 615070000
H	7. 985596000	-1. 813943000	0. 070796000
H	8. 967866000	-1. 621817000	-1. 388177000
H	7. 463056000	-2. 545870000	-1. 456921000
H	7. 380263000	2. 364015000	-0. 935461000
H	8. 921351000	1. 510821000	-1. 097474000
H	7. 975794000	1. 346286000	0. 388255000
H	0. 904965000	0. 811706000	2. 547930000
H	0. 009966000	1. 786407000	3. 708903000
H	0. 446198000	2. 479421000	2. 148129000
H	0. 164312000	-1. 439546000	2. 384579000
H	-1. 328339000	-2. 379994000	2. 492165000
H	-0. 858843000	-1. 304426000	3. 803021000
H	-5. 248054000	1. 999368000	1. 791108000
H	-5. 356152000	0. 864323000	0. 453061000
H	-4. 603240000	2. 446347000	0. 218257000
H	-2. 958686000	3. 858678000	0. 999514000
H	-1. 356103000	3. 866057000	1. 733655000
H	-2. 787878000	3. 630663000	2. 738935000
H	4. 891799000	-2. 244130000	-0. 965355000
H	4. 293187000	-1. 255991000	-2. 284646000
H	2. 491803000	-2. 268773000	-1. 143369000
C	-3. 052328000	0. 437227000	-3. 277540000
O	-3. 103476000	0. 004709000	-1. 875403000
C	-4. 224328000	-0. 924566000	-1. 712832000
C	-5. 140498000	-0. 636188000	-2. 884709000
C	-4. 131517000	-0. 356981000	-3. 999236000
H	-3. 258832000	1. 511144000	-3. 296235000
H	-2. 046753000	0. 245382000	-3. 656550000
H	-3. 822926000	-1. 941040000	-1. 751790000
H	-4. 655719000	-0. 737033000	-0. 731772000
H	-5. 798656000	-1. 480686000	-3. 106161000
H	-5. 762014000	0. 244333000	-2. 686008000
H	-3. 724795000	-1. 295213000	-4. 391181000
H	-4. 554219000	0. 207606000	-4. 834582000
C	3. 164112000	-0. 792637000	1. 855311000
C	2. 921395000	-1. 747755000	0. 857174000
C	2. 710070000	-3. 071378000	1. 265946000
C	2. 738595000	-3. 439395000	2. 609414000
C	2. 983982000	-2. 466340000	3. 576044000
C	3. 199358000	-1. 140532000	3. 205249000
H	3. 348403000	0. 243976000	1. 586183000
H	2. 529573000	-3. 838984000	0. 516080000

H	2.578488000	-4.471463000	2.905196000
C	-0.951961000	-2.358008000	-0.811500000
C	-0.055921000	-1.488240000	-1.467700000
C	0.159323000	-1.708115000	-2.852793000
C	-0.482911000	-2.727491000	-3.534553000
C	-1.378656000	-3.564908000	-2.854270000
C	-1.608790000	-3.387724000	-1.497408000
H	-1.055643000	-2.312950000	0.269963000
H	0.875128000	-1.094614000	-3.392874000
H	-2.258740000	-4.071998000	-0.962857000
C	0.590560000	-0.368513000	-0.760317000
C	2.086982000	-0.179357000	-0.991047000
H	0.420825000	-0.444229000	0.333849000
H	2.277494000	0.047713000	-2.049259000
H	2.427837000	0.699985000	-0.431596000
Si	-4.234400000	-1.705245000	2.150218000
C	-3.862667000	-3.403467000	1.384686000
H	-4.084168000	-3.421299000	0.312498000
H	-2.832494000	-3.742674000	1.534661000
H	-4.517069000	-4.143166000	1.861728000
C	-6.054203000	-1.328759000	1.761299000
H	-6.400385000	-0.404551000	2.233729000
H	-6.301610000	-1.285957000	0.695204000
H	-6.643084000	-2.150185000	2.188825000
C	-4.104718000	-1.831494000	4.037093000
H	-4.295528000	-0.860139000	4.506832000
H	-4.855530000	-2.537331000	4.411839000
H	-3.123928000	-2.181709000	4.372580000
C	0.051834000	6.315366000	-0.001973000
C	-1.157321000	6.091802000	-0.658442000
C	-1.472424000	4.808680000	-1.091690000
C	-0.602581000	3.725415000	-0.886551000
C	0.612660000	3.984902000	-0.232107000
C	0.942024000	5.262876000	0.209186000
H	-1.840369000	6.916909000	-0.833596000
H	-2.412062000	4.649786000	-1.617431000
H	1.321881000	3.179554000	-0.056990000
C	-0.953392000	2.403530000	-1.436355000
C	0.028555000	1.493540000	-1.859310000
H	-1.909309000	2.384707000	-1.964723000
H	-0.170680000	0.860948000	-2.722441000
H	1.065029000	1.799568000	-1.774432000
H	1.885750000	5.445619000	0.713520000
H	-0.283925000	-2.895718000	-4.588710000

H	3.401250000	-0.391266000	3.964445000
Cl	0.456483000	7.912975000	0.548893000
Cl	-2.172375000	-4.848033000	-3.711891000
Cl	3.020170000	-2.908078000	5.259070000

pP3^a, $E_{(\text{SCF Done})} = -3794.074747$ a.u.

Sc	1.929418000	-0.049731000	0.075914000
Si	-7.623035000	1.784183000	0.905251000
C	-5.852537000	1.349445000	0.314400000
C	-7.534569000	2.669082000	2.582544000
C	-8.649865000	0.197315000	1.064509000
C	-8.404079000	2.931887000	-0.385829000
C	0.575903000	0.709800000	-3.126356000
C	1.580489000	-0.099781000	-2.363347000
C	1.386038000	-1.422524000	-1.871416000
C	2.636007000	-1.921702000	-1.352547000
C	3.589059000	-0.858929000	-1.520721000
C	2.943930000	0.248926000	-2.144753000
C	0.116755000	-2.206139000	-2.067576000
C	5.066905000	-0.878794000	-1.242176000
C	3.638130000	1.486052000	-2.631479000
C	-5.084078000	0.402688000	1.239667000
C	-3.649493000	-0.001448000	0.797896000
H	-5.310815000	2.298184000	0.188283000
H	-5.942874000	0.908641000	-0.688109000
H	-7.101503000	2.028198000	3.359442000
H	-8.536827000	2.959891000	2.917831000
H	-6.929094000	3.581015000	2.519929000
H	-8.674802000	-0.354935000	0.117878000
H	-9.684587000	0.433825000	1.338327000
H	-8.250551000	-0.471836000	1.835243000
H	-7.822895000	3.853603000	-0.506104000
H	-9.420489000	3.216704000	-0.090541000
H	-8.467484000	2.443986000	-1.365393000
H	-0.453155000	0.452517000	-2.857552000
H	0.679836000	0.520638000	-4.203468000
H	0.712726000	1.783015000	-2.971770000
H	-0.785532000	-1.607960000	-1.898807000
H	0.061240000	-3.082867000	-1.416641000
H	0.051305000	-2.570495000	-3.100800000
H	5.620284000	-1.207588000	-2.131996000
H	5.343223000	-1.554435000	-0.430457000
H	5.443408000	0.119904000	-0.995904000
H	4.293759000	1.933688000	-1.877350000

H	2.930059000	2.257761000	-2.936754000
H	4.263205000	1.242689000	-3.501020000
H	-5.656495000	-0.524940000	1.371101000
H	-5.000158000	0.850010000	2.240545000
H	-3.271727000	-0.651631000	1.601430000
C	3.846079000	0.696949000	2.667900000
O	3.292971000	-0.332889000	1.777024000
C	3.827274000	-1.640932000	2.170060000
C	5.044443000	-1.326922000	3.017524000
C	4.593813000	-0.062771000	3.752146000
H	4.518922000	1.314631000	2.066986000
H	3.014495000	1.300886000	3.036993000
H	3.053851000	-2.154155000	2.748186000
H	4.030931000	-2.193338000	1.253277000
H	5.291241000	-2.149190000	3.694384000
H	5.917328000	-1.123951000	2.386913000
H	3.924897000	-0.317417000	4.581002000
H	5.426108000	0.523163000	4.151148000
C	-3.678714000	-0.287206000	-1.752614000
C	-3.663920000	-0.843400000	-0.465395000
C	-3.720430000	-2.240128000	-0.364006000
C	-3.791206000	-3.057744000	-1.489665000
C	-3.801228000	-2.472572000	-2.754397000
C	-3.746330000	-1.087404000	-2.892866000
H	-3.651756000	0.791490000	-1.882127000
H	-3.724480000	-2.702901000	0.621287000
H	-3.843885000	-4.137449000	-1.389568000
C	-0.200142000	-1.237805000	1.454475000
C	-0.645711000	0.079962000	1.655687000
C	-0.542037000	0.611538000	2.953521000
C	-0.035833000	-0.140343000	4.006869000
C	0.389940000	-1.453714000	3.780036000
C	0.308129000	-2.011355000	2.509933000
H	-0.368013000	-1.716111000	0.488425000
H	-0.880248000	1.626304000	3.147576000
H	0.597424000	-3.043735000	2.344054000
C	-1.223232000	0.886190000	0.511621000
C	-2.714181000	1.214667000	0.726528000
H	-1.154894000	0.256380000	-0.388363000
H	-2.821380000	1.790214000	1.656674000
H	-3.025503000	1.894314000	-0.076121000
Si	2.990877000	-3.794219000	-1.127433000
C	1.975207000	-4.598817000	0.264863000
H	2.296222000	-4.257860000	1.255592000

H	0.897069000	-4.430960000	0.170654000
H	2.135042000	-5.683341000	0.232392000
C	4.816052000	-4.173841000	-0.769419000
H	5.479504000	-3.792740000	-1.551780000
H	5.181296000	-3.811879000	0.197768000
H	4.919953000	-5.266087000	-0.759929000
C	2.572781000	-4.633389000	-2.773182000
H	3.122076000	-4.166792000	-3.598443000
H	2.865637000	-5.689323000	-2.731419000
H	1.505869000	-4.594264000	-3.012229000
C	3.447501000	5.318747000	-1.230381000
C	3.894807000	4.583731000	-0.135137000
C	3.114684000	3.538443000	0.349332000
C	1.885547000	3.172508000	-0.233351000
C	1.456378000	3.961615000	-1.318452000
C	2.219270000	5.015342000	-1.814127000
H	4.832888000	4.843384000	0.346035000
H	3.457991000	3.014606000	1.237866000
H	0.498393000	3.768253000	-1.791322000
C	1.112292000	2.010422000	0.293759000
C	-0.412682000	2.171642000	0.243973000
H	1.393613000	1.906299000	1.370498000
H	-0.734633000	2.957825000	0.947115000
H	-0.720158000	2.525159000	-0.745640000
H	1.856813000	5.607264000	-2.649054000
H	0.019580000	0.278965000	5.007116000
H	-3.766626000	-0.640220000	-3.881937000
Cl	4.406275000	6.632135000	-1.847422000
Cl	1.016901000	-2.394932000	5.099595000
Cl	-3.880225000	-3.480308000	-4.172732000

$pC3^a_{syn}, E_{(SCF Done)} = -3794.039282 \text{ a.u.}$

Sc	-0.925813000	-1.327870000	0.586601000
Si	3.765987000	5.360876000	1.127889000
C	3.396553000	3.535560000	0.682591000
C	2.138341000	6.295513000	1.423901000
C	4.727789000	6.184628000	-0.283770000
C	4.806953000	5.379672000	2.713365000
C	0.132688000	-2.172882000	3.939492000
C	-0.905940000	-1.523222000	3.068526000
C	-2.114414000	-2.142707000	2.632975000
C	-2.920631000	-1.151361000	2.014298000
C	-2.230576000	0.112490000	2.071187000
C	-0.981038000	-0.137552000	2.738046000

C	-2. 534811000	-3. 548290000	2. 946181000
C	-4. 311001000	-1. 416280000	1. 508291000
C	2. 507113000	3. 340248000	-0. 548428000
C	2. 182222000	1. 879040000	-0. 964768000
H	2. 942242000	3. 068285000	1. 568953000
H	4. 364601000	3. 037806000	0. 534275000
H	1. 516012000	6. 321443000	0. 521916000
H	2. 338777000	7. 333316000	1. 714686000
H	1. 551666000	5. 835236000	2. 228060000
H	5. 670947000	5. 661220000	-0. 478936000
H	4. 970352000	7. 223456000	-0. 031495000
H	4. 151685000	6. 197626000	-1. 216098000
H	4. 274118000	4. 910271000	3. 548765000
H	5. 049701000	6. 406743000	3. 009316000
H	5. 751954000	4. 842269000	2. 572826000
H	0. 429307000	-3. 168398000	3. 590142000
H	-0. 257279000	-2. 295887000	4. 958637000
H	1. 039251000	-1. 567429000	4. 019728000
H	-1. 681256000	-4. 201272000	3. 151815000
H	-3. 128511000	-4. 004424000	2. 146991000
H	-3. 162777000	-3. 560364000	3. 847193000
H	-4. 423541000	-2. 447232000	1. 153251000
H	-4. 597058000	-0. 744966000	0. 697551000
H	-5. 047074000	-1. 284448000	2. 312574000
H	2. 970903000	3. 831060000	-1. 414300000
H	1. 546043000	3. 851403000	-0. 390623000
H	1. 506816000	1. 971707000	-1. 830229000
C	-0. 250827000	-4. 478994000	0. 450978000
O	-1. 132553000	-3. 449053000	-0. 113436000
C	-2. 171013000	-4. 087031000	-0. 914791000
C	-1. 753148000	-5. 544838000	-1. 041595000
C	-0. 994514000	-5. 788755000	0. 263637000
H	0. 684549000	-4. 443751000	-0. 109637000
H	-0. 063443000	-4. 217090000	1. 493822000
H	-3. 122746000	-3. 972529000	-0. 385127000
H	-2. 221731000	-3. 573525000	-1. 877252000
H	-2. 615872000	-6. 204397000	-1. 168282000
H	-1. 091520000	-5. 679726000	-1. 904093000
H	-1. 689350000	-5. 968652000	1. 090875000
H	-0. 306327000	-6. 636263000	0. 204466000
C	4. 349196000	0. 557134000	-0. 602476000
C	3. 408714000	1. 138645000	-1. 463793000
C	3. 656922000	1. 057729000	-2. 840002000
C	4. 787535000	0. 422776000	-3. 348765000

C	5. 698284000	-0. 149264000	-2. 464225000
C	5. 486259000	-0. 084070000	-1. 089095000
H	4. 198480000	0. 594076000	0. 472577000
H	2. 952004000	1. 508070000	-3. 536700000
H	4. 962646000	0. 372363000	-4. 418876000
H	6. 204540000	-0. 529929000	-0. 408289000
C	1. 935064000	-2. 254638000	-1. 282010000
C	1. 620497000	-1. 407045000	-0. 191788000
C	2. 120781000	-1. 796557000	1. 071796000
C	2. 938250000	-2. 916605000	1. 234911000
C	3. 261542000	-3. 693831000	0. 127104000
C	2. 754786000	-3. 365794000	-1. 136385000
H	1. 595632000	-1. 979931000	-2. 278339000
H	1. 932954000	-1. 160549000	1. 933348000
H	3. 340054000	-3. 169009000	2. 211543000
H	3. 029741000	-3. 965266000	-1. 999124000
C	0. 774076000	-0. 198813000	-0. 338423000
C	1. 375646000	1. 135876000	0. 123232000
H	0. 491825000	-0. 104397000	-1. 398594000
H	1. 996451000	0. 980370000	1. 013176000
H	0. 577232000	1. 817441000	0. 438245000
C	-0. 004165000	0. 894096000	3. 224055000
H	-0. 065080000	1. 821903000	2. 652699000
H	-0. 207908000	1. 138126000	4. 274921000
H	1. 033455000	0. 549116000	3. 175376000
Cl	4. 291064000	-5. 081336000	0. 309171000
Cl	7. 113248000	-0. 957826000	-3. 082672000
Si	-2. 991906000	1. 868324000	1. 884799000
C	-2. 052035000	2. 968973000	0. 657753000
H	-1. 964899000	2. 505715000	-0. 331240000
H	-2. 601996000	3. 910042000	0. 535379000
H	-1. 045754000	3. 224649000	1. 003450000
C	-4. 808647000	1. 829065000	1. 349039000
H	-5. 434547000	1. 246789000	2. 032466000
H	-5. 173043000	2. 863600000	1. 377871000
H	-4. 961164000	1. 458889000	0. 331257000
C	-2. 961026000	2. 672283000	3. 602821000
H	-3. 457452000	2. 034129000	4. 342578000
H	-1. 950530000	2. 886219000	3. 962972000
H	-3. 506708000	3. 622857000	3. 565250000
C	-6. 552697000	1. 917190000	-2. 614486000
C	-6. 853307000	0. 594450000	-2. 287780000
C	-5. 813490000	-0. 304430000	-2. 088072000
C	-4. 469305000	0. 094519000	-2. 196205000

C	-4.197477000	1.431969000	-2.539637000
C	-5.225358000	2.338903000	-2.746570000
H	-7.887250000	0.277868000	-2.200171000
H	-6.048860000	-1.338010000	-1.844291000
H	-3.172798000	1.766407000	-2.671156000
C	-3.423803000	-0.902076000	-2.000884000
C	-2.087290000	-0.701419000	-1.921956000
H	-3.791060000	-1.926996000	-1.948522000
H	-1.401990000	-1.545031000	-2.012856000
H	-1.644206000	0.285259000	-2.019174000
H	-5.010318000	3.366579000	-3.020152000
Cl	-7.835530000	3.047999000	-2.874371000

pTS3^a_{syn}, $E_{(\text{SCF Done})} = -3794.022319$ a.u. **IF** = $i209.22$ cm⁻¹

Sc	1.299848000	1.292100000	0.119207000
Si	-3.443334000	-4.308259000	2.230749000
C	-2.926832000	-2.659591000	1.397606000
C	-1.927222000	-5.411609000	2.522773000
C	-4.684159000	-5.206670000	1.113801000
C	-4.254054000	-3.882360000	3.890836000
C	1.366282000	2.934075000	3.397447000
C	1.944568000	1.893077000	2.483097000
C	3.117665000	2.044599000	1.693313000
C	3.477848000	0.765776000	1.181771000
C	2.538502000	-0.209828000	1.666116000
C	1.583407000	0.513599000	2.458688000
C	3.968451000	3.277198000	1.608746000
C	4.753716000	0.517974000	0.431876000
C	-2.221182000	-2.804509000	0.046407000
C	-2.004790000	-1.503815000	-0.772850000
H	-2.301280000	-2.102033000	2.110504000
H	-3.851631000	-2.078008000	1.279343000
H	-1.418116000	-5.663853000	1.585309000
H	-2.228951000	-6.353073000	2.996390000
H	-1.198477000	-4.928980000	3.184313000
H	-5.548948000	-4.572409000	0.887414000
H	-5.056647000	-6.112126000	1.606694000
H	-4.233065000	-5.513637000	0.163258000
H	-3.560077000	-3.350155000	4.552152000
H	-4.575021000	-4.791845000	4.411640000
H	-5.139052000	-3.250461000	3.752654000
H	1.294482000	3.926945000	2.940688000
H	2.000187000	3.039439000	4.288141000
H	0.370304000	2.658636000	3.755086000

