# Condensation of diaminoferrocenes with phosphorus trihalides: controllable access to P-functional [3]-ferrocenophane and [4]-ferrocenophane frameworks

Stefan Weller,[a] Simon H. Schlindwein,[a] Christoph M. Feil,[a] Zsolt Kelemen,[b] Dániel Buzsáki,[b] László Nyulászi,*[,b] Stefan Isenberg,[c] Rudolf Pietschnig,*[,c] Martin Nieger[d] and Dietrich Gudat*[,a]

[a] *Institut für Anorganische Chemie, University of Stuttgart, 70550 Stuttgart, Germany. Fax: +49 711 685 4241; E-mail: gudat@iac.uni-stuttgart.de*

[b] *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, and MTA-BME Computation Driven Chemistry Research Group, Szent Gellért tér 4, 1111 Budapest (Hungary)*

[c] *Institut für Chemie und CINSaT, Universität Kassel, Heinrich Plett-Straße 40 34132 Kassel (Germany)*

[d] *Laboratory of Inorganic Chemistry, Dept. of Chemistry, University of Helsinki, P.O Box 