H	3. 427623000	4. 178311000	1. 911984000
H	4. 378344000	3. 445991000	0. 607440000
H	4. 828339000	3. 183580000	2. 285511000
H	5. 016189000	1. 362884000	-0. 216044000
H	4. 701683000	-0. 379068000	-0. 184435000
H	5. 592266000	0. 392206000	1. 130275000
H	-2. 798323000	-3. 481202000	-0. 597277000
H	-1. 243554000	-3. 284366000	0. 188892000
H	-1. 483306000	-1. 811621000	-1. 692263000
C	1. 445486000	4. 520940000	-0. 326426000
O	1. 864023000	3. 237237000	-0. 897845000
C	2. 772627000	3. 486004000	-2. 016823000
C	2. 674660000	4. 976261000	-2. 298896000
C	2. 388668000	5. 555862000	-0. 913300000
H	0. 411860000	4. 690551000	-0. 631910000
H	1. 494883000	4. 430391000	0. 759074000
H	3. 780162000	3. 193584000	-1. 702335000
H	2. 459782000	2. 863177000	-2. 856906000
H	3. 592829000	5. 363729000	-2. 748623000
H	1. 845716000	5. 184243000	-2. 984522000
H	3. 308814000	5. 629534000	-0. 324049000
H	1. 927040000	6. 546374000	-0. 950435000
C	-4. 066907000	-0. 013361000	-0. 423263000
C	-3. 322975000	-0. 894349000	-1. 219424000
C	-3. 855426000	-1. 254183000	-2. 464173000
C	-5. 081689000	-0. 764633000	-2. 906376000
C	-5. 796946000	0. 109996000	-2. 091201000
C	-5. 294907000	0. 489816000	-0. 848477000
H	-3. 692688000	0. 295601000	0. 549038000
H	-3. 303870000	-1. 939693000	-3. 105132000
H	-5. 479256000	-1. 055569000	-3. 873450000
H	-5. 860704000	1. 170510000	-0. 220301000
C	-1. 721049000	3. 100210000	-1. 185979000
C	-1. 210750000	2. 076019000	-0. 341603000
C	-1. 059497000	2. 387850000	1. 026962000
C	-1. 446328000	3. 639290000	1. 539372000
C	-1. 975835000	4. 594410000	0. 689710000
C	-2. 118045000	4. 322755000	-0. 684554000
H	-1. 871750000	2. 886060000	-2. 241165000
H	-0. 813690000	1. 604794000	1. 741117000
H	-1. 375783000	3. 842147000	2. 602339000
H	-2. 561134000	5. 069622000	-1. 336447000
C	-0. 869146000	0. 771788000	-0. 909003000
C	-1. 072859000	-0. 490705000	-0. 062157000

H	-1.374909000	0.669498000	-1.864282000
H	-1.494196000	-0.235176000	0.917933000
H	-0.126984000	-1.023012000	0.155753000
C	0.512555000	-0.091348000	3.325758000
H	0.179537000	-1.061643000	2.951725000
H	0.891512000	-0.247393000	4.344006000
H	-0.373421000	0.545817000	3.428512000
Cl	-2.491153000	6.128161000	1.313390000
Cl	-7.326282000	0.739524000	-2.631673000
Si	2.886569000	-2.085863000	1.939641000
C	1.437012000	-3.230093000	1.516604000
H	1.236052000	-3.238006000	0.441411000
H	1.720786000	-4.250757000	1.801695000
H	0.510549000	-2.994074000	2.048256000
C	4.403496000	-2.730126000	1.015670000
H	5.321734000	-2.207854000	1.301177000
H	4.527806000	-3.783029000	1.298300000
H	4.298923000	-2.693604000	-0.071868000
C	3.265801000	-2.241721000	3.794124000
H	4.069845000	-1.559478000	4.092352000
H	2.396472000	-2.039746000	4.427273000
H	3.599878000	-3.263825000	4.009844000
C	3.605712000	-3.677938000	-2.862660000
C	4.447645000	-2.567900000	-2.898553000
C	3.955134000	-1.322464000	-2.520336000
C	2.625470000	-1.149045000	-2.098614000
C	1.804621000	-2.287271000	-2.075885000
C	2.280485000	-3.539179000	-2.453008000
H	5.474797000	-2.675441000	-3.232285000
H	4.613757000	-0.459883000	-2.590929000
H	0.767494000	-2.201894000	-1.763219000
C	2.117266000	0.215722000	-1.843275000
C	0.835479000	0.601942000	-2.278412000
H	2.899097000	0.978499000	-1.858562000
H	0.662881000	1.613237000	-2.642411000
H	0.248853000	-0.149050000	-2.797684000
H	1.627832000	-4.406208000	-2.430085000
Cl	4.205700000	-5.238055000	-3.336392000

$pP3$ '^a_{syn}, $E_{(SCF Done)} = -3794.071466$ a.u.

Sc	-2.539624000	-0.375222000	-0.137390000
Si	5.628187000	1.726921000	2.876252000
C	4.553062000	0.464036000	1.916775000
C	4.586149000	3.249462000	3.329108000

C	7.104512000	2.255868000	1.810434000
C	6.241583000	0.882588000	4.459546000
C	-5.610588000	-1.251420000	1.590785000
C	-4.786902000	-0.153132000	0.978022000
C	-4.900937000	0.346033000	-0.350320000
C	-4.062188000	1.496880000	-0.463564000
C	-3.406453000	1.718757000	0.795951000
C	-3.873529000	0.682114000	1.679828000
C	-5.869389000	-0.139075000	-1.390014000
C	-4.037559000	2.389546000	-1.670893000
C	3.961044000	0.981873000	0.603863000
C	3.136212000	-0.024092000	-0.247191000
H	3.758390000	0.130685000	2.600336000
H	5.185084000	-0.414404000	1.726273000
H	4.245615000	3.787061000	2.436672000
H	5.174700000	3.952119000	3.930344000
H	3.703207000	2.970606000	3.916530000
H	7.710521000	1.391263000	1.516114000
H	7.753750000	2.943473000	2.364759000
H	6.784795000	2.769984000	0.896739000
H	5.405848000	0.562018000	5.092546000
H	6.862109000	1.566308000	5.050259000
H	6.847942000	-0.001120000	4.229522000
H	-6.152589000	-1.828846000	0.835817000
H	-6.370149000	-0.827227000	2.260486000
H	-5.019418000	-1.952940000	2.191301000
H	-6.061331000	-1.213963000	-1.315495000
H	-5.529430000	0.072128000	-2.408649000
H	-6.837817000	0.365231000	-1.273510000
H	-4.259886000	1.839624000	-2.591600000
H	-3.076815000	2.885483000	-1.803523000
H	-4.806033000	3.168615000	-1.577819000
H	4.768024000	1.357843000	-0.038262000
H	3.312960000	1.846613000	0.810459000
H	2.785418000	0.553045000	-1.113540000
C	-3.748219000	-3.323422000	-0.876744000
O	-3.081851000	-2.118057000	-1.380724000
C	-3.060389000	-2.154770000	-2.849358000
C	-3.526979000	-3.552247000	-3.224684000
C	-4.470886000	-3.910321000	-2.075520000
H	-2.970652000	-3.992906000	-0.499797000
H	-4.402639000	-3.022664000	-0.057030000
H	-3.745368000	-1.380204000	-3.206443000
H	-2.043868000	-1.927490000	-3.174747000

H	-4.016915000	-3.564362000	-4.201899000
H	-2.679329000	-4.245424000	-3.261028000
H	-5.449255000	-3.437696000	-2.213928000
H	-4.624971000	-4.987371000	-1.967370000
C	4.317938000	-2.295769000	-0.062167000
C	3.999924000	-1.145411000	-0.797846000
C	4.544261000	-1.027592000	-2.083319000
C	5.374270000	-2.007200000	-2.622169000
C	5.668199000	-3.139293000	-1.865698000
C	5.143614000	-3.289801000	-0.584231000
H	3.923220000	-2.429410000	0.941881000
H	4.319832000	-0.145185000	-2.679581000
H	5.787883000	-1.896830000	-3.619531000
H	5.383344000	-4.173106000	-0.000464000
C	-0.168934000	-3.523364000	0.560791000
C	-0.041747000	-2.127340000	0.589335000
C	-0.853419000	-1.425569000	1.505553000
C	-1.748888000	-2.095781000	2.354892000
C	-1.850209000	-3.484756000	2.288787000
C	-1.050658000	-4.202912000	1.398905000
H	0.463955000	-4.097297000	-0.111980000
H	-0.687426000	-0.354966000	1.663279000
H	-2.312852000	-1.548985000	3.100528000
H	-1.107219000	-5.287363000	1.376233000
C	0.958851000	-1.432790000	-0.304650000
C	1.891282000	-0.516731000	0.510598000
H	1.603386000	-2.224141000	-0.709692000
H	2.204088000	-1.070083000	1.405324000
H	1.343645000	0.356514000	0.888901000
C	-3.663729000	0.614155000	3.168354000
H	-2.624994000	0.774577000	3.474353000
H	-4.260834000	1.388878000	3.664438000
H	-4.000329000	-0.340868000	3.583329000
Cl	-2.943345000	-4.321550000	3.344219000
Cl	6.694657000	-4.380187000	-2.529039000
Si	-2.523714000	3.308994000	1.417506000
C	-0.898068000	2.885381000	2.302760000
H	-0.227669000	2.307376000	1.658587000
H	-0.377186000	3.814535000	2.563271000
H	-1.052146000	2.333289000	3.235807000
C	-2.185176000	4.561288000	0.045355000
H	-3.111995000	4.927048000	-0.407994000
H	-1.684146000	5.424932000	0.500289000
H	-1.531378000	4.181899000	-0.743823000

C	-3.698657000	4.152539000	2.647380000
H	-4.687312000	4.314015000	2.203312000
H	-3.830491000	3.593486000	3.578564000
H	-3.290699000	5.135666000	2.911912000
C	0.588503000	4.103466000	-2.815579000
C	-0.396403000	3.422227000	-3.526396000
C	-0.857919000	2.197303000	-3.050602000
C	-0.380818000	1.621267000	-1.858734000
C	0.605903000	2.345275000	-1.169807000
C	1.094081000	3.564053000	-1.635067000
H	-0.783656000	3.836238000	-4.452262000
H	-1.600960000	1.663551000	-3.640767000
H	1.011447000	1.955179000	-0.243295000
C	-0.851377000	0.260722000	-1.432080000
C	0.266069000	-0.827071000	-1.556354000
H	-1.592553000	-0.014974000	-2.224930000
H	-0.155222000	-1.694013000	-2.086470000
H	1.058530000	-0.452824000	-2.218434000
H	1.859970000	4.096878000	-1.080140000
Cl	1.191015000	5.625971000	-3.404003000

$pC3^{a}_{iso}, E_{(SCF Done)} = -3794.04118 \text{ a.u.}$

Sc	1.039280000	-1.083077000	0.885705000
Si	-6.803717000	-0.925746000	-1.513427000
C	-5.137544000	-0.196565000	-0.914342000
C	-6.548665000	-2.691725000	-2.164626000
C	-7.524875000	0.164235000	-2.887612000
C	-7.988307000	-0.962621000	-0.032107000
C	0.641744000	-2.075026000	4.307708000
C	0.743935000	-2.541639000	2.881284000
C	1.913176000	-3.016661000	2.218939000
C	1.518953000	-3.513024000	0.946210000
C	0.091762000	-3.379774000	0.804003000
C	-0.372511000	-2.775328000	2.017703000
C	3.300562000	-3.138610000	2.784325000
C	2.449381000	-4.277072000	0.044852000
C	-4.042507000	-0.110586000	-1.981065000
C	-2.685591000	0.516464000	-1.555623000
H	-4.802852000	-0.801463000	-0.058402000
H	-5.355071000	0.803979000	-0.516182000
H	-5.873413000	-2.713520000	-3.027811000
H	-7.504418000	-3.122940000	-2.484506000
H	-6.132617000	-3.348030000	-1.391077000
H	-7.658178000	1.197517000	-2.546771000

H	-8.505950000	-0.211364000	-3.200744000
H	-6.881050000	0.182715000	-3.774381000
H	-7.595928000	-1.587333000	0.779019000
H	-8.963833000	-1.369996000	-0.321868000
H	-8.155152000	0.043768000	0.369097000
H	1.624240000	-1.940696000	4.768129000
H	0.106491000	-2.817030000	4.913672000
H	0.101189000	-1.127648000	4.410901000
H	3.345204000	-2.821847000	3.830115000
H	4.047890000	-2.558976000	2.227545000
H	3.628052000	-4.185196000	2.761597000
H	3.482587000	-3.924022000	0.128406000
H	2.158024000	-4.238341000	-1.008900000
H	2.463068000	-5.336686000	0.331633000
H	-4.413141000	0.470803000	-2.835566000
H	-3.827728000	-1.116222000	-2.371005000
H	-2.051981000	0.467075000	-2.455462000
C	3.043487000	0.351021000	3.015827000
O	2.785659000	0.069396000	1.598673000
C	3.616728000	0.947329000	0.771312000
C	4.204540000	1.969063000	1.729003000
C	4.320281000	1.172702000	3.029194000
H	2.186988000	0.908939000	3.402765000
H	3.126517000	-0.606852000	3.527215000
H	4.385723000	0.326749000	0.305679000
H	2.981060000	1.381592000	-0.003656000
H	5.163796000	2.352625000	1.370850000
H	3.519880000	2.813163000	1.858107000
H	5.200946000	0.520650000	3.010882000
H	4.382655000	1.808429000	3.916417000
C	-3.276353000	2.434676000	0.037985000
C	-2.817105000	1.987008000	-1.208334000
C	-2.512313000	2.957519000	-2.171139000
C	-2.651863000	4.319531000	-1.913875000
C	-3.106340000	4.729301000	-0.662946000
C	-3.422524000	3.791668000	0.317576000
H	-3.523618000	1.717828000	0.816010000
H	-2.164250000	2.643053000	-3.153550000
H	-2.413603000	5.056286000	-2.674617000
H	-3.779803000	4.121617000	1.288040000
C	0.401310000	2.328753000	0.650040000
C	-0.299798000	1.113419000	0.854773000
C	-0.677677000	0.823667000	2.188833000
C	-0.430483000	1.713316000	3.241780000

C	0.235653000	2.905160000	2.987504000
C	0.651258000	3.215876000	1.684968000
H	0.671714000	2.611968000	-0.364711000
H	-1.277877000	-0.061130000	2.388516000
H	-0.776432000	1.488685000	4.246446000
H	1.132055000	4.169884000	1.489025000
C	-0.518472000	0.126925000	-0.216960000
C	-1.960142000	-0.327997000	-0.483535000
H	-0.079861000	0.505369000	-1.150426000
H	-2.534093000	-0.318907000	0.450917000
H	-1.976785000	-1.366960000	-0.833955000
C	-1.797542000	-2.605399000	2.463828000
H	-2.460444000	-2.267001000	1.665609000
H	-2.192474000	-3.562915000	2.828102000
H	-1.880237000	-1.904651000	3.300885000
Cl	0.548159000	4.023611000	4.280213000
Cl	-3.275626000	6.429550000	-0.319080000
Si	-0.928289000	-4.342496000	-0.509660000
C	-2.798901000	-4.236500000	-0.236134000
H	-3.212444000	-3.230860000	-0.352391000
H	-3.272037000	-4.872616000	-0.994620000
H	-3.096547000	-4.624327000	0.742986000
C	-0.562286000	-3.782843000	-2.288620000
H	0.477703000	-3.948916000	-2.590266000
H	-1.187909000	-4.372786000	-2.969759000
H	-0.805171000	-2.727643000	-2.456539000
C	-0.464252000	-6.173947000	-0.333866000
H	0.566469000	-6.390066000	-0.630390000
H	-0.600271000	-6.518017000	0.697652000
H	-1.122393000	-6.774544000	-0.973251000
C	6.450908000	1.131430000	-3.343249000
C	6.795995000	-0.038055000	-2.665701000
C	5.787373000	-0.844565000	-2.152716000
C	4.430951000	-0.504548000	-2.298972000
C	4.113674000	0.674446000	-2.999138000
C	5.109458000	1.488933000	-3.516469000
H	7.839608000	-0.311523000	-2.550354000
H	6.057427000	-1.761436000	-1.633229000
H	3.076189000	0.952850000	-3.161505000
H	4.858516000	2.392432000	-4.062578000
C	3.420922000	-1.395691000	-1.735740000
C	2.080626000	-1.217781000	-1.711885000
H	3.817146000	-2.315186000	-1.308120000
H	1.424749000	-2.046583000	-1.438149000

H	1.601591000	-0.365075000	-2.181990000
Cl	7.693837000	2.149030000	-3.986627000

***p*TS3^a_{iso}, $E_{(\text{SCF Done})} = -3794.020125$ a.u. **IF** = $i268.9$ cm⁻¹**

Sc	-1.541743000	-1.054468000	-0.454199000
Si	6.695810000	-0.944566000	1.168047000
C	4.993582000	-0.227128000	0.655238000
C	6.449917000	-2.431816000	2.322354000
C	7.711362000	0.391764000	2.049400000
C	7.589426000	-1.501432000	-0.409112000
C	-2.385456000	-2.545128000	-3.715024000
C	-1.944747000	-2.764360000	-2.293199000
C	-2.754802000	-3.126707000	-1.176521000
C	-1.886570000	-3.504819000	-0.113820000
C	-0.519772000	-3.370980000	-0.550100000
C	-0.582222000	-2.914760000	-1.907830000
C	-4.251850000	-3.259302000	-1.142448000
C	-2.359799000	-4.194208000	1.135483000
C	4.099406000	0.206403000	1.819010000
C	2.724433000	0.835054000	1.464239000
H	4.492560000	-0.987487000	0.037956000
H	5.195489000	0.625094000	-0.007913000
H	5.960241000	-2.142926000	3.259365000
H	7.416612000	-2.878388000	2.582776000
H	5.842880000	-3.212521000	1.848791000
H	7.867800000	1.263373000	1.403356000
H	8.698108000	0.003722000	2.327473000
H	7.223498000	0.737059000	2.968102000
H	7.026396000	-2.280943000	-0.935718000
H	8.578284000	-1.910039000	-0.171283000
H	7.735228000	-0.664712000	-1.102119000
H	-3.471051000	-2.609520000	-3.826406000
H	-1.961352000	-3.327212000	-4.357023000
H	-2.063098000	-1.584381000	-4.133547000
H	-4.719349000	-2.912454000	-2.068140000
H	-4.710531000	-2.705537000	-0.314139000
H	-4.540260000	-4.310912000	-1.020204000
H	-3.415141000	-3.987335000	1.342261000
H	-1.785492000	-3.921350000	2.025282000
H	-2.272924000	-5.282696000	1.020412000
H	4.634389000	0.940352000	2.435684000
H	3.904014000	-0.653891000	2.475688000
H	2.251524000	1.058315000	2.433769000
C	-3.867222000	0.130434000	-2.464936000

O	-3.260957000	0.162294000	-1.129935000
C	-3.921364000	1.208977000	-0.335675000
C	-4.632880000	2.082972000	-1.347872000
C	-5.065798000	1.063066000	-2.399733000
H	-3.110871000	0.477403000	-3.173303000
H	-4.129424000	-0.902227000	-2.681099000
H	-4.616633000	0.716487000	0.347454000
H	-3.153707000	1.718566000	0.245488000
H	-5.472001000	2.619257000	-0.896313000
H	-3.945748000	2.817883000	-1.780831000
H	-5.958821000	0.522300000	-2.067115000
H	-5.281251000	1.511006000	-3.373499000
C	3.107996000	2.254867000	-0.635737000
C	2.860461000	2.162203000	0.740744000
C	2.777142000	3.357273000	1.466516000
C	2.928552000	4.599970000	0.855699000
C	3.168065000	4.656915000	-0.515263000
C	3.261470000	3.487376000	-1.266914000
H	3.184390000	1.353155000	-1.237128000
H	2.597407000	3.319969000	2.539499000
H	2.863084000	5.515287000	1.435330000
H	3.455763000	3.542862000	-2.333396000
C	-0.672133000	2.203771000	-0.759667000
C	-0.028278000	0.939758000	-0.686498000
C	0.184970000	0.261881000	-1.909827000
C	-0.175012000	0.832671000	-3.141247000
C	-0.769626000	2.084713000	-3.167459000
C	-1.011763000	2.778506000	-1.969404000
H	-0.826420000	2.768097000	0.156513000
H	0.771848000	-0.651218000	-1.918641000
H	0.047197000	0.316020000	-4.069633000
H	-1.434274000	3.778085000	-2.004605000
C	0.362179000	0.377052000	0.615656000
C	1.784017000	-0.170477000	0.762690000
H	0.175485000	1.149634000	1.360674000
H	2.187916000	-0.452849000	-0.216170000
H	1.792610000	-1.088820000	1.364070000
C	0.546032000	-2.856110000	-2.899179000
H	1.496460000	-2.547461000	-2.457317000
H	0.712758000	-3.850363000	-3.336016000
H	0.322207000	-2.184704000	-3.734417000
Cl	-1.203585000	2.812832000	-4.680071000
Cl	3.347278000	6.201784000	-1.298339000
Si	0.940870000	-4.362321000	0.211527000

C	2.639079000	-3.891836000	-0.491928000
H	2.865618000	-2.824286000	-0.404231000
H	3.394941000	-4.431405000	0.092103000
H	2.765641000	-4.191750000	-1.536228000
C	1.098347000	-4.238296000	2.100986000
H	0.199343000	-4.541157000	2.644792000
H	1.898667000	-4.927596000	2.398635000
H	1.394509000	-3.243192000	2.450260000
C	0.603708000	-6.171474000	-0.247292000
H	-0.316437000	-6.551153000	0.209061000
H	0.514859000	-6.292989000	-1.332586000
H	1.430085000	-6.805988000	0.094411000
C	-4.678145000	1.871642000	3.794867000
C	-5.176323000	0.625008000	3.412871000
C	-4.335549000	-0.282299000	2.780002000
C	-2.984655000	0.015737000	2.512852000
C	-2.512185000	1.274939000	2.926729000
C	-3.343032000	2.195681000	3.558485000
H	-6.210562000	0.368231000	3.619949000
H	-4.731019000	-1.257477000	2.501953000
H	-1.471520000	1.546581000	2.769985000
H	-2.956432000	3.158973000	3.876569000
C	-2.134847000	-0.989170000	1.865164000
C	-0.721317000	-0.943780000	1.900710000
H	-2.587469000	-1.972387000	1.782697000
H	-0.206857000	-1.878449000	1.680336000
H	-0.216349000	-0.372475000	2.674266000
Cl	-5.721978000	3.018744000	4.577801000

pP3^a_{iso}, $E_{(\text{SCF Done})} = -3794.039282$ a.u.

Sc	2.592051000	-0.367822000	-0.116837000
Si	-7.178647000	-2.571623000	0.689449000
C	-5.694814000	-1.361084000	0.625779000
C	-6.564356000	-4.356740000	0.485482000
C	-8.411558000	-2.156036000	-0.690494000
C	-8.014939000	-2.375353000	2.380342000
C	5.323609000	-2.258860000	1.423250000
C	4.496920000	-1.993782000	0.195150000
C	4.826816000	-1.131234000	-0.892680000
C	3.899603000	-1.387699000	-1.947249000
C	2.968725000	-2.393057000	-1.522021000
C	3.359188000	-2.760389000	-0.189158000
C	6.027927000	-0.231881000	-0.996267000
C	4.032908000	-0.828536000	-3.338132000

C	-4.895783000	-1.384747000	-0.679480000
C	-3.673784000	-0.429667000	-0.785103000
H	-5.050639000	-1.599692000	1.484823000
H	-6.094275000	-0.354199000	0.809239000
H	-6.102604000	-4.520040000	-0.495117000
H	-7.399409000	-5.061264000	0.575646000
H	-5.827765000	-4.617684000	1.254663000
H	-8.773871000	-1.125034000	-0.604352000
H	-9.282813000	-2.819298000	-0.639153000
H	-7.966070000	-2.274333000	-1.684890000
H	-7.322563000	-2.604000000	3.199084000
H	-8.872190000	-3.052227000	2.472202000
H	-8.382723000	-1.353055000	2.526274000
H	6.125459000	-1.527534000	1.551063000
H	5.806912000	-3.240904000	1.341019000
H	4.736260000	-2.272785000	2.348617000
H	6.513890000	-0.076464000	-0.028754000
H	5.785775000	0.756946000	-1.402477000
H	6.782673000	-0.672768000	-1.660182000
H	4.741941000	0.004595000	-3.376312000
H	3.084637000	-0.483569000	-3.761767000
H	4.423550000	-1.598566000	-4.016087000
H	-5.562720000	-1.147307000	-1.518330000
H	-4.524531000	-2.402772000	-0.866413000
H	-3.252305000	-0.617795000	-1.782324000
C	4.426653000	0.825341000	2.364512000
O	3.277636000	0.985421000	1.469886000
C	2.577224000	2.236191000	1.806032000
C	3.121371000	2.641406000	3.162452000
C	4.568495000	2.154466000	3.087072000
H	4.197636000	0.006437000	3.051822000
H	5.288425000	0.565640000	1.751316000
H	2.820481000	2.961803000	1.027782000
H	1.508407000	2.024350000	1.795523000
H	3.040176000	3.720065000	3.322274000
H	2.582987000	2.130983000	3.968496000
H	5.180712000	2.850308000	2.502683000
H	5.033351000	2.031809000	4.069023000
C	-4.338670000	1.723880000	0.437509000
C	-4.071947000	1.034688000	-0.754628000
C	-4.209184000	1.742702000	-1.955609000
C	-4.596326000	3.080585000	-1.980802000
C	-4.851025000	3.735852000	-0.778343000
C	-4.725698000	3.062508000	0.435011000

H	-4.254229000	1.212507000	1.392922000
H	-4.015612000	1.235818000	-2.899121000
H	-4.699223000	3.611035000	-2.922191000
H	-4.935549000	3.580329000	1.365882000
C	-0.580465000	0.440780000	2.507535000
C	-0.398369000	-0.268174000	1.311875000
C	0.554024000	-1.304898000	1.314741000
C	1.291710000	-1.616898000	2.465998000
C	1.091568000	-0.878540000	3.630573000
C	0.144730000	0.144344000	3.659735000
H	-1.322317000	1.235649000	2.542490000
H	0.638727000	-1.955195000	0.440238000
H	1.983282000	-2.451201000	2.470734000
H	-0.026620000	0.698871000	4.577547000
C	-1.278888000	0.033176000	0.122552000
C	-2.588049000	-0.787940000	0.244508000
H	-1.573714000	1.085050000	0.216063000
H	-2.984470000	-0.665817000	1.259801000
H	-2.348504000	-1.856691000	0.143326000
C	2.860101000	-3.950369000	0.585941000
H	1.770809000	-3.997166000	0.673504000
H	3.174068000	-4.877592000	0.089270000
H	3.284321000	-3.984968000	1.593998000
Cl	2.009832000	-1.254489000	5.057912000
Cl	-5.324976000	5.411783000	-0.789427000
Si	1.857720000	-3.453669000	-2.669537000
C	0.411785000	-4.275100000	-1.748528000
H	-0.202990000	-3.572188000	-1.175197000
H	-0.243640000	-4.735308000	-2.498006000
H	0.740384000	-5.073068000	-1.076366000
C	1.119009000	-2.500602000	-4.134049000
H	1.876438000	-2.149794000	-4.840843000
H	0.468204000	-3.195263000	-4.679816000
H	0.500406000	-1.647348000	-3.836991000
C	2.982086000	-4.818818000	-3.355094000
H	3.801081000	-4.401095000	-3.951164000
H	3.425932000	-5.419917000	-2.553813000
H	2.409918000	-5.494595000	-4.001766000
C	2.306697000	4.273588000	-1.210431000
C	3.141067000	3.235826000	-1.605940000
C	2.628240000	1.936214000	-1.683033000
C	1.280073000	1.627489000	-1.364507000
C	0.471670000	2.717994000	-0.956537000
C	0.965322000	4.012544000	-0.899461000

H	4.168055000	3.441663000	-1.892391000
H	3.258612000	1.173040000	-2.139982000
H	-0.580835000	2.558548000	-0.749546000
H	0.309036000	4.834869000	-0.629629000
C	0.859081000	0.222809000	-1.413647000
C	-0.603636000	-0.175507000	-1.250404000
H	1.258583000	-0.235097000	-2.326373000
H	-0.679267000	-1.240418000	-1.510095000
H	-1.225524000	0.345835000	-1.994001000
Cl	2.914557000	5.899413000	-1.125831000

oC3^a, $E_{(\text{SCF Done})} = -3794.02999$ a.u.

Sc	0.520609000	-1.815098000	-0.040352000
Si	-4.795010000	4.297635000	-1.622300000
C	-4.222233000	2.511669000	-1.238109000
C	-3.434599000	5.529977000	-1.130673000
C	-6.384969000	4.690761000	-0.667594000
C	-5.113071000	4.420112000	-3.488337000
C	-1.698260000	-2.168878000	-2.819526000
C	-0.288378000	-2.273103000	-2.321969000
C	0.322255000	-3.455226000	-1.823406000
C	1.725371000	-3.206633000	-1.609815000
C	1.957114000	-1.844020000	-2.000275000
C	0.718808000	-1.266559000	-2.412398000
C	-0.391816000	-4.772849000	-1.698675000
C	3.281430000	-1.140216000	-2.088561000
C	0.524407000	0.119110000	-2.958479000
C	-3.933023000	2.226788000	0.238416000
C	-3.460287000	0.793485000	0.604704000
H	-3.332766000	2.316895000	-1.856177000
H	-5.005998000	1.835679000	-1.606554000
H	-3.234441000	5.505015000	-0.053179000
H	-3.733544000	6.553431000	-1.385407000
H	-2.495150000	5.319934000	-1.656079000
H	-7.182658000	3.979442000	-0.910982000
H	-6.746905000	5.694479000	-0.919078000
H	-6.225865000	4.659731000	0.416207000
H	-4.208103000	4.195609000	-4.065185000
H	-5.439981000	5.429472000	-3.763634000
H	-5.895170000	3.720201000	-3.804593000
H	-2.422488000	-2.634914000	-2.143635000
H	-1.792322000	-2.673485000	-3.790447000
H	-2.001149000	-1.129456000	-2.969089000
H	-1.444365000	-4.646451000	-1.423871000

H	0.069998000	-5.434728000	-0.960608000
H	-0.378511000	-5.303292000	-2.659734000
H	3.809800000	-1.439940000	-3.002659000
H	3.942935000	-1.365006000	-1.249072000
H	3.163167000	-0.054356000	-2.140984000
H	1.229717000	0.838437000	-2.529727000
H	-0.484844000	0.495297000	-2.766975000
H	0.677106000	0.132892000	-4.045822000
H	-4.830434000	2.436148000	0.834710000
H	-3.162106000	2.922479000	0.602784000
H	-3.301345000	0.810123000	1.688059000
C	3.131334000	-1.194011000	1.788143000
O	2.080486000	-0.651272000	0.927545000
C	2.153967000	0.812315000	0.904980000
C	3.070503000	1.168664000	2.061716000
C	4.042874000	-0.013465000	2.084106000
H	2.649020000	-1.583206000	2.690626000
H	3.617668000	-2.008394000	1.244879000
H	2.572859000	1.111762000	-0.059447000
H	1.135301000	1.192848000	1.008364000
H	3.569973000	2.126665000	1.897775000
H	2.502725000	1.222738000	2.996861000
H	4.799019000	0.098619000	1.300097000
H	4.554782000	-0.128673000	3.043339000
C	-4.740917000	-0.802496000	-0.919820000
C	-4.537375000	-0.244124000	0.351691000
C	-5.418509000	-0.669227000	1.360256000
C	-6.429912000	-1.600000000	1.125793000
C	-6.594701000	-2.134748000	-0.147858000
C	-5.747455000	-1.730290000	-1.176551000
H	-7.082409000	-1.894809000	1.941345000
H	-5.873403000	-2.128531000	-2.179771000
C	-0.576153000	-2.121290000	2.455102000
C	-1.032561000	-0.916019000	1.865551000
C	-0.879133000	0.217928000	2.712968000
C	-0.389199000	0.125879000	4.005061000
C	0.010395000	-1.105590000	4.542159000
C	-0.082143000	-2.244176000	3.754792000
H	-1.208079000	1.183750000	2.343109000
H	-0.338071000	1.022085000	4.617846000
H	0.205000000	-3.219178000	4.136554000
C	-1.456286000	-0.843088000	0.463212000
C	-2.094917000	0.446173000	-0.035706000
H	-2.081575000	-1.708286000	0.200667000

H	-1.424885000	1.302934000	0.134297000
H	-2.196518000	0.385148000	-1.124490000
Si	2.994910000	-4.579207000	-1.186895000
C	2.668138000	-5.313154000	0.538087000
H	2.773099000	-4.565284000	1.334051000
H	1.677029000	-5.768511000	0.632769000
H	3.406236000	-6.099742000	0.737282000
C	4.787288000	-3.959507000	-1.196755000
H	5.071997000	-3.512732000	-2.154167000
H	5.013427000	-3.240366000	-0.401928000
H	5.436654000	-4.829072000	-1.036257000
C	2.858506000	-5.941313000	-2.495418000
H	3.022738000	-5.535756000	-3.499944000
H	3.625119000	-6.703682000	-2.312811000
H	1.885260000	-6.440971000	-2.487390000
C	6.618867000	5.053537000	1.510612000
C	6.639556000	3.918258000	0.705001000
C	5.571075000	3.667563000	-0.151854000
C	4.460117000	4.524610000	-0.239230000
C	4.479622000	5.665408000	0.582773000
C	5.533713000	5.927617000	1.449249000
H	7.478715000	3.230515000	0.732371000
H	3.658721000	6.372597000	0.504350000
H	5.518779000	6.824737000	2.061422000
C	3.345489000	4.270200000	-1.164832000
C	2.077535000	4.656763000	-0.974136000
H	3.598145000	3.734897000	-2.078256000
H	1.318869000	4.476998000	-1.730628000
H	1.754083000	5.175560000	-0.074559000
Cl	5.638138000	2.207792000	-1.126574000
Cl	-0.657039000	-3.614507000	1.475282000
H	-7.385403000	-2.856697000	-0.331376000
H	0.373499000	-1.177744000	5.562617000
H	7.455334000	5.257213000	2.172974000
H	-4.096212000	-0.490188000	-1.735600000
Cl	-5.297108000	-0.031087000	2.990360000

***o*TS3^a_{syn}, $E_{(\text{SCF Done})} = -3794.04616$ a.u. IF = $i248.1$ cm⁻¹**

Sc	1.499031000	-0.064224000	-0.419793000
Si	-6.980111000	1.645377000	-1.216278000
C	-5.373176000	0.607274000	-1.090904000
C	-6.614620000	3.454004000	-0.767626000
C	-8.289162000	0.943218000	-0.037947000
C	-7.597314000	1.544460000	-3.006098000

C	-0.652867000	-1.543327000	-2.957457000
C	0.689121000	-1.519188000	-2.292480000
C	1.112642000	-2.367870000	-1.235175000
C	2.538273000	-2.228409000	-1.067375000
C	2.964286000	-1.259884000	-2.041688000
C	1.830038000	-0.821900000	-2.781952000
C	0.219770000	-3.370717000	-0.557327000
C	4.368100000	-0.878386000	-2.419420000
C	1.862512000	0.014856000	-4.027017000
C	-4.738802000	0.577711000	0.301750000
C	-3.370782000	-0.143017000	0.474335000
H	-4.668022000	1.006897000	-1.835490000
H	-5.627242000	-0.409592000	-1.417260000
H	-6.274224000	3.557151000	0.269242000
H	-7.518773000	4.064209000	-0.876275000
H	-5.846896000	3.883324000	-1.422383000
H	-8.501828000	-0.108763000	-0.261041000
H	-9.229378000	1.498810000	-0.132295000
H	-7.972376000	1.007609000	1.009302000
H	-6.857436000	1.945341000	-3.708780000
H	-8.521288000	2.120276000	-3.133192000
H	-7.810241000	0.508971000	-3.296011000
H	-1.432075000	-1.929336000	-2.296587000
H	-0.616462000	-2.207641000	-3.832117000
H	-0.966399000	-0.561242000	-3.329262000
H	-0.771288000	-2.968332000	-0.322925000
H	0.648742000	-3.743753000	0.375316000
H	0.057392000	-4.235929000	-1.212934000
H	4.649130000	-1.376439000	-3.357278000
H	5.098455000	-1.176175000	-1.668951000
H	4.473478000	0.197855000	-2.588777000
H	2.727106000	0.684267000	-4.058145000
H	0.960710000	0.624291000	-4.151659000
H	1.928865000	-0.634195000	-4.910905000
H	-5.439056000	0.120584000	1.012367000
H	-4.586026000	1.608131000	0.655616000
H	-3.091105000	0.050903000	1.513987000
C	3.138326000	1.692413000	1.846920000
O	3.204253000	0.666842000	0.809121000
C	4.568549000	0.138179000	0.805517000
C	5.230460000	0.629325000	2.098531000
C	4.059336000	1.167433000	2.927281000
H	3.498978000	2.633680000	1.422859000
H	2.094680000	1.801780000	2.139423000

H	4.476986000	-0.946052000	0.757364000
H	5.069809000	0.507219000	-0.091071000
H	5.775001000	-0.172170000	2.604729000
H	5.942468000	1.431555000	1.880967000
H	3.571546000	0.365715000	3.492497000
H	4.360371000	1.951817000	3.627200000
C	-3.689723000	-2.241322000	-0.932866000
C	-3.486365000	-1.648619000	0.324935000
C	-3.463229000	-2.525817000	1.422869000
C	-3.626853000	-3.904374000	1.280990000
C	-3.827184000	-4.451141000	0.017709000
C	-3.860282000	-3.613727000	-1.095111000
H	-3.604179000	-4.536665000	2.162807000
H	-4.027319000	-4.024566000	-2.087002000
C	0.065278000	0.236727000	2.531398000
C	-0.688032000	0.879978000	1.533065000
C	-1.338894000	2.061103000	1.954104000
C	-1.250445000	2.536745000	3.256573000
C	-0.508771000	1.843429000	4.214028000
C	0.155211000	0.676585000	3.847324000
H	-1.958339000	2.598904000	1.242287000
H	-1.780660000	3.444016000	3.531649000
H	0.730776000	0.108494000	4.571217000
C	-0.845176000	0.350278000	0.151414000
C	-2.266844000	0.490872000	-0.410003000
H	-0.604771000	-0.731189000	0.124186000
H	-2.514777000	1.553425000	-0.534831000
H	-2.293447000	0.069615000	-1.418889000
Si	3.596550000	-3.585734000	-0.206539000
C	3.332235000	-3.692606000	1.672417000
H	3.625431000	-2.774580000	2.194254000
H	2.299921000	-3.927781000	1.951955000
H	3.961055000	-4.502522000	2.062416000
C	5.465643000	-3.405315000	-0.494797000
H	5.721036000	-3.417968000	-1.559004000
H	5.925911000	-2.522288000	-0.039407000
H	5.939934000	-4.283081000	-0.037896000
C	3.112560000	-5.236939000	-1.002505000
H	3.249144000	-5.199042000	-2.089127000
H	3.758689000	-6.032685000	-0.613000000
H	2.076345000	-5.522805000	-0.801343000
C	3.131113000	5.565954000	0.475759000
C	3.811583000	4.888195000	-0.532002000
C	3.238375000	3.765577000	-1.124701000

C	1. 973402000	3. 267624000	-0. 747109000
C	1. 319127000	3. 985516000	0. 273965000
C	1. 874965000	5. 109232000	0. 872714000
H	4. 783358000	5. 230362000	-0. 873713000
H	0. 347740000	3. 643582000	0. 617290000
H	1. 324507000	5. 629113000	1. 651997000
C	1. 360889000	2. 110023000	-1. 416943000
C	-0. 003620000	1. 793735000	-1. 314974000
H	1. 871174000	1. 775792000	-2. 315729000
H	-0. 468102000	1. 261673000	-2. 140423000
H	-0. 669759000	2. 487527000	-0. 812734000
Cl	4. 157086000	2. 997193000	-2. 405484000
Cl	0. 960458000	-1. 225561000	2. 099758000
H	-3. 962938000	-5. 523492000	-0. 090453000
H	-0. 453800000	2. 197868000	5. 238740000
H	3. 576405000	6. 443722000	0. 934491000
H	-3. 733218000	-1. 600656000	-1. 808617000
Cl	-3. 237865000	-1. 926567000	3. 056475000

oP3_{syn}, $E_{(\text{SCF Done})} = -3794.082503$ a.u.

Sc	2. 346562000	0. 043424000	-0. 678205000
Si	-7. 814783000	0. 604175000	-1. 116199000
C	-5. 954028000	0. 162512000	-1. 030220000
C	-8. 061203000	2. 457594000	-0. 784355000
C	-8. 773708000	-0. 409300000	0. 168947000
C	-8. 433957000	0. 181644000	-2. 859019000
C	-0. 016579000	-1. 627665000	-2. 816923000
C	1. 303694000	-1. 702260000	-2. 111088000
C	1. 550623000	-2. 291669000	-0. 841345000
C	2. 975055000	-2. 343079000	-0. 616171000
C	3. 587501000	-1. 777347000	-1. 785889000
C	2. 562036000	-1. 383944000	-2. 695586000
C	0. 486880000	-2. 951727000	-0. 009981000
C	5. 052946000	-1. 725833000	-2. 120796000
C	2. 752067000	-0. 904615000	-4. 105408000
C	-5. 278060000	0. 461607000	0. 310142000
C	-3. 768443000	0. 109245000	0. 433363000
H	-5. 451019000	0. 700236000	-1. 847641000
H	-5. 871032000	-0. 907179000	-1. 267069000
H	-7. 734420000	2. 736401000	0. 224146000
H	-9. 120910000	2. 724396000	-0. 871026000
H	-7. 505766000	3. 072028000	-1. 502843000
H	-8. 622212000	-1. 484785000	0. 019917000
H	-9. 849103000	-0. 211539000	0. 090782000

H	-8.467282000	-0.165340000	1.192582000
H	-7.895995000	0.753218000	-3.624457000
H	-9.500659000	0.412606000	-2.961142000
H	-8.303215000	-0.883897000	-3.081090000
H	-0.857753000	-1.586530000	-2.119758000
H	-0.160340000	-2.521732000	-3.439613000
H	-0.080244000	-0.762164000	-3.483944000
H	-0.456323000	-2.397758000	-0.008395000
H	0.789856000	-3.088409000	1.030766000
H	0.265541000	-3.946583000	-0.417192000
H	5.327092000	-2.578554000	-2.756256000
H	5.685738000	-1.772889000	-1.234342000
H	5.323923000	-0.823493000	-2.680842000
H	3.761498000	-0.525899000	-4.286911000
H	2.045738000	-0.114410000	-4.381105000
H	2.592080000	-1.735803000	-4.805306000
H	-5.805017000	-0.064209000	1.116650000
H	-5.372744000	1.533131000	0.538005000
H	-3.473090000	0.463756000	1.426961000
C	3.642192000	1.876665000	1.732401000
O	3.856653000	0.805593000	0.752635000
C	5.282143000	0.480505000	0.693709000
C	5.978681000	1.550326000	1.520507000
C	4.914535000	1.906858000	2.559256000
H	3.483124000	2.807471000	1.181585000
H	2.745497000	1.625807000	2.297479000
H	5.403605000	-0.517968000	1.121489000
H	5.581193000	0.470927000	-0.355711000
H	6.907528000	1.179642000	1.962514000
H	6.218057000	2.421404000	0.900854000
H	4.879814000	1.154668000	3.355609000
H	5.075123000	2.886012000	3.018673000
C	-3.501628000	-2.118166000	-0.785373000
C	-3.549190000	-1.393691000	0.417137000
C	-3.460274000	-2.152847000	1.596638000
C	-3.331137000	-3.541672000	1.584827000
C	-3.293657000	-4.222567000	0.371914000
C	-3.380050000	-3.505538000	-0.818978000
H	-3.271076000	-4.078581000	2.526128000
H	-3.363890000	-4.023235000	-1.774243000
C	-0.164408000	1.232531000	1.975090000
C	-1.145354000	1.646905000	1.071055000
C	-1.878211000	2.778437000	1.470106000
C	-1.654533000	3.426190000	2.681104000

C	-0.679414000	2.955807000	3.558306000
C	0.076238000	1.843170000	3.203257000
H	-2.656125000	3.154851000	0.812230000
H	-2.255285000	4.291483000	2.946277000
H	0.823861000	1.439514000	3.879054000
C	-1.407946000	0.957964000	-0.253909000
C	-2.911334000	0.873851000	-0.589734000
H	-1.036594000	-0.070980000	-0.173399000
H	-3.322948000	1.885773000	-0.703454000
H	-3.002759000	0.425444000	-1.585621000
Si	3.765534000	-3.407735000	0.770195000
C	3.375852000	-2.722286000	2.499806000
H	3.726287000	-1.690495000	2.617488000
H	2.306787000	-2.740957000	2.736520000
H	3.886069000	-3.333465000	3.254181000
C	5.652790000	-3.565267000	0.630152000
H	5.962501000	-3.982658000	-0.333210000
H	6.207315000	-2.635857000	0.796853000
H	5.974041000	-4.271081000	1.406435000
C	3.083990000	-5.169127000	0.610372000
H	3.269940000	-5.569158000	-0.392766000
H	3.591263000	-5.823151000	1.329643000
H	2.009845000	-5.230743000	0.805513000
C	3.084143000	5.221437000	-0.493916000
C	3.687355000	4.197390000	-1.220147000
C	2.953733000	3.047593000	-1.480623000
C	1.612551000	2.830155000	-1.100765000
C	1.062593000	3.889703000	-0.342531000
C	1.772202000	5.049106000	-0.049543000
H	4.706885000	4.288021000	-1.582317000
H	0.041105000	3.800952000	0.008389000
H	1.287258000	5.835452000	0.522640000
C	0.885581000	1.587771000	-1.471615000
C	-0.649886000	1.626894000	-1.430328000
H	1.175835000	1.349827000	-2.508677000
H	-1.009345000	1.119625000	-2.332845000
H	-1.012533000	2.662311000	-1.526621000
Cl	3.777532000	1.729198000	-2.347089000
Cl	0.827193000	-0.201382000	1.615468000
H	-3.205983000	-5.305429000	0.363407000
H	-0.511769000	3.439130000	4.516153000
H	3.632008000	6.134663000	-0.282910000
H	-3.582954000	-1.578961000	-1.724678000
Cl	-3.523775000	-1.381417000	3.170954000

oC3^{iso}, $E_{(\text{SCF Done})} = -3794.045165$ a.u.

Sc	0.741721000	-1.752979000	-0.001805000
Si	-4.636555000	4.416425000	-0.928109000
C	-4.043745000	2.595883000	-0.941486000
C	-3.457002000	5.465707000	0.130006000
C	-6.393342000	4.519366000	-0.222852000
C	-4.614554000	5.050556000	-2.715839000
C	-0.873865000	-1.084580000	-3.131603000
C	0.351259000	-1.584787000	-2.428391000
C	0.637312000	-2.944034000	-2.126025000
C	1.984880000	-3.036578000	-1.627721000
C	2.518636000	-1.700404000	-1.650614000
C	1.512243000	-0.812161000	-2.123765000
C	-0.322302000	-4.064140000	-2.415537000
C	3.930547000	-1.296201000	-1.329390000
C	1.660094000	0.658395000	-2.392702000
C	-4.004878000	1.921099000	0.432443000
C	-3.480004000	0.460866000	0.496979000
H	-3.048740000	2.579524000	-1.411268000
H	-4.711806000	2.043180000	-1.615775000
H	-3.457342000	5.144603000	1.178093000
H	-3.757399000	6.519767000	0.110063000
H	-2.427125000	5.407850000	-0.242635000
H	-7.091285000	3.907172000	-0.805624000
H	-6.758714000	5.552548000	-0.245384000
H	-6.434036000	4.176458000	0.817318000
H	-3.607541000	4.996176000	-3.146154000
H	-4.941637000	6.095573000	-2.765166000
H	-5.284594000	4.462932000	-3.354051000
H	-1.794975000	-1.527249000	-2.740706000
H	-0.823120000	-1.334226000	-4.200148000
H	-0.966427000	0.002867000	-3.061201000
H	-1.363476000	-3.742469000	-2.309653000
H	-0.173165000	-4.931231000	-1.770357000
H	-0.200891000	-4.409616000	-3.451064000
H	4.548558000	-1.316941000	-2.236262000
H	4.402018000	-1.967165000	-0.606015000
H	3.995437000	-0.280055000	-0.928251000
H	2.549787000	1.079773000	-1.917176000
H	0.792210000	1.236678000	-2.054559000
H	1.760375000	0.839635000	-3.471003000
H	-5.010164000	1.928503000	0.872540000
H	-3.375824000	2.514131000	1.113577000

H	-3.505032000	0.193880000	1.558723000
C	2.857263000	-1.120073000	2.401082000
O	2.022168000	-0.594758000	1.318676000
C	1.988647000	0.869156000	1.378617000
C	2.564780000	1.215222000	2.739699000
C	3.584621000	0.094269000	2.955673000
H	2.189743000	-1.577281000	3.138086000
H	3.514624000	-1.878407000	1.970630000
H	2.607052000	1.247530000	0.559992000
H	0.951269000	1.184275000	1.239743000
H	3.014137000	2.212033000	2.743034000
H	1.783153000	1.178844000	3.506159000
H	4.499239000	0.292459000	2.386779000
H	3.855145000	-0.042275000	4.006182000
C	-4.379666000	-0.660728000	-1.607190000
C	-4.399244000	-0.516965000	-0.210498000
C	-5.341887000	-1.299591000	0.477213000
C	-6.202315000	-2.179931000	-0.178520000
C	-6.146748000	-2.298147000	-1.563387000
C	-5.232643000	-1.530757000	-2.281495000
H	-3.681708000	-0.059927000	-2.182409000
H	-6.911376000	-2.762327000	0.401002000
H	-5.187939000	-1.601455000	-3.364957000
C	-0.651881000	-2.556822000	2.254955000
C	-1.112671000	-1.291998000	1.813292000
C	-1.184238000	-0.326780000	2.857027000
C	-0.893404000	-0.626627000	4.177675000
C	-0.481882000	-1.912072000	4.554525000
C	-0.355604000	-2.889176000	3.577762000
H	-1.532435000	0.670862000	2.610139000
H	-1.010926000	0.144370000	4.934649000
H	-0.047522000	-3.899834000	3.827563000
C	-1.337507000	-0.982031000	0.394023000
C	-2.002577000	0.344114000	0.048560000
H	-1.857749000	-1.813271000	-0.105488000
H	-1.452213000	1.183781000	0.500154000
H	-1.921010000	0.504128000	-1.031060000
Si	3.037013000	-4.598114000	-1.266189000
C	2.081419000	-6.217820000	-1.489153000
H	1.279824000	-6.353546000	-0.754899000
H	1.656853000	-6.324557000	-2.492069000
H	2.791723000	-7.041535000	-1.345588000
C	3.674020000	-4.586417000	0.528857000
H	4.370348000	-3.766813000	0.736793000

H	2.848341000	-4.537490000	1.250068000
H	4.214097000	-5.520829000	0.724115000
C	4.499151000	-4.609879000	-2.469307000
H	5.167979000	-3.754875000	-2.331260000
H	5.090329000	-5.522203000	-2.326660000
H	4.146560000	-4.599323000	-3.506689000
C	3.857733000	5.149754000	-2.403519000
C	4.584536000	4.074623000	-1.899165000
C	4.766030000	3.955743000	-0.523663000
C	4.246495000	4.891291000	0.387418000
C	3.525963000	5.967505000	-0.160172000
C	3.324328000	6.096222000	-1.528854000
H	5.019000000	3.334789000	-2.564023000
H	3.150375000	6.732702000	0.513185000
H	2.771374000	6.947659000	-1.915081000
C	4.469578000	4.780947000	1.836978000
C	3.648623000	5.252645000	2.784276000
H	5.387845000	4.282354000	2.141137000
H	3.907043000	5.174662000	3.836435000
H	2.704262000	5.738791000	2.550120000
H	3.724164000	5.252204000	-3.476710000
H	-6.820041000	-2.981219000	-2.073486000
H	-0.275162000	-2.150687000	5.593105000
Cl	5.664827000	2.561655000	0.056897000
Cl	-5.494694000	-1.202949000	2.222471000
Cl	-0.450051000	-3.850448000	1.035622000

***o*TS3^a_{iso}, $E_{(\text{SCF Done})} = -3794.026618$ a.u. $\text{IF} = i268.2 \text{ cm}^{-1}$**

Sc	1.691094000	0.123957000	0.066222000
Si	-6.778919000	1.540055000	0.284705000
C	-5.097590000	0.816091000	-0.286599000
C	-6.601411000	2.291138000	2.019905000
C	-8.090502000	0.171569000	0.312564000
C	-7.274029000	2.892517000	-0.948580000
C	-0.023099000	0.685132000	-3.010074000
C	1.237807000	0.199267000	-2.359886000
C	1.558484000	-1.146213000	-2.025012000
C	2.933397000	-1.198822000	-1.592512000
C	3.441251000	0.141587000	-1.699264000
C	2.404884000	0.997495000	-2.162133000
C	0.637296000	-2.311955000	-2.255308000
C	4.877858000	0.573158000	-1.611959000
C	2.591593000	2.399221000	-2.656403000
C	-4.535873000	-0.288260000	0.611339000

C	-3.127042000	-0.859657000	0.277909000
H	-4.390788000	1.656527000	-0.364024000
H	-5.245435000	0.440775000	-1.307720000
H	-6.345594000	1.531467000	2.767640000
H	-7.545192000	2.752335000	2.333298000
H	-5.829466000	3.069463000	2.047253000
H	-8.202368000	-0.295471000	-0.672783000
H	-9.066624000	0.580338000	0.598410000
H	-7.840156000	-0.616229000	1.032147000
H	-6.528240000	3.695362000	-0.982929000
H	-8.233089000	3.343183000	-0.668462000
H	-7.381228000	2.488192000	-1.961778000
H	-0.875692000	0.036603000	-2.796833000
H	0.101726000	0.697448000	-4.101828000
H	-0.276933000	1.705683000	-2.707332000
H	-0.413810000	-2.010837000	-2.265999000
H	0.750630000	-3.099178000	-1.507968000
H	0.845022000	-2.762291000	-3.235068000
H	5.327231000	0.549714000	-2.613766000
H	5.479455000	-0.079187000	-0.975901000
H	4.985582000	1.601019000	-1.251953000
H	3.317636000	2.961682000	-2.063423000
H	1.657930000	2.965068000	-2.666157000
H	2.969562000	2.370816000	-3.688123000
H	-5.233692000	-1.135123000	0.629799000
H	-4.483665000	0.076180000	1.648057000
H	-2.919474000	-1.564007000	1.088094000
C	3.139334000	-0.284111000	3.075110000
O	3.235820000	0.254031000	1.714099000
C	4.413378000	1.112557000	1.647378000
C	4.552879000	1.664069000	3.050812000
C	4.205046000	0.439399000	3.900880000
H	2.123334000	-0.090122000	3.427692000
H	3.299706000	-1.362293000	3.026193000
H	5.270821000	0.495310000	1.361194000
H	4.231813000	1.867060000	0.880921000
H	5.559095000	2.045445000	3.244767000
H	3.839819000	2.480014000	3.213811000
H	5.086051000	-0.198010000	4.027914000
H	3.835428000	0.702369000	4.895458000
C	-3.209017000	-1.034242000	-2.261540000
C	-3.128897000	-1.663428000	-1.008119000
C	-3.125291000	-3.068965000	-1.022393000
C	-3.190611000	-3.803243000	-2.207019000

C	-3.269474000	-3.141774000	-3.428158000
C	-3.280452000	-1.749058000	-3.454689000
H	-3.230993000	0.051085000	-2.298495000
H	-3.185700000	-4.887551000	-2.161816000
H	-3.351771000	-1.218082000	-4.399901000
C	0.233583000	-2.006698000	2.443376000
C	-0.664096000	-0.974563000	2.132859000
C	-1.548676000	-0.627677000	3.173608000
C	-1.549993000	-1.293399000	4.396527000
C	-0.665530000	-2.343861000	4.632620000
C	0.244402000	-2.706951000	3.640809000
H	-2.268806000	0.167590000	3.007941000
H	-2.258132000	-0.996021000	5.164544000
H	0.950753000	-3.516370000	3.796626000
C	-0.657394000	-0.269381000	0.825406000
C	-2.025839000	0.234284000	0.349444000
H	-0.288151000	-0.959570000	0.035285000
H	-2.392056000	1.017565000	1.026296000
H	-1.901642000	0.722727000	-0.623030000
Si	4.068534000	-2.735766000	-1.405138000
C	3.128222000	-4.381350000	-1.423904000
H	2.431726000	-4.512133000	-0.589713000
H	2.578838000	-4.532407000	-2.358052000
H	3.874251000	-5.182739000	-1.351895000
C	5.090530000	-2.687434000	0.199263000
H	5.790951000	-1.846847000	0.238838000
H	4.454789000	-2.646974000	1.090580000
H	5.686780000	-3.605816000	0.263098000
C	5.239266000	-2.748422000	-2.896702000
H	5.901560000	-1.877808000	-2.926691000
H	5.869869000	-3.644948000	-2.864029000
H	4.672628000	-2.773626000	-3.834310000
C	0.103079000	5.783703000	-1.639427000
C	1.365808000	5.717358000	-1.057593000
C	1.720873000	4.605752000	-0.299533000
C	0.847797000	3.521378000	-0.086134000
C	-0.421793000	3.630940000	-0.684737000
C	-0.793282000	4.733847000	-1.445679000
H	2.078437000	6.526394000	-1.182177000
H	-1.135434000	2.824418000	-0.543109000
H	-1.785697000	4.773701000	-1.886240000
C	1.214568000	2.381558000	0.765857000
C	0.256904000	1.646263000	1.490995000
H	2.195402000	2.453822000	1.228433000

H	0.572540000	1.189628000	2.427676000
H	-0.770919000	1.991778000	1.516482000
H	-0.174896000	6.650628000	-2.231137000
H	-3.327800000	-3.714725000	-4.349199000
H	-0.675132000	-2.877785000	5.577847000
Cl	3.326672000	4.611936000	0.415009000
Cl	-3.047269000	-3.989986000	0.468142000
Cl	1.450889000	-2.425686000	1.227337000

oP3_{iso}, $E_{(\text{SCF Done})} = -3024.957533$ a.u.

Sc	2.471594000	0.325821000	-0.058607000
Si	-7.650067000	1.327757000	-0.410709000
C	-5.806726000	0.861010000	-0.639782000
C	-7.835683000	2.510720000	1.063230000
C	-8.673208000	-0.240768000	-0.110455000
C	-8.235689000	2.188862000	-1.996473000
C	1.788633000	1.443687000	-3.393941000
C	2.435312000	0.398307000	-2.536691000
C	1.855515000	-0.832595000	-2.128254000
C	2.865640000	-1.638331000	-1.484009000
C	4.072743000	-0.858798000	-1.509424000
C	3.808958000	0.383909000	-2.148853000
C	0.447204000	-1.230583000	-2.464479000
C	5.452681000	-1.300911000	-1.107020000
C	4.841902000	1.394858000	-2.550786000
C	-5.148475000	0.220512000	0.584786000
C	-3.650140000	-0.172431000	0.450949000
H	-5.271099000	1.776406000	-0.931608000
H	-5.750588000	0.182105000	-1.502013000
H	-7.523372000	2.040621000	2.003033000
H	-8.881406000	2.817595000	1.181224000
H	-7.238205000	3.419685000	0.924465000
H	-8.564014000	-0.948876000	-0.940058000
H	-9.738042000	0.002835000	-0.018801000
H	-8.371055000	-0.752661000	0.810330000
H	-7.659299000	3.101155000	-2.189909000
H	-9.291592000	2.473085000	-1.920723000
H	-8.130020000	1.533116000	-2.868576000
H	0.712313000	1.520285000	-3.216418000
H	1.924169000	1.194662000	-4.455434000
H	2.219962000	2.434781000	-3.232921000
H	-0.208851000	-0.359209000	-2.546626000
H	0.005192000	-1.909951000	-1.734762000
H	0.416767000	-1.738533000	-3.437876000

H	6. 054354000	-1. 525351000	-1. 997567000
H	5. 436613000	-2. 206417000	-0. 495993000
H	5. 998232000	-0. 525861000	-0. 554342000
H	5. 698412000	1. 407603000	-1. 870350000
H	4. 436871000	2. 409670000	-2. 599298000
H	5. 227100000	1. 152260000	-3. 550665000
H	-5. 701255000	-0. 682129000	0. 874762000
H	-5. 221971000	0. 906517000	1. 440761000
H	-3. 356070000	-0. 524442000	1. 446377000
C	3. 166005000	0. 831583000	3. 148002000
O	3. 434310000	0. 004098000	1. 963863000
C	4. 314463000	-1. 100303000	2. 337938000
C	4. 899947000	-0. 703843000	3. 681620000
C	3. 736554000	0. 053818000	4. 322332000
H	3. 673604000	1. 788224000	3. 002723000
H	2. 088231000	0. 994324000	3. 208711000
H	3. 706199000	-2. 006579000	2. 406374000
H	5. 054940000	-1. 217207000	1. 546271000
H	5. 218527000	-1. 575126000	4. 260408000
H	5. 766137000	-0. 045888000	3. 548241000
H	2. 994376000	-0. 645251000	4. 722965000
H	4. 048860000	0. 719189000	5. 131810000
C	-3. 383107000	-1. 149696000	-1. 892880000
C	-3. 467031000	-1. 339144000	-0. 504215000
C	-3. 443823000	-2. 673027000	-0. 062231000
C	-3. 340260000	-3. 751231000	-0. 940499000
C	-3. 261979000	-3. 520589000	-2. 310592000
C	-3. 285043000	-2. 212445000	-2. 787741000
H	-3. 411064000	-0. 137721000	-2. 286025000
H	-3. 331807000	-4. 761917000	-0. 545066000
H	-3. 237053000	-2. 016489000	-3. 855486000
C	-0. 162018000	-0. 472685000	2. 302749000
C	-0. 979736000	0. 571746000	1. 863822000
C	-1. 554551000	1. 349242000	2. 883061000
C	-1. 364820000	1. 063133000	4. 231645000
C	-0. 592473000	-0. 032885000	4. 615990000
C	0. 024436000	-0. 810706000	3. 640652000
H	-2. 183282000	2. 190471000	2. 606181000
H	-1. 838707000	1. 685897000	4. 984887000
H	0. 630415000	-1. 670661000	3. 907836000
C	-1. 259002000	0. 839315000	0. 397330000
C	-2. 765609000	1. 042581000	0. 128329000
H	-0. 956395000	-0. 049761000	-0. 165927000
H	-3. 132022000	1. 899581000	0. 709124000

H	-2.879761000	1.342859000	-0.919783000
Si	2.843149000	-3.545367000	-1.250514000
C	1.128337000	-4.314074000	-1.487330000
H	0.395054000	-3.990768000	-0.741444000
H	0.714024000	-4.125881000	-2.481975000
H	1.243274000	-5.400205000	-1.380616000
C	3.450310000	-4.132070000	0.453237000
H	4.461308000	-3.798842000	0.707841000
H	2.767386000	-3.827053000	1.254196000
H	3.466568000	-5.228964000	0.445700000
C	3.986986000	-4.245190000	-2.590905000
H	5.027808000	-3.932506000	-2.458757000
H	3.962755000	-5.341190000	-2.569509000
H	3.662440000	-3.922282000	-3.586385000
C	2.813776000	5.724335000	-1.640269000
C	3.595154000	4.823259000	-0.920351000
C	2.989589000	3.680488000	-0.419172000
C	1.632470000	3.345633000	-0.550877000
C	0.891995000	4.289364000	-1.294509000
C	1.463035000	5.442805000	-1.827317000
H	4.653930000	4.999559000	-0.758499000
H	-0.167183000	4.123506000	-1.453734000
H	0.838082000	6.132466000	-2.388063000
C	1.047452000	2.098110000	0.043225000
C	-0.471575000	2.042475000	-0.158875000
H	1.246572000	2.148969000	1.139444000
H	-0.934155000	2.955466000	0.255026000
H	-0.686776000	2.066694000	-1.235836000
H	3.260675000	6.625934000	-2.047581000
H	-3.192017000	-4.360750000	-2.995802000
H	-0.469906000	-0.284548000	5.665343000
Cl	4.028106000	2.531820000	0.452141000
Cl	-3.560947000	-3.056419000	1.646597000
Cl	0.713183000	-1.449853000	1.100177000

oC3'_{syn}, $E_{(\text{SCF Done})} = -3794.045414$ a.u.

Sc	-1.342391000	0.631839000	-0.783921000
Si	6.003587000	-2.852025000	-0.716805000
C	4.838400000	-1.354413000	-0.470431000
C	5.009842000	-4.340408000	-1.356714000
C	6.839204000	-3.303408000	0.924934000
C	7.319172000	-2.369854000	-1.995557000
C	-1.102243000	1.661192000	-4.207344000
C	-1.590229000	0.604390000	-3.255930000

C	-2.907177000	0.463613000	-2.727852000
C	-2.959939000	-0.755358000	-1.999164000
C	-1.678440000	-1.406692000	-2.082273000
C	-0.838876000	-0.544325000	-2.871508000
C	-4.089615000	1.351659000	-2.988002000
C	-4.220322000	-1.270584000	-1.363856000
C	3.726170000	-1.565181000	0.560492000
C	2.759283000	-0.373227000	0.805275000
H	4.416203000	-1.105905000	-1.455552000
H	5.463701000	-0.498411000	-0.181655000
H	4.242153000	-4.651348000	-0.638631000
H	5.667913000	-5.200266000	-1.527654000
H	4.513350000	-4.110307000	-2.307095000
H	7.392435000	-2.450883000	1.335699000
H	7.551870000	-4.123970000	0.781792000
H	6.111123000	-3.625426000	1.678207000
H	6.866037000	-2.106320000	-2.958475000
H	8.015628000	-3.197836000	-2.171112000
H	7.905455000	-1.509120000	-1.653607000
H	-1.871919000	2.408312000	-4.422450000
H	-0.827995000	1.205816000	-5.167331000
H	-0.216679000	2.191353000	-3.840041000
H	-3.808294000	2.289937000	-3.474241000
H	-4.641975000	1.601007000	-2.074646000
H	-4.799956000	0.849677000	-3.657374000
H	-4.855054000	-0.455393000	-0.999978000
H	-4.025852000	-1.941163000	-0.526252000
H	-4.819579000	-1.829572000	-2.095503000
H	4.170287000	-1.828433000	1.529167000
H	3.109849000	-2.427832000	0.268583000
H	2.037516000	-0.736669000	1.548986000
C	-2.184733000	3.714316000	-1.262538000
O	-2.349195000	2.541212000	-0.391408000
C	-3.277297000	2.864400000	0.692962000
C	-3.537759000	4.358743000	0.572279000
C	-3.359878000	4.612013000	-0.925606000
H	-1.222856000	4.171318000	-1.018418000
H	-2.171457000	3.354892000	-2.291441000
H	-4.182935000	2.268855000	0.538276000
H	-2.799888000	2.590836000	1.635687000
H	-4.532137000	4.626114000	0.939801000
H	-2.795103000	4.919436000	1.149195000
H	-4.254230000	4.311270000	-1.482396000
H	-3.146730000	5.659075000	-1.157393000

C	4. 154157000	1. 756431000	0. 664207000
C	3. 484079000	0. 798174000	1. 438960000
C	3. 586478000	0. 948347000	2. 831471000
C	4. 303035000	1. 986955000	3. 422975000
C	4. 953813000	2. 917483000	2. 618944000
C	4. 878296000	2. 800361000	1. 233403000
H	4. 102684000	1. 681084000	-0. 417527000
H	4. 348111000	2. 057048000	4. 505013000
H	5. 382891000	3. 518869000	0. 593488000
C	0. 852400000	3. 486400000	0. 347874000
C	1. 087910000	2. 402536000	-0. 527261000
C	1. 626656000	2. 764353000	-1. 783678000
C	1. 927762000	4. 076267000	-2. 130170000
C	1. 695557000	5. 110670000	-1. 223117000
C	1. 155636000	4. 807700000	0. 023881000
H	2. 354455000	4. 290525000	-3. 106519000
H	0. 981807000	5. 588995000	0. 757597000
C	0. 794954000	0. 982646000	-0. 195456000
C	1. 928125000	-0. 030931000	-0. 450210000
H	0. 567264000	0. 940690000	0. 883005000
H	2. 576136000	0. 320406000	-1. 261369000
H	1. 521100000	-0. 986299000	-0. 802591000
C	0. 513920000	-0. 862628000	-3. 437520000
H	1. 034603000	-1. 636596000	-2. 871001000
H	0. 410585000	-1. 225823000	-4. 469257000
H	1. 164684000	0. 015981000	-3. 473557000
Si	-1. 300615000	-3. 267381000	-1. 789267000
C	0. 212262000	-3. 566194000	-0. 683113000
H	0. 125918000	-3. 077380000	0. 294194000
H	0. 305270000	-4. 644218000	-0. 502140000
H	1. 147811000	-3. 235644000	-1. 144472000
C	-2. 755107000	-4. 206326000	-1. 021140000
H	-3. 667140000	-4. 130871000	-1. 621067000
H	-2. 472779000	-5. 266279000	-0. 990087000
H	-2. 984599000	-3. 901143000	0. 004152000
C	-0. 998591000	-4. 039665000	-3. 494281000
H	-1. 858279000	-3. 872436000	-4. 153027000
H	-0. 107884000	-3. 648412000	-3. 994543000
H	-0. 868209000	-5. 123128000	-3. 385811000
C	-4. 849442000	-4. 196215000	3. 040279000
C	-5. 649671000	-3. 098631000	2. 733254000
C	-5. 053873000	-1. 885863000	2. 402052000
C	-3. 650360000	-1. 740842000	2. 355688000
C	-2. 873129000	-2. 869919000	2. 681616000

C	-3.458148000	-4.081802000	3.018441000
H	-6.731601000	-3.176392000	2.753813000
H	-1.791818000	-2.773487000	2.707097000
C	-3.030392000	-0.452070000	2.077783000
C	-1.742716000	-0.208241000	1.731413000
H	-3.683313000	0.406226000	2.223470000
H	-1.352452000	0.805339000	1.839655000
H	-1.002796000	-1.003124000	1.635916000
H	-2.834311000	-4.931263000	3.278839000
Cl	-6.104711000	-0.543227000	2.030899000
Cl	2.806102000	-0.191866000	3.919127000
H	5.515895000	3.726104000	3.077767000
H	1.938867000	6.138805000	-1.474139000
H	-5.317602000	-5.138881000	3.308439000
H	1.836904000	1.969714000	-2.495131000
Cl	0.179434000	3.209250000	1.951238000

***o*TS3^a_{syn}, $E_{(\text{SCF Done})} = -3794.025203$ a.u. IF = $i290.5$ cm⁻¹**

Sc	-1.649873000	0.307214000	-0.537919000
Si	5.683673000	-1.671544000	-1.579516000
C	4.258962000	-0.475416000	-1.116705000
C	5.046377000	-3.454537000	-1.709225000
C	7.040762000	-1.574481000	-0.259180000
C	6.372422000	-1.118250000	-3.257722000
C	-2.501083000	0.600311000	-4.095281000
C	-2.380702000	-0.276898000	-2.882340000
C	-3.455237000	-0.639167000	-2.022358000
C	-3.005721000	-1.680608000	-1.163837000
C	-1.640811000	-1.995035000	-1.488219000
C	-1.263812000	-1.098364000	-2.546607000
C	-4.881428000	-0.191569000	-2.150960000
C	-3.919968000	-2.423464000	-0.235729000
C	3.567512000	-0.762695000	0.219065000
C	2.558008000	0.304033000	0.725747000
H	3.535355000	-0.479934000	-1.945839000
H	4.699777000	0.530960000	-1.101918000
H	4.619450000	-3.803644000	-0.762175000
H	5.867015000	-4.132968000	-1.970214000
H	4.278136000	-3.553965000	-2.484955000
H	7.408026000	-0.548744000	-0.139029000
H	7.894444000	-2.201448000	-0.541640000
H	6.687633000	-1.922025000	0.718384000
H	5.603285000	-1.151819000	-4.038434000
H	7.194711000	-1.769838000	-3.574971000

H	6.760195000	-0.094035000	-3.210822000
H	-3.023298000	1.544001000	-3.904817000
H	-3.066726000	0.075114000	-4.876425000
H	-1.525956000	0.842975000	-4.525495000
H	-4.982925000	0.712576000	-2.758183000
H	-5.357910000	-0.009100000	-1.182220000
H	-5.473951000	-0.971830000	-2.647211000
H	-4.688096000	-1.770813000	0.191668000
H	-3.381828000	-2.889138000	0.588851000
H	-4.450992000	-3.218460000	-0.777377000
H	4.321554000	-0.876254000	1.008039000
H	3.042448000	-1.725915000	0.164606000
H	2.189775000	-0.065715000	1.690719000
C	-3.718428000	2.773452000	-0.973760000
O	-3.299626000	1.752485000	-0.009943000
C	-4.216279000	1.768512000	1.133864000
C	-5.032238000	3.040383000	0.978778000
C	-5.110373000	3.197985000	-0.539981000
H	-3.002499000	3.594465000	-0.912067000
H	-3.674519000	2.325753000	-1.967006000
H	-4.838404000	0.869474000	1.076112000
H	-3.622474000	1.739750000	2.048603000
H	-6.012429000	2.951455000	1.454989000
H	-4.508256000	3.889750000	1.430567000
H	-5.873088000	2.534450000	-0.961223000
H	-5.336547000	4.220822000	-0.853721000
C	3.397095000	2.609452000	0.011211000
C	3.252211000	1.625909000	1.001425000
C	3.831810000	1.907378000	2.249621000
C	4.515067000	3.095754000	2.502008000
C	4.638546000	4.046985000	1.494219000
C	4.076444000	3.802335000	0.243732000
H	2.966483000	2.434493000	-0.970885000
H	4.944466000	3.265911000	3.484018000
H	4.167858000	4.535989000	-0.552251000
C	-0.453659000	3.843224000	-0.194613000
C	-0.141506000	2.514446000	-0.612001000
C	-0.304490000	2.249070000	-1.991823000
C	-0.675024000	3.248198000	-2.907157000
C	-0.901436000	4.540053000	-2.467121000
C	-0.787916000	4.835168000	-1.099465000
H	-0.734176000	3.012724000	-3.964615000
H	-0.952177000	5.846674000	-0.740474000
C	0.331950000	1.491185000	0.320561000

C	1.323529000	0.439428000	-0.196288000
H	0.726646000	1.978329000	1.205270000
H	1.649994000	0.684869000	-1.214630000
H	0.880926000	-0.573208000	-0.275255000
C	0.015779000	-1.156534000	-3.336617000
H	0.875212000	-1.425721000	-2.717720000
H	-0.057836000	-1.908819000	-4.132277000
H	0.249395000	-0.210526000	-3.836786000
Si	-0.827588000	-3.726070000	-1.263781000
C	1.030711000	-3.687730000	-0.894951000
H	1.235664000	-3.252120000	0.086629000
H	1.390603000	-4.723821000	-0.873330000
H	1.622337000	-3.157591000	-1.646714000
C	-1.650617000	-4.809760000	0.049676000
H	-2.685641000	-5.056579000	-0.205431000
H	-1.091267000	-5.753218000	0.084853000
H	-1.627727000	-4.377220000	1.053146000
C	-1.097580000	-4.595117000	-2.931827000
H	-2.161479000	-4.619762000	-3.193424000
H	-0.557538000	-4.120623000	-3.757106000
H	-0.747747000	-5.632270000	-2.862526000
C	-0.687492000	-4.025144000	3.820324000
C	-2.001263000	-3.567896000	3.858663000
C	-2.359997000	-2.424676000	3.146691000
C	-1.436326000	-1.710822000	2.358230000
C	-0.121050000	-2.202959000	2.348236000
C	0.257829000	-3.330961000	3.067268000
H	-2.750341000	-4.078656000	4.455165000
H	0.622006000	-1.675056000	1.758093000
C	-1.799460000	-0.433188000	1.708315000
C	-0.989690000	0.702175000	1.897939000
H	-2.874320000	-0.264032000	1.640699000
H	-1.439364000	1.686286000	1.997432000
H	-0.087400000	0.575731000	2.488042000
H	1.289212000	-3.670239000	3.034221000
Cl	-4.007257000	-1.852489000	3.339474000
Cl	3.720649000	0.756632000	3.568342000
H	5.172021000	4.972619000	1.690369000
H	-1.151382000	5.330686000	-3.168260000
H	-0.407905000	-4.911493000	4.381846000
H	0.038488000	1.295390000	-2.387390000
Cl	-0.337882000	4.286420000	1.487107000

oP3^a_{syn}, $E_{(\text{SCF Done})} = -3794.073374$ a.u.

Sc	2.691951000	0.394256000	0.133049000
Si	-7.164567000	0.815230000	1.936931000
C	-5.652720000	0.774723000	0.763501000
C	-6.575869000	0.960581000	3.736837000
C	-8.197573000	-0.761716000	1.727178000
C	-8.211449000	2.331963000	1.486833000
C	5.098789000	1.948199000	2.426418000
C	4.392669000	0.695325000	1.987195000
C	4.890367000	-0.281594000	1.076553000
C	4.017707000	-1.411170000	1.127255000
C	2.957526000	-1.142575000	2.056172000
C	3.211315000	0.172453000	2.583937000
C	6.196845000	-0.219541000	0.337105000
C	4.295890000	-2.722293000	0.450129000
C	-4.696551000	-0.400258000	0.981866000
C	-3.440413000	-0.472235000	0.067195000
H	-5.130315000	1.734807000	0.886548000
H	-6.037013000	0.764401000	-0.265647000
H	-5.989056000	0.087385000	4.044625000
H	-7.432691000	1.036097000	4.416482000
H	-5.956842000	1.853599000	3.884307000
H	-8.539664000	-0.879083000	0.692339000
H	-9.085845000	-0.726162000	2.368611000
H	-7.631182000	-1.660027000	1.998008000
H	-7.641507000	3.261275000	1.603146000
H	-9.095520000	2.402003000	2.131180000
H	-8.560697000	2.279773000	0.449042000
H	5.945514000	2.193042000	1.779703000
H	5.506889000	1.814387000	3.436675000
H	4.443311000	2.825800000	2.464517000
H	6.521798000	0.807482000	0.139456000
H	6.158667000	-0.744426000	-0.622144000
H	6.991934000	-0.692322000	0.928830000
H	4.952297000	-2.604524000	-0.416287000
H	3.385362000	-3.220757000	0.115325000
H	4.808095000	-3.399668000	1.147125000
H	-5.241350000	-1.344324000	0.855127000
H	-4.335546000	-0.397890000	2.020497000
H	-2.911904000	-1.375973000	0.388908000
C	4.334797000	3.165918000	-0.684590000
O	3.278122000	2.209021000	-1.006382000
C	2.621430000	2.615173000	-2.259231000
C	3.143515000	4.010983000	-2.551244000
C	4.552354000	3.964178000	-1.957755000

H	3. 975619000	3. 792823000	0. 137105000
H	5. 207263000	2. 599440000	-0. 359634000
H	2. 912537000	1. 895668000	-3. 028690000
H	1. 544408000	2. 567250000	-2. 097449000
H	3. 135490000	4. 227466000	-3. 622823000
H	2. 534249000	4. 766048000	-2. 043362000
H	5. 239936000	3. 438908000	-2. 630150000
H	4. 966625000	4. 954725000	-1. 751159000
C	-4. 117875000	0. 420299000	-2. 222360000
C	-3. 814015000	-0. 667960000	-1. 389496000
C	-3. 923686000	-1. 941507000	-1. 971500000
C	-4. 303448000	-2. 128028000	-3. 299388000
C	-4. 593344000	-1. 022895000	-4. 093456000
C	-4. 501107000	0. 256303000	-3. 550862000
H	-4. 056459000	1. 424188000	-1. 812735000
H	-4. 372909000	-3. 134527000	-3. 699303000
H	-4. 731409000	1. 127383000	-4. 158071000
C	-0. 542069000	3. 189675000	-0. 585279000
C	-0. 364652000	1. 915870000	-0. 017452000
C	0. 522258000	1. 840589000	1. 074921000
C	1. 174942000	2. 968636000	1. 586149000
C	0. 964871000	4. 215326000	1. 001781000
C	0. 103189000	4. 323121000	-0. 085668000
H	1. 805908000	2. 877971000	2. 462771000
H	-0. 089782000	5. 287484000	-0. 546037000
C	-1. 156707000	0. 704174000	-0. 455627000
C	-2. 496973000	0. 715300000	0. 325650000
H	-1. 391627000	0. 824016000	-1. 520592000
H	-3. 007798000	1. 664248000	0. 123222000
H	-2. 271057000	0. 723513000	1. 401879000
C	2. 546065000	0. 788102000	3. 786076000
H	1. 454759000	0. 829047000	3. 722100000
H	2. 784053000	0. 202080000	4. 683068000
H	2. 913858000	1. 800668000	3. 977400000
Si	1. 880206000	-2. 460176000	2. 942181000
C	0. 255549000	-1. 755682000	3. 632494000
H	-0. 359893000	-1. 250715000	2. 880403000
H	-0. 335631000	-2. 596161000	4. 016649000
H	0. 415195000	-1. 067407000	4. 467655000
C	1. 457246000	-3. 954578000	1. 861583000
H	2. 331076000	-4. 584490000	1. 669168000
H	0. 725641000	-4. 568658000	2. 401029000
H	1. 016547000	-3. 677781000	0. 899673000
C	2. 929414000	-3. 059447000	4. 406229000

H	3.868881000	-3.506958000	4.062996000
H	3.177788000	-2.246129000	5.096805000
H	2.383655000	-3.822716000	4.973744000
C	2.187435000	-4.212378000	-3.130377000
C	3.004867000	-3.083645000	-3.101334000
C	2.585353000	-1.992723000	-2.357893000
C	1.380117000	-1.898542000	-1.644745000
C	0.603423000	-3.073723000	-1.690069000
C	0.996124000	-4.200770000	-2.409819000
H	3.952048000	-3.059370000	-3.630965000
H	-0.343243000	-3.110164000	-1.161719000
C	0.998104000	-0.635883000	-0.939772000
C	-0.403669000	-0.626848000	-0.312096000
H	1.024704000	0.162722000	-1.716253000
H	-1.048275000	-1.365558000	-0.801240000
H	-0.368881000	-0.934196000	0.743195000
H	0.352091000	-5.075711000	-2.411719000
Cl	3.691702000	-0.599302000	-2.254678000
Cl	-3.586874000	-3.389066000	-1.032738000
H	-4.892376000	-1.166628000	-5.127865000
H	1.442703000	5.104027000	1.404117000
H	2.489427000	-5.085883000	-3.699893000
H	0.588542000	0.893490000	1.616754000
Cl	-1.602094000	3.417031000	-1.951128000

***oC3*^{iso}, $E_{(\text{SCF Done})} = -3794.043034$ a.u.**

Sc	-1.287744000	0.910600000	0.797493000
Si	6.436419000	1.055370000	-1.329399000
C	4.872090000	0.379163000	-0.456766000
C	5.950076000	2.260284000	-2.714613000
C	7.431025000	-0.382891000	-2.062907000
C	7.478968000	1.964374000	-0.030967000
C	-1.993561000	2.933385000	3.717020000
C	-1.769722000	2.921212000	2.230151000
C	-2.773277000	2.922692000	1.217709000
C	-2.128591000	3.098771000	-0.036048000
C	-0.706521000	3.225727000	0.174637000
C	-0.506744000	3.120176000	1.591759000
C	-4.262843000	2.894346000	1.409628000
C	-2.883661000	3.376463000	-1.306241000
C	3.901382000	-0.387027000	-1.359351000
C	2.671094000	-1.040950000	-0.672424000
H	4.368775000	1.229690000	0.026947000
H	5.221774000	-0.270184000	0.357912000

H	5. 363930000	1. 761868000	-3. 495293000
H	6. 845078000	2. 676636000	-3. 191499000
H	5. 359526000	3. 100356000	-2. 330346000
H	7. 717867000	-1. 106088000	-1. 290668000
H	8. 351376000	-0. 015037000	-2. 531329000
H	6. 862367000	-0. 919416000	-2. 830952000
H	6. 929238000	2. 804357000	0. 409785000
H	8. 395818000	2. 365613000	-0. 477935000
H	7. 773236000	1. 290906000	0. 782285000
H	-3. 041178000	2. 754782000	3. 975634000
H	-1. 729238000	3. 913712000	4. 133460000
H	-1. 393336000	2. 185484000	4. 245703000
H	-4. 543260000	2. 756977000	2. 457683000
H	-4. 752112000	2. 104396000	0. 827399000
H	-4. 705539000	3. 845668000	1. 088436000
H	-3. 841587000	2. 847511000	-1. 340880000
H	-2. 320792000	3. 123325000	-2. 207857000
H	-3. 120073000	4. 447048000	-1. 370848000
H	4. 439580000	-1. 187623000	-1. 882710000
H	3. 520066000	0. 281558000	-2. 145069000
H	2. 115751000	-1. 534844000	-1. 480125000
C	-3. 512105000	-0. 296914000	2. 782721000
O	-3. 013704000	-0. 265474000	1. 403293000
C	-3. 679389000	-1. 311846000	0. 614601000
C	-4. 387129000	-2. 182274000	1. 637274000
C	-4. 748626000	-1. 177688000	2. 732449000
H	-2. 723373000	-0. 725734000	3. 406675000
H	-3. 705571000	0. 732757000	3. 082018000
H	-4. 380571000	-0. 811424000	-0. 058142000
H	-2. 914826000	-1. 833423000	0. 037985000
H	-5. 260259000	-2. 678829000	1. 205397000
H	-3. 708033000	-2. 950765000	2. 020758000
H	-5. 629958000	-0. 592165000	2. 447491000
H	-4. 948375000	-1. 648917000	3. 698692000
C	3. 416922000	-1. 836793000	1. 632553000
C	3. 090311000	-2. 126723000	0. 299222000
C	3. 237254000	-3. 466247000	-0. 096025000
C	3. 673575000	-4. 460448000	0. 778068000
C	3. 984984000	-4. 132511000	2. 093923000
C	3. 857129000	-2. 813527000	2. 521839000
H	3. 327793000	-0. 812068000	1. 981059000
H	3. 768966000	-5. 480867000	0. 421110000
H	4. 103522000	-2. 541753000	3. 544586000
C	-0. 364768000	-2. 174082000	2. 259162000

C	0.186490000	-0.947937000	1.783561000
C	0.402558000	0.038197000	2.782746000
C	0.186036000	-0.202318000	4.147850000
C	-0.305112000	-1.429535000	4.564133000
C	-0.581970000	-2.416285000	3.605948000
H	0.436788000	0.564661000	4.875700000
H	-0.945872000	-3.391598000	3.915768000
C	0.365174000	-0.599604000	0.380323000
C	1.698827000	0.006082000	-0.082435000
H	0.074423000	-1.427979000	-0.268939000
H	2.175317000	0.562802000	0.734327000
H	1.531927000	0.746216000	-0.878273000
C	0.760154000	3.397088000	2.353515000
H	1.650565000	2.973560000	1.881178000
H	0.924705000	4.480169000	2.426361000
H	0.703287000	3.021762000	3.379938000
Si	0.493636000	4.026226000	-1.097375000
C	2.283627000	4.105346000	-0.482804000
H	2.706139000	3.119185000	-0.264388000
H	2.885860000	4.545624000	-1.287098000
H	2.405261000	4.741508000	0.398625000
C	0.546257000	3.153016000	-2.784791000
H	-0.418662000	3.098992000	-3.298708000
H	1.216453000	3.734793000	-3.430153000
H	0.962464000	2.141703000	-2.724007000
C	-0.125826000	5.800344000	-1.346959000
H	-1.117730000	5.833007000	-1.809240000
H	-0.179516000	6.338493000	-0.394054000
H	0.563150000	6.346523000	-2.002142000
C	-4.527887000	-3.534228000	-3.909497000
C	-5.331733000	-2.460890000	-3.537628000
C	-4.745727000	-1.312203000	-3.012503000
C	-3.349709000	-1.195955000	-2.848140000
C	-2.570443000	-2.302519000	-3.238306000
C	-3.142612000	-3.454908000	-3.756776000
H	-6.409517000	-2.506389000	-3.654380000
H	-1.489814000	-2.244827000	-3.149265000
H	-2.509959000	-4.286126000	-4.053059000
C	-2.743372000	0.031061000	-2.328746000
C	-1.443203000	0.227451000	-2.024835000
H	-3.423873000	0.869113000	-2.211397000
H	-1.081369000	1.231895000	-1.805030000
H	-0.682301000	-0.531726000	-2.164155000
H	-4.985658000	-4.428019000	-4.323341000

H	-0.461532000	-1.641726000	5.617490000
H	4.328742000	-4.905993000	2.774934000
Cl	-5.818818000	-0.008883000	-2.548956000
Cl	2.881241000	-3.959919000	-1.742853000
Cl	-0.699994000	-3.469392000	1.137411000
H	0.907943000	0.955779000	2.489700000

***o*TS3^a_{iso}, $E_{(\text{SCF Done})} = -3794.022963$ a.u. $\text{IF} = i119.9$ cm⁻¹**

Sc	-1.734902000	0.686043000	0.487641000
Si	6.542471000	1.524447000	-0.496811000
C	4.911486000	0.666282000	0.027634000
C	6.212758000	2.711305000	-1.941265000
C	7.810397000	0.213374000	-1.014953000
C	7.192528000	2.499678000	0.994769000
C	-2.969952000	2.553486000	3.372505000
C	-2.509708000	2.608740000	1.941411000
C	-3.319827000	2.599682000	0.768673000
C	-2.483766000	2.911485000	-0.339941000
C	-1.135358000	3.115081000	0.127848000
C	-1.177538000	2.928693000	1.548060000
C	-4.813623000	2.457703000	0.691078000
C	-3.019368000	3.254812000	-1.700869000
C	4.202634000	-0.103592000	-1.089680000
C	2.918673000	-0.886158000	-0.698238000
H	4.251929000	1.440626000	0.447186000
H	5.156806000	-0.011275000	0.857089000
H	5.836911000	2.182644000	-2.824982000
H	7.136491000	3.223782000	-2.233875000
H	5.480291000	3.480591000	-1.669220000
H	8.005037000	-0.493645000	-0.200200000
H	8.764205000	0.682914000	-1.282195000
H	7.470863000	-0.360597000	-1.884596000
H	6.479618000	3.270660000	1.310032000
H	8.136486000	3.000676000	0.751234000
H	7.378111000	1.841678000	1.851691000
H	-4.057818000	2.475014000	3.450501000
H	-2.687404000	3.477343000	3.891941000
H	-2.533907000	1.722935000	3.940849000
H	-5.260325000	2.242798000	1.665918000
H	-5.127287000	1.669812000	-0.003015000
H	-5.265881000	3.392936000	0.337521000
H	-3.924976000	2.691734000	-1.944088000
H	-2.295372000	3.082698000	-2.501291000
H	-3.289867000	4.318718000	-1.736192000

H	4.894072000	-0.828830000	-1.537041000
H	3.928063000	0.588336000	-1.898732000
H	2.552027000	-1.327304000	-1.634132000
C	-4.001941000	-0.553256000	2.518534000
O	-3.330565000	-0.625443000	1.217719000
C	-3.832313000	-1.797629000	0.483295000
C	-4.494109000	-2.663050000	1.536431000
C	-5.087062000	-1.617821000	2.481310000
H	-3.246435000	-0.756720000	3.281161000
H	-4.384565000	0.458077000	2.636450000
H	-4.546132000	-1.433070000	-0.258321000
H	-2.987077000	-2.263846000	-0.021507000
H	-5.247485000	-3.322796000	1.097531000
H	-3.752867000	-3.283002000	2.052264000
H	-6.015520000	-1.208872000	2.067775000
H	-5.302948000	-2.008970000	3.479407000
C	3.298452000	-1.858247000	1.630931000
C	3.229061000	-2.036747000	0.240977000
C	3.524502000	-3.325376000	-0.234538000
C	3.862392000	-4.375635000	0.617289000
C	3.919895000	-4.158821000	1.990398000
C	3.637463000	-2.893422000	2.498726000
H	3.091666000	-0.875330000	2.044782000
H	4.081414000	-5.352558000	0.198536000
H	3.687554000	-2.707719000	3.568136000
C	-0.479424000	-2.268781000	1.697491000
C	-0.000763000	-0.984261000	1.299533000
C	0.020542000	0.000981000	2.319267000
C	-0.329622000	-0.277687000	3.647385000
C	-0.746680000	-1.553034000	3.997312000
C	-0.821774000	-2.546150000	3.012981000
H	-0.233841000	0.496957000	4.402356000
H	-1.115915000	-3.557200000	3.278001000
C	0.450016000	-0.670850000	-0.065414000
C	1.796902000	0.050861000	-0.206685000
H	0.443892000	-1.595215000	-0.636715000
H	2.078420000	0.532093000	0.736123000
H	1.730667000	0.863372000	-0.941822000
C	-0.101152000	3.265446000	2.541421000
H	0.905541000	3.038360000	2.182914000
H	-0.119161000	4.341355000	2.762404000
H	-0.251212000	2.750548000	3.495433000
Si	0.176164000	4.142470000	-0.835589000
C	1.845626000	4.261231000	0.058521000

H	2.292089000	3.283380000	0.268881000
H	2.535300000	4.793973000	-0.607910000
H	1.791964000	4.830976000	0.990658000
C	0.577799000	3.515003000	-2.585790000
H	-0.292553000	3.297177000	-3.211366000
H	1.140770000	4.312663000	-3.086945000
H	1.224583000	2.630760000	-2.580118000
C	-0.546317000	5.890216000	-0.967836000
H	-1.453583000	5.917106000	-1.579822000
H	-0.794022000	6.292628000	0.020691000
H	0.186181000	6.562621000	-1.430071000
C	-3.611915000	-3.503081000	-3.688572000
C	-4.420575000	-2.386720000	-3.491053000
C	-3.899450000	-1.255359000	-2.871867000
C	-2.561592000	-1.172819000	-2.429425000
C	-1.779565000	-2.325934000	-2.650269000
C	-2.285170000	-3.465765000	-3.264615000
H	-5.454612000	-2.383710000	-3.821056000
H	-0.738245000	-2.324683000	-2.345058000
H	-1.636131000	-4.323193000	-3.418800000
C	-2.000624000	0.045291000	-1.832895000
C	-0.605853000	0.227300000	-1.664685000
H	-2.586069000	0.945316000	-1.990219000
H	-0.281936000	1.261620000	-1.540123000
H	0.101733000	-0.339491000	-2.263194000
H	-4.016719000	-4.385261000	-4.175353000
H	-0.994220000	-1.795413000	5.026684000
H	4.188389000	-4.975945000	2.653972000
Cl	-4.991480000	0.102789000	-2.656558000
Cl	3.485354000	-3.678311000	-1.952202000
Cl	-0.539377000	-3.586746000	0.565291000
H	0.476624000	0.959379000	2.089068000

oP3^a_{iso}, $E_{(\text{SCF Done})} = -3794.077119$ a.u.

Sc	-2.768257000	0.208158000	0.166155000
Si	7.094644000	1.460052000	1.630722000
C	5.545415000	0.471391000	1.092979000
C	6.562844000	3.078808000	2.469326000
C	8.174414000	1.844222000	0.119611000
C	8.066826000	0.392242000	2.860709000
C	-5.330475000	1.867639000	2.242729000
C	-4.506624000	1.884629000	0.985134000
C	-4.917291000	1.393727000	-0.289929000
C	-3.955711000	1.825133000	-1.254201000

C	-2.918859000	2.556334000	-0.583080000
C	-3.288009000	2.594069000	0.808571000
C	-6.225423000	0.709174000	-0.573951000
C	-4.101484000	1.675060000	-2.743298000
C	4.639597000	1.189515000	0.089959000
C	3.367959000	0.430403000	-0.387286000
H	4.993827000	0.216437000	2.009704000
H	5.897799000	-0.480155000	0.671677000
H	6.016206000	3.732444000	1.779538000
H	7.438006000	3.635019000	2.824844000
H	5.918413000	2.885818000	3.335211000
H	8.470486000	0.926232000	-0.401332000
H	9.090241000	2.364360000	0.423450000
H	7.654112000	2.486397000	-0.600056000
H	7.464017000	0.148532000	3.743382000
H	8.966203000	0.914634000	3.206831000
H	8.386599000	-0.550329000	2.401358000
H	-6.172765000	1.173943000	2.170845000
H	-5.759356000	2.861857000	2.424639000
H	-4.754106000	1.604151000	3.136795000
H	-6.506473000	-0.007996000	0.205583000
H	-6.217409000	0.169352000	-1.524834000
H	-7.037552000	1.445789000	-0.633639000
H	-4.917904000	0.999242000	-3.008627000
H	-3.195180000	1.299727000	-3.226538000
H	-4.332821000	2.648077000	-3.195126000
H	5.216587000	1.444702000	-0.807952000
H	4.301234000	2.146692000	0.512103000
H	2.888107000	1.107910000	-1.101735000
C	-4.468687000	-1.445464000	2.487904000
O	-3.449548000	-1.444426000	1.440365000
C	-2.898474000	-2.798997000	1.291921000
C	-3.307911000	-3.523230000	2.559631000
C	-4.678083000	-2.908125000	2.851262000
H	-4.073787000	-0.861178000	3.323654000
H	-5.358491000	-0.959725000	2.086642000
H	-3.350761000	-3.245846000	0.402675000
H	-1.821337000	-2.703685000	1.146791000
H	-3.347074000	-4.605686000	2.410823000
H	-2.603949000	-3.310344000	3.370408000
H	-5.446541000	-3.358101000	2.213000000
H	-4.990410000	-3.025798000	3.892482000
C	3.933681000	-2.054463000	-0.485245000
C	3.724479000	-0.833416000	-1.145566000

C	3.912354000	-0.841238000	-2.538560000
C	4.278679000	-1.991435000	-3.236318000
C	4.474928000	-3.183664000	-2.545429000
C	4.301955000	-3.213937000	-1.163477000
H	3.809512000	-2.092633000	0.593002000
H	4.412119000	-1.942799000	-4.312299000
H	4.459944000	-4.135805000	-0.610518000
C	0.297863000	-1.518896000	2.626564000
C	0.183792000	-0.508940000	1.654972000
C	-0.683864000	0.555989000	1.970429000
C	-1.367952000	0.630213000	3.189372000
C	-1.212971000	-0.381939000	4.133205000
C	-0.378121000	-1.458045000	3.847172000
H	-1.979092000	1.497023000	3.414334000
H	-0.226349000	-2.249509000	4.575083000
C	1.037951000	-0.476800000	0.406454000
C	2.375754000	0.221959000	0.770511000
H	1.272641000	-1.513747000	0.148035000
H	2.848356000	-0.337931000	1.586631000
H	2.148914000	1.215187000	1.184654000
C	-2.681781000	3.478183000	1.864583000
H	-1.595773000	3.386123000	1.955271000
H	-2.887099000	4.530505000	1.629126000
H	-3.123473000	3.291990000	2.848204000
Si	-1.698503000	3.767770000	-1.437041000
C	-0.234313000	4.251551000	-0.326149000
H	0.313830000	3.399520000	0.090277000
H	0.476458000	4.819119000	-0.939363000
H	-0.536784000	4.902083000	0.499839000
C	-0.997845000	3.117884000	-3.074026000
H	-1.762014000	3.037059000	-3.852526000
H	-0.251331000	3.839356000	-3.428621000
H	-0.494598000	2.149911000	-2.982456000
C	-2.704226000	5.337223000	-1.790502000
H	-3.546511000	5.132974000	-2.460565000
H	-3.106704000	5.774509000	-0.869898000
H	-2.071035000	6.092581000	-2.270844000
C	-1.244730000	-4.341151000	-2.939849000
C	-2.405763000	-3.616211000	-2.676248000
C	-2.274814000	-2.368800000	-2.085429000
C	-1.065642000	-1.745913000	-1.742848000
C	0.075855000	-2.517740000	-2.039521000
C	-0.010077000	-3.783280000	-2.616166000
H	-3.386479000	-4.012818000	-2.920327000

H	1.061415000	-2.107792000	-1.846507000
H	0.905603000	-4.328565000	-2.826321000
C	-1.041101000	-0.363603000	-1.167297000
C	0.347779000	0.175010000	-0.803435000
H	-1.438624000	0.298070000	-1.962351000
H	0.272262000	1.258079000	-0.635890000
H	1.034351000	0.077834000	-1.657121000
H	-1.312584000	-5.324280000	-3.395579000
H	-1.712440000	-0.324932000	5.096195000
H	4.768248000	-4.078294000	-3.087699000
Cl	-3.770640000	-1.463481000	-1.732335000
Cl	3.695536000	0.622865000	-3.480519000
Cl	1.328789000	-2.901019000	2.361821000
H	-0.708874000	1.416646000	1.298370000

$mC3^a_{syn}$, $E_{(SCF Done)} = -3794.048489$ a.u.

Sc	1.385926000	-0.841882000	-0.352536000
Si	-5.991301000	2.892787000	-0.515216000
C	-4.786363000	1.406224000	-0.436993000
C	-5.082171000	4.485713000	-0.021451000
C	-7.453133000	2.597416000	0.656414000
C	-6.616893000	3.045065000	-2.299066000
C	-0.880371000	-2.287556000	-2.698802000
C	0.477614000	-2.405919000	-2.071954000
C	0.811065000	-3.183643000	-0.931824000
C	2.233887000	-3.111665000	-0.717042000
C	2.765740000	-2.320492000	-1.796876000
C	1.690211000	-1.876100000	-2.611685000
C	-0.175580000	-4.049235000	-0.199116000
C	4.210782000	-2.217952000	-2.198967000
C	1.824724000	-1.200859000	-3.946167000
C	-4.185986000	1.136589000	0.945701000
C	-3.143642000	-0.008220000	1.066394000
H	-3.994553000	1.591205000	-1.178572000
H	-5.340215000	0.525744000	-0.789411000
H	-4.733013000	4.450651000	1.016955000
H	-5.748653000	5.351137000	-0.113557000
H	-4.213828000	4.667879000	-0.666005000
H	-7.980734000	1.670202000	0.404417000
H	-8.175217000	3.419325000	0.587883000
H	-7.131586000	2.527883000	1.701921000
H	-5.793148000	3.222584000	-3.000475000
H	-7.320403000	3.880162000	-2.395101000
H	-7.137899000	2.134306000	-2.616262000

H	-1.683406000	-2.283303000	-1.956444000
H	-1.070484000	-3.135040000	-3.370731000
H	-0.980694000	-1.379693000	-3.303695000
H	-1.207978000	-3.744438000	-0.391407000
H	-0.030870000	-4.064149000	0.884188000
H	-0.084638000	-5.087595000	-0.544349000
H	4.454097000	-3.033568000	-2.892935000
H	4.894739000	-2.307635000	-1.352313000
H	4.441656000	-1.285880000	-2.724296000
H	2.719036000	-0.572677000	-4.008320000
H	0.954932000	-0.585685000	-4.199506000
H	1.913501000	-1.954631000	-4.740172000
H	-4.994766000	0.923338000	1.656883000
H	-3.694804000	2.048904000	1.316427000
H	-2.813965000	0.008765000	2.114914000
C	3.081252000	1.349701000	1.414771000
O	3.062625000	0.461421000	0.244778000
C	4.294367000	0.653734000	-0.522733000
C	4.961567000	1.882828000	0.071209000
C	4.520576000	1.814993000	1.533350000
H	2.398243000	2.179594000	1.212210000
H	2.726737000	0.774972000	2.268125000
H	4.902604000	-0.243380000	-0.391113000
H	4.018932000	0.762554000	-1.573799000
H	6.047635000	1.848223000	-0.052447000
H	4.589506000	2.795736000	-0.404462000
H	5.118109000	1.082812000	2.088147000
H	4.591582000	2.776523000	2.048836000
C	-4.053183000	-1.855115000	-0.444594000
C	-3.743196000	-1.383743000	0.838869000
C	-4.027726000	-2.212713000	1.931472000
C	-4.605726000	-3.468502000	1.753511000
C	-4.912772000	-3.934591000	0.477052000
C	-4.628950000	-3.113337000	-0.611109000
H	-3.866099000	-1.244064000	-1.321412000
H	-3.798978000	-1.865808000	2.936663000
H	-4.821469000	-4.093015000	2.616346000
C	0.913724000	-1.409418000	2.274453000
C	-0.015745000	-0.428399000	1.833303000
C	-0.124733000	0.747391000	2.622042000
C	0.583125000	0.869217000	3.807195000
C	1.470221000	-0.123193000	4.254284000
C	1.631133000	-1.256114000	3.469373000
H	0.943035000	-2.376476000	1.772177000

H	-0.816693000	1.533232000	2.339116000
H	2.292784000	-2.050420000	3.804736000
C	-0.696718000	-0.629547000	0.558764000
C	-1.883789000	0.254032000	0.205262000
H	-0.961920000	-1.686386000	0.442916000
H	-1.629352000	1.318457000	0.314167000
H	-2.130979000	0.126502000	-0.855645000
Si	3.318167000	-4.181226000	0.446317000
C	2.317234000	-5.095252000	1.772753000
H	1.764622000	-4.438194000	2.452976000
H	1.611726000	-5.811372000	1.340974000
H	3.027088000	-5.667307000	2.383231000
C	4.614054000	-3.119602000	1.351701000
H	5.407531000	-2.757525000	0.689593000
H	4.160028000	-2.254391000	1.848311000
H	5.097891000	-3.728818000	2.124838000
C	4.189733000	-5.486631000	-0.614101000
H	4.857462000	-5.043589000	-1.359876000
H	4.792340000	-6.144965000	0.022727000
H	3.459433000	-6.109600000	-1.142368000
C	3.528343000	5.655288000	-1.669720000
C	3.899287000	4.849203000	-2.743154000
C	3.229276000	3.653821000	-2.990832000
C	2.172182000	3.240651000	-2.163511000
C	1.791337000	4.062151000	-1.088324000
C	2.470350000	5.250467000	-0.850339000
H	4.711057000	5.162790000	-3.392977000
H	3.518521000	3.038030000	-3.839096000
H	0.954065000	3.797411000	-0.450886000
C	1.492501000	1.981449000	-2.470247000
C	0.510665000	1.378959000	-1.765359000
H	1.816890000	1.509157000	-3.396170000
H	-0.023102000	0.528192000	-2.188608000
H	0.077486000	1.825844000	-0.875087000
H	4.038960000	6.592134000	-1.471640000
H	1.995708000	-0.004949000	5.195663000
H	-5.364739000	-4.909312000	0.325609000
Cl	0.368342000	2.296206000	4.777435000
Cl	-5.001488000	-3.668087000	-2.225258000
Cl	1.989325000	6.253842000	0.483961000

$mTS3^a_{syn}$, $E_{(SCF\ Done)} = -3794.035799$ a.u. IF = $i180.5\text{cm}^{-1}$

Sc	1.588377000	-0.527443000	-0.483894000
Si	-6.737445000	2.260556000	-0.397716000

C	-5.204227000	1.109814000	-0.440105000
C	-6.192111000	4.042003000	-0.032024000
C	-7.945772000	1.668356000	0.938539000
C	-7.567586000	2.184003000	-2.100251000
C	-0.359550000	-2.439517000	-2.827951000
C	0.862314000	-2.430429000	-1.955436000
C	0.944358000	-2.936542000	-0.628325000
C	2.313005000	-2.877494000	-0.190311000
C	3.069989000	-2.373272000	-1.305929000
C	2.183280000	-2.093206000	-2.378365000
C	-0.206476000	-3.600488000	0.075759000
C	4.561915000	-2.439751000	-1.477014000
C	2.606684000	-1.764328000	-3.780619000
C	-4.424117000	1.028375000	0.874105000
C	-3.153572000	0.132986000	0.896617000
H	-4.559909000	1.464682000	-1.258317000
H	-5.559845000	0.113466000	-0.735925000
H	-5.731868000	4.134985000	0.958476000
H	-7.055099000	4.717545000	-0.056215000
H	-5.471647000	4.401592000	-0.776328000
H	-8.250530000	0.629465000	0.766662000
H	-8.852477000	2.284370000	0.936236000
H	-7.508914000	1.730305000	1.941844000
H	-6.889088000	2.519798000	-2.893198000
H	-8.454673000	2.827222000	-2.128504000
H	-7.889049000	1.164282000	-2.341784000
H	-1.279228000	-2.245207000	-2.266876000
H	-0.484907000	-3.422337000	-3.301079000
H	-0.296841000	-1.705612000	-3.638166000
H	-1.176580000	-3.248164000	-0.285678000
H	-0.193492000	-3.473523000	1.160477000
H	-0.177265000	-4.681752000	-0.114415000
H	4.828968000	-3.399041000	-1.940539000
H	5.102940000	-2.383916000	-0.530030000
H	4.948358000	-1.659029000	-2.139115000
H	3.432614000	-1.044993000	-3.816964000
H	1.785943000	-1.366298000	-4.385509000
H	2.956581000	-2.673007000	-4.288755000
H	-5.087812000	0.668015000	1.670571000
H	-4.108585000	2.036984000	1.178525000
H	-2.730198000	0.254223000	1.903673000
C	3.363771000	1.563451000	1.346783000
O	3.333785000	0.603195000	0.235110000
C	4.602346000	0.683318000	-0.495341000

C	5.252424000	1.971657000	-0.030771000
C	4.801938000	2.045059000	1.427712000
H	2.677475000	2.376109000	1.097538000
H	3.017811000	1.042953000	2.238273000
H	5.191617000	-0.192710000	-0.219520000
H	4.372455000	0.664674000	-1.561968000
H	6.339741000	1.936259000	-0.143641000
H	4.870278000	2.822899000	-0.602307000
H	5.401957000	1.376371000	2.055183000
H	4.861944000	3.053442000	1.845807000
C	-3.751670000	-1.916909000	-0.507345000
C	-3.485508000	-1.340240000	0.742356000
C	-3.586163000	-2.152356000	1.879512000
C	-3.943808000	-3.495417000	1.776358000
C	-4.207038000	-4.066891000	0.533034000
C	-4.106580000	-3.262380000	-0.599214000
H	-3.707149000	-1.326254000	-1.416646000
H	-3.392685000	-1.722273000	2.859728000
H	-4.022959000	-4.105862000	2.671973000
C	0.637796000	-0.634640000	2.114319000
C	-0.058365000	0.364890000	1.393923000
C	-0.115169000	1.662156000	1.965033000
C	0.428846000	1.902319000	3.216005000
C	1.087180000	0.894667000	3.941153000
C	1.198170000	-0.363925000	3.372247000
H	0.592077000	-1.666894000	1.777725000
H	-0.637076000	2.465476000	1.455816000
H	1.682617000	-1.162515000	3.926947000
C	-0.702752000	0.042607000	0.111526000
C	-2.091423000	0.638283000	-0.102509000
H	-0.752514000	-1.047360000	-0.025729000
H	-2.050829000	1.732631000	-0.016591000
H	-2.426282000	0.440246000	-1.126148000
Si	3.119917000	-3.716376000	1.331375000
C	1.865256000	-4.313787000	2.625430000
H	1.230222000	-3.527102000	3.047393000
H	1.215499000	-5.102750000	2.234433000
H	2.435211000	-4.747603000	3.456607000
C	4.326966000	-2.544563000	2.220673000
H	5.209574000	-2.303702000	1.619349000
H	3.845267000	-1.603782000	2.508706000
H	4.685969000	-3.029200000	3.136779000
C	4.056299000	-5.245828000	0.718764000
H	4.870967000	-4.992925000	0.032996000

H	4.492447000	-5.782315000	1.569810000
H	3.380828000	-5.935427000	0.200290000
C	3.498233000	4.744232000	-2.257602000
C	3.806431000	3.729543000	-3.163633000
C	3.117514000	2.520244000	-3.143515000
C	2.083472000	2.290090000	-2.217347000
C	1.782826000	3.311295000	-1.299805000
C	2.482188000	4.514541000	-1.330985000
H	4.585147000	3.894054000	-3.903515000
H	3.349676000	1.758955000	-3.884845000
H	0.990607000	3.185839000	-0.567460000
C	1.305415000	1.041413000	-2.299320000
C	-0.016379000	0.942903000	-1.852730000
H	1.605630000	0.364998000	-3.094297000
H	-0.666341000	0.217341000	-2.330624000
H	-0.518904000	1.839259000	-1.504614000
H	4.024289000	5.692782000	-2.271921000
H	1.481374000	1.105279000	4.929769000
H	-4.489413000	-5.110409000	0.440608000
Cl	0.287978000	3.483159000	3.916002000
Cl	-4.430826000	-3.947781000	-2.170990000
Cl	2.075387000	5.756399000	-0.178287000

$mP3^a_{syn}$, $E_{(SCF Done)} = -3794.076087$ a.u.

Sc	-2.132723000	0.370351000	-0.419032000
Si	7.579512000	-1.881931000	-0.132962000
C	5.873703000	-1.049176000	-0.393213000
C	7.335636000	-3.692767000	0.382395000
C	8.551026000	-0.956769000	1.208291000
C	8.519954000	-1.808037000	-1.777522000
C	-1.365441000	2.155135000	-3.458953000
C	-2.035141000	2.188320000	-2.117884000
C	-1.470891000	2.699029000	-0.920341000
C	-2.493561000	2.750234000	0.095804000
C	-3.699622000	2.271501000	-0.522137000
C	-3.415111000	1.905691000	-1.867403000
C	-0.074494000	3.248452000	-0.834370000
C	-5.075194000	2.278933000	0.085300000
C	-4.418337000	1.504489000	-2.912239000
C	4.974449000	-1.022772000	0.844921000
C	3.582590000	-0.348105000	0.686590000
H	5.382630000	-1.580991000	-1.220954000
H	6.060368000	-0.027156000	-0.751314000
H	6.815565000	-3.778380000	1.343522000

H	8. 304065000	-4. 195492000	0. 488037000
H	6. 756610000	-4. 246241000	-0. 366379000
H	8. 682404000	0. 099650000	0. 946753000
H	9. 548364000	-1. 394804000	1. 331287000
H	8. 049339000	-1. 003517000	2. 181701000
H	7. 979546000	-2. 337118000	-2. 571154000
H	9. 508248000	-2. 272426000	-1. 682205000
H	8. 669561000	-0. 772810000	-2. 105288000
H	-0. 289795000	1. 969752000	-3. 384673000
H	-1. 490059000	3. 122153000	-3. 964559000
H	-1. 790358000	1. 394197000	-4. 120805000
H	0. 616320000	2. 729316000	-1. 505356000
H	0. 346917000	3. 206404000	0. 172060000
H	-0. 066363000	4. 304835000	-1. 135797000
H	-5. 383012000	3. 304311000	0. 323663000
H	-5. 143633000	1. 702306000	1. 013357000
H	-5. 821496000	1. 885937000	-0. 610780000
H	-5. 242705000	0. 911649000	-2. 505847000
H	-3. 964621000	0. 921915000	-3. 717919000
H	-4. 861074000	2. 398017000	-3. 372272000
H	5. 494458000	-0. 509792000	1. 664437000
H	4. 796460000	-2. 049775000	1. 195159000
H	3. 090479000	-0. 463102000	1. 664061000
C	-3. 996085000	-0. 988588000	1. 931471000
O	-3. 777581000	-0. 758779000	0. 500842000
C	-4. 907497000	-1. 309434000	-0. 258889000
C	-5. 604970000	-2. 243091000	0. 711442000
C	-5. 417115000	-1. 518037000	2. 045278000
H	-3. 255215000	-1. 721795000	2. 259072000
H	-3. 831046000	-0. 041922000	2. 451073000
H	-5. 547568000	-0. 470463000	-0. 547411000
H	-4. 501868000	-1. 796712000	-1. 145053000
H	-6. 656417000	-2. 387954000	0. 448604000
H	-5. 113965000	-3. 221660000	0. 723704000
H	-6. 132936000	-0. 694234000	2. 143085000
H	-5. 532582000	-2. 174663000	2. 911866000
C	3. 854996000	1. 689890000	-0. 836914000
C	3. 710317000	1. 146274000	0. 445893000
C	3. 740688000	2. 020131000	1. 541438000
C	3. 919808000	3. 390617000	1. 366063000
C	4. 062854000	3. 929268000	0. 088445000
C	4. 025259000	3. 063658000	-1. 001388000
H	3. 847416000	1. 054647000	-1. 716798000
H	3. 637386000	1. 616385000	2. 546584000

H	3.952312000	4.048932000	2.230274000
C	-0.171346000	0.309529000	1.459626000
C	0.505238000	-0.778137000	0.875576000
C	0.473007000	-2.009308000	1.545680000
C	-0.163651000	-2.126644000	2.779803000
C	-0.799169000	-1.034299000	3.380114000
C	-0.802067000	0.181474000	2.708815000
H	-0.051362000	1.303127000	1.026243000
H	0.979340000	-2.875051000	1.129935000
H	-1.256733000	1.050873000	3.174281000
C	1.248876000	-0.621295000	-0.434381000
C	2.715724000	-1.082582000	-0.346772000
H	1.251346000	0.448806000	-0.683596000
H	2.749635000	-2.158104000	-0.122272000
H	3.151979000	-0.986848000	-1.348152000
Si	-2.475014000	3.821299000	1.683972000
C	-0.745068000	4.097461000	2.416894000
H	-0.181962000	3.182084000	2.628127000
H	-0.127829000	4.735716000	1.777339000
H	-0.871830000	4.625018000	3.370543000
C	-3.569795000	3.107874000	3.066755000
H	-4.631747000	3.110997000	2.804331000
H	-3.294844000	2.088586000	3.362122000
H	-3.455154000	3.741028000	3.955069000
C	-3.163557000	5.514575000	1.183855000
H	-4.185431000	5.446367000	0.795736000
H	-3.177949000	6.190162000	2.047249000
H	-2.541671000	5.974436000	0.407902000
C	-3.834296000	-3.990801000	-2.659148000
C	-3.720528000	-2.888006000	-3.505398000
C	-2.788573000	-1.883827000	-3.250926000
C	-1.920881000	-1.943044000	-2.138495000
C	-2.058491000	-3.057305000	-1.280556000
C	-2.991099000	-4.053578000	-1.549459000
H	-4.351630000	-2.826547000	-4.388257000
H	-2.685054000	-1.062428000	-3.955457000
H	-1.419105000	-3.161281000	-0.408467000
C	-0.923950000	-0.868644000	-1.874457000
C	0.499620000	-1.371636000	-1.551065000
H	-0.872150000	-0.236681000	-2.766187000
H	1.116131000	-1.318601000	-2.459685000
H	0.471380000	-2.436644000	-1.286147000
H	-4.543584000	-4.786889000	-2.858723000
H	-1.257025000	-1.139971000	4.358344000

H	4.205498000	4.994389000	-0.061946000
Cl	-0.154937000	-3.653215000	3.598466000
Cl	4.192359000	3.708999000	-2.615437000
Cl	-3.107776000	-5.416381000	-0.464470000

mC3^a_{iso}, $E_{(\text{SCF Done})} = -3794.047194$ a.u.

Sc	1.819089000	0.143676000	0.039427000
Si	-6.386479000	-0.513782000	1.433990000
C	-4.661328000	-0.872518000	0.681393000
C	-6.195181000	0.340322000	3.119195000
C	-7.345294000	-2.136860000	1.637460000
C	-7.310755000	0.633972000	0.239947000
C	-0.300577000	1.021421000	-2.652996000
C	1.117442000	0.744791000	-2.248056000
C	1.775905000	-0.511710000	-2.326034000
C	3.156915000	-0.341782000	-1.943508000
C	3.326078000	1.061238000	-1.669442000
C	2.078079000	1.719363000	-1.836117000
C	1.132541000	-1.757327000	-2.865587000
C	4.615209000	1.808346000	-1.466027000
C	1.881305000	3.204970000	-1.773789000
C	-3.754315000	-1.770102000	1.527397000
C	-2.357688000	-2.118209000	0.943084000
H	-4.182388000	0.099819000	0.492508000
H	-4.835133000	-1.327711000	-0.303182000
H	-5.694567000	-0.306391000	3.848931000
H	-7.177730000	0.599725000	3.530182000
H	-5.616721000	1.268122000	3.035033000
H	-7.436021000	-2.664061000	0.680670000
H	-8.358691000	-1.943020000	2.007672000
H	-6.858271000	-2.812610000	2.349678000
H	-6.780605000	1.583949000	0.103747000
H	-8.313011000	0.865048000	0.618915000
H	-7.427925000	0.170100000	-0.746324000
H	-0.983193000	0.222372000	-2.348203000
H	-0.378327000	1.108790000	-3.744658000
H	-0.670228000	1.961904000	-2.233784000
H	0.041409000	-1.696978000	-2.837368000
H	1.427006000	-2.664343000	-2.331036000
H	1.412840000	-1.901496000	-3.917247000
H	4.870102000	2.360374000	-2.380685000
H	5.457365000	1.145513000	-1.255824000
H	4.555815000	2.553895000	-0.663651000
H	2.437535000	3.663833000	-0.949359000

H	0.831588000	3.483402000	-1.659200000
H	2.240626000	3.671143000	-2.701472000
H	-4.267137000	-2.719273000	1.731503000
H	-3.586964000	-1.301548000	2.508380000
H	-1.858482000	-2.725796000	1.712035000
C	2.660032000	1.467525000	2.997603000
O	3.080117000	0.862005000	1.729655000
C	4.508719000	0.543402000	1.804984000
C	5.041244000	1.416478000	2.923951000
C	3.874415000	1.400756000	3.912757000
H	2.368191000	2.497192000	2.776904000
H	1.803801000	0.904892000	3.375651000
H	4.600471000	-0.520665000	2.039147000
H	4.938568000	0.746695000	0.825887000
H	5.966404000	1.016249000	3.347621000
H	5.239713000	2.432496000	2.563781000
H	3.869466000	0.469950000	4.489310000
H	3.893911000	2.236884000	4.616964000
C	-2.723952000	-2.465331000	-1.561792000
C	-2.450996000	-2.994563000	-0.293172000
C	-2.296807000	-4.381907000	-0.177389000
C	-2.415826000	-5.215980000	-1.287343000
C	-2.685487000	-4.687020000	-2.547825000
C	-2.835478000	-3.308104000	-2.665964000
H	-2.865778000	-1.398507000	-1.701519000
H	-2.086322000	-4.814534000	0.798176000
H	-2.296951000	-6.290194000	-1.173454000
C	2.084855000	-2.318770000	0.964978000
C	0.851315000	-1.746356000	1.393672000
C	0.676038000	-1.585227000	2.796534000
C	1.644585000	-2.029263000	3.682179000
C	2.839502000	-2.628935000	3.252475000
C	3.040775000	-2.770274000	1.887857000
H	2.206313000	-2.578123000	-0.086871000
H	-0.246939000	-1.168295000	3.186479000
H	3.935249000	-3.272822000	1.528430000
C	-0.032045000	-1.176080000	0.397044000
C	-1.479004000	-0.862144000	0.739228000
H	0.037373000	-1.730743000	-0.544469000
H	-1.552705000	-0.254764000	1.652301000
H	-1.912340000	-0.239443000	-0.052678000
Si	4.600041000	-1.555949000	-2.295423000
C	4.027069000	-3.340167000	-2.586090000
H	3.491313000	-3.778929000	-1.736789000

H	3.400132000	-3.441779000	-3.476302000
H	4.924692000	-3.949830000	-2.748922000
C	5.875736000	-1.639482000	-0.886246000
H	6.426606000	-0.707413000	-0.724355000
H	5.419807000	-1.940507000	0.063052000
H	6.617074000	-2.404637000	-1.147327000
C	5.452032000	-0.937441000	-3.870155000
H	5.862438000	0.070488000	-3.747742000
H	6.278336000	-1.605231000	-4.140746000
H	4.750389000	-0.913816000	-4.711283000
C	-1.515903000	6.784880000	-0.891865000
C	-0.471771000	6.952392000	0.014378000
C	0.014661000	5.867643000	0.737925000
C	-0.528942000	4.586340000	0.556257000
C	-1.593627000	4.421473000	-0.345840000
C	-2.071008000	5.513926000	-1.059222000
H	-0.042300000	7.939393000	0.159229000
H	0.825474000	6.011597000	1.447917000
H	-2.073508000	3.456255000	-0.469802000
C	0.017077000	3.467758000	1.325866000
C	-0.176519000	2.151280000	1.109759000
H	0.628372000	3.766419000	2.177897000
H	0.146420000	1.425908000	1.855256000
H	-0.810958000	1.777806000	0.311114000
H	-1.908356000	7.625791000	-1.454214000
H	-2.779498000	-5.326008000	-3.419629000
H	3.559023000	-2.997286000	3.975659000
Cl	-3.392431000	5.295777000	-2.167270000
Cl	1.370706000	-1.846889000	5.391387000
Cl	-3.168192000	-2.610806000	-4.233285000

mTS3^a_{iso}, $E_{(\text{SCF Done})} = -3794.028236$ a.u. $\text{IF} = i253.3$ cm^{-1}

Sc	-1.789184000	0.297950000	-0.401553000
Si	6.765828000	-1.385190000	-0.943295000
C	5.014806000	-0.917609000	-0.316144000
C	6.638797000	-2.212529000	-2.647535000
C	7.588331000	-2.571883000	0.286464000
C	7.775916000	0.212896000	-1.074894000
C	-0.265773000	2.910016000	1.519064000
C	-1.509580000	2.102882000	1.290352000
C	-1.854489000	0.915340000	1.989924000
C	-3.199298000	0.529412000	1.631171000
C	-3.653912000	1.518201000	0.691999000
C	-2.623449000	2.477666000	0.482278000

C	-0.985334000	0.329713000	3.069465000
C	-5.045695000	1.715776000	0.155433000
C	-2.825062000	3.782874000	-0.224695000
C	4.048153000	-2.093304000	-0.159493000
C	2.611514000	-1.771928000	0.340608000
H	4.613028000	-0.168879000	-1.014839000
H	5.148135000	-0.403015000	0.645132000
H	6.065390000	-3.145828000	-2.605351000
H	7.637053000	-2.457899000	-3.028170000
H	6.159724000	-1.552304000	-3.380211000
H	7.657555000	-2.124600000	1.284881000
H	8.606338000	-2.816301000	-0.038436000
H	7.037205000	-3.515006000	0.377023000
H	7.323278000	0.917036000	-1.782700000
H	8.794552000	0.002761000	-1.420685000
H	7.851449000	0.714860000	-0.103362000
H	0.634930000	2.291811000	1.596048000
H	-0.346710000	3.460014000	2.466096000
H	-0.100291000	3.643125000	0.727517000
H	0.076550000	0.526133000	2.894650000
H	-1.103144000	-0.748541000	3.193389000
H	-1.231128000	0.787347000	4.037451000
H	-5.469398000	2.646525000	0.555007000
H	-5.725623000	0.911389000	0.443495000
H	-5.072756000	1.809816000	-0.937404000
H	-3.363445000	3.668349000	-1.171107000
H	-1.885348000	4.293408000	-0.438216000
H	-3.427132000	4.451051000	0.406971000
H	4.474203000	-2.827697000	0.536175000
H	3.942540000	-2.615358000	-1.121526000
H	2.078511000	-2.733378000	0.339491000
C	-2.941228000	-0.944509000	-3.328448000
O	-3.169623000	-0.635485000	-1.910962000
C	-4.431951000	-1.255369000	-1.521041000
C	-5.272430000	-1.198487000	-2.778287000
C	-4.241456000	-1.560889000	-3.851448000
H	-2.691379000	-0.005120000	-3.825618000
H	-2.095053000	-1.632008000	-3.395453000
H	-4.225093000	-2.285577000	-1.213578000
H	-4.816707000	-0.690893000	-0.675735000
H	-6.113543000	-1.896342000	-2.745619000
H	-5.668160000	-0.188031000	-2.929875000
H	-4.142770000	-2.647903000	-3.932782000
H	-4.501113000	-1.173119000	-4.839825000

C	2. 907665000	0. 051960000	2. 107389000
C	2. 601181000	-1. 275134000	1. 775298000
C	2. 335412000	-2. 173395000	2. 817200000
C	2. 382766000	-1. 766051000	4. 149098000
C	2. 692790000	-0. 447909000	4. 477556000
C	2. 952265000	0. 448695000	3. 443850000
H	3. 135177000	0. 783134000	1. 338322000
H	2. 102894000	-3. 209452000	2. 580906000
H	2. 181809000	-2. 481062000	4. 942457000
C	-1. 427411000	-2. 271157000	0. 489013000
C	-0. 421508000	-1. 987854000	-0. 462179000
C	-0. 269842000	-2. 888353000	-1. 547503000
C	-1. 078414000	-4. 008495000	-1. 644824000
C	-2. 076454000	-4. 285564000	-0. 696198000
C	-2. 239440000	-3. 409394000	0. 363767000
H	-1. 478075000	-1. 693073000	1. 406490000
H	0. 507229000	-2. 732382000	-2. 288914000
H	-2. 973316000	-3. 630037000	1. 133617000
C	0. 365421000	-0. 750528000	-0. 378947000
C	1. 863457000	-0. 849376000	-0. 643277000
H	0. 217485000	-0. 254370000	0. 601726000
H	2. 041758000	-1. 229294000	-1. 658953000
H	2. 301725000	0. 154909000	-0. 622325000
Si	-4. 372949000	-0. 533699000	2. 719859000
C	-3. 463277000	-1. 734956000	3. 874661000
H	-2. 806294000	-2. 446788000	3. 362276000
H	-2. 875108000	-1. 214944000	4. 636148000
H	-4. 225198000	-2. 323159000	4. 401430000
C	-5. 643302000	-1. 591900000	1. 777618000
H	-6. 337636000	-1. 019033000	1. 154553000
H	-5. 178933000	-2. 366361000	1. 158414000
H	-6. 251488000	-2. 105997000	2. 532321000
C	-5. 313218000	0. 716828000	3. 788461000
H	-5. 923183000	1. 391775000	3. 178458000
H	-5. 981050000	0. 201926000	4. 489019000
H	-4. 619872000	1. 330733000	4. 374015000
C	0. 764492000	5. 520984000	-2. 575606000
C	-0. 458424000	5. 195919000	-3. 160008000
C	-1. 002230000	3. 923255000	-3. 016001000
C	-0. 334764000	2. 930944000	-2. 278729000
C	0. 898247000	3. 259886000	-1. 694990000
C	1. 430386000	4. 537059000	-1. 847901000
H	-0. 987700000	5. 945573000	-3. 741825000
H	-1. 947962000	3. 687274000	-3. 498468000

H	1.448823000	2.530907000	-1.108779000
C	-0.887332000	1.563928000	-2.228774000
C	-0.042984000	0.440102000	-2.201582000
H	-1.857158000	1.460324000	-2.721468000
H	-0.349878000	-0.472942000	-2.709719000
H	1.024127000	0.622426000	-2.254700000
H	1.196536000	6.509942000	-2.684268000
H	2.738532000	-0.120266000	5.510932000
H	-2.675649000	-5.185792000	-0.784331000
Cl	2.961444000	4.905641000	-1.102499000
Cl	-0.852078000	-5.108013000	-2.970339000
Cl	3.343589000	2.105608000	3.823736000

mP3_{iso}, $E_{(\text{SCF Done})} = -3794.06801$ a.u.

Sc	-2.299803000	0.121723000	-0.513012000
Si	7.567618000	-1.339127000	-0.951530000
C	5.801149000	-0.758396000	-0.489782000
C	7.511758000	-2.338891000	-2.564898000
C	8.278120000	-2.409872000	0.444012000
C	8.640332000	0.205331000	-1.193242000
C	-2.415787000	3.592422000	0.484920000
C	-3.117972000	2.270855000	0.419734000
C	-3.153594000	1.305853000	1.466507000
C	-4.139200000	0.301336000	1.148005000
C	-4.673839000	0.662111000	-0.134602000
C	-4.040785000	1.855511000	-0.585505000
C	-2.384847000	1.466571000	2.750167000
C	-5.833973000	0.028425000	-0.850243000
C	-4.421528000	2.627720000	-1.814776000
C	4.804283000	-1.885282000	-0.210219000
C	3.358033000	-1.470254000	0.181698000
H	5.451132000	-0.115551000	-1.310644000
H	5.893710000	-0.109245000	0.391511000
H	6.912145000	-3.250593000	-2.460202000
H	8.521736000	-2.642587000	-2.863653000
H	7.088075000	-1.747377000	-3.385149000
H	8.296975000	-1.863356000	1.394069000
H	9.307028000	-2.709219000	0.212987000
H	7.694764000	-3.325812000	0.592869000
H	8.246328000	0.842896000	-1.993256000
H	9.667007000	-0.068869000	-1.462166000
H	8.685677000	0.805741000	-0.277280000
H	-1.419231000	3.523934000	0.929093000
H	-3.001958000	4.281183000	1.108908000

H	-2.301441000	4.052785000	-0.497938000
H	-1.444322000	2.005100000	2.592415000
H	-2.153317000	0.514144000	3.232724000
H	-2.960995000	2.058824000	3.473448000
H	-6.734586000	0.645442000	-0.733604000
H	-6.074277000	-0.964067000	-0.461856000
H	-5.661285000	-0.063718000	-1.928921000
H	-4.706797000	1.973559000	-2.646789000
H	-3.611939000	3.276577000	-2.156449000
H	-5.289796000	3.267506000	-1.606074000
H	5.189389000	-2.517256000	0.600559000
H	4.724973000	-2.538778000	-1.091256000
H	2.828226000	-2.416713000	0.363389000
C	-2.835456000	-1.289035000	-3.423833000
O	-2.913638000	-1.409668000	-1.960176000
C	-3.647884000	-2.629622000	-1.614556000
C	-4.405971000	-2.999838000	-2.874640000
C	-3.421260000	-2.583550000	-3.969175000
H	-3.425173000	-0.412573000	-3.709138000
H	-1.789548000	-1.130659000	-3.691895000
H	-2.912551000	-3.391279000	-1.342227000
H	-4.274732000	-2.397318000	-0.753522000
H	-4.649986000	-4.065201000	-2.903271000
H	-5.339111000	-2.431117000	-2.948558000
H	-2.638063000	-3.339680000	-4.090537000
H	-3.898416000	-2.430639000	-4.940825000
C	3.547438000	0.667385000	1.577128000
C	3.314633000	-0.712040000	1.496450000
C	3.072118000	-1.414188000	2.684793000
C	3.066168000	-0.765114000	3.917492000
C	3.297093000	0.606518000	3.995666000
C	3.536110000	1.307613000	2.815963000
H	3.749094000	1.252479000	0.685007000
H	2.897131000	-2.487235000	2.642462000
H	2.884965000	-1.329955000	4.828221000
C	-0.530684000	-1.056119000	0.987966000
C	0.314939000	-1.372647000	-0.092804000
C	0.289214000	-2.683659000	-0.589439000
C	-0.520357000	-3.647911000	0.007293000
C	-1.347853000	-3.339397000	1.091152000
C	-1.350905000	-2.034970000	1.573895000
H	-0.437175000	-0.078944000	1.466258000
H	0.926890000	-2.966526000	-1.421341000
H	-1.960123000	-1.783936000	2.435394000

C	1.192056000	-0.312307000	-0.717550000
C	2.638351000	-0.770792000	-0.984086000
H	1.236356000	0.518446000	-0.004188000
H	2.660404000	-1.447241000	-1.851269000
H	3.197176000	0.118201000	-1.300851000
Si	-5.073020000	-0.830360000	2.387004000
C	-4.262435000	-0.925791000	4.100165000
H	-3.282668000	-1.414392000	4.127019000
H	-4.165869000	0.058261000	4.568252000
H	-4.930458000	-1.521741000	4.734719000
C	-5.310534000	-2.620771000	1.787505000
H	-5.963100000	-2.700446000	0.911304000
H	-4.363499000	-3.122783000	1.561419000
H	-5.794429000	-3.187782000	2.592201000
C	-6.776559000	-0.036943000	2.630528000
H	-7.360997000	-0.005205000	1.705531000
H	-7.353119000	-0.605212000	3.369989000
H	-6.675856000	0.989227000	3.000977000
C	0.153342000	5.295039000	-2.214254000
C	-0.763009000	4.682574000	-3.066364000
C	-1.053438000	3.325695000	-2.943129000
C	-0.453826000	2.530125000	-1.950038000
C	0.479054000	3.153920000	-1.104632000
C	0.770947000	4.508813000	-1.244744000
H	-1.239566000	5.268564000	-3.848140000
H	-1.740253000	2.864324000	-3.650229000
H	0.981016000	2.595318000	-0.321121000
C	-0.758863000	1.066229000	-1.857039000
C	0.523710000	0.197756000	-2.016674000
H	-1.390691000	0.850991000	-2.743574000
H	0.304592000	-0.682962000	-2.639822000
H	1.277257000	0.772883000	-2.574417000
H	0.395499000	6.348416000	-2.305208000
H	3.299153000	1.124458000	4.949190000
H	-1.949633000	-4.112751000	1.556979000
Cl	1.932967000	5.237594000	-0.168534000
Cl	-0.501387000	-5.270362000	-0.607319000
Cl	3.830133000	3.024589000	2.888653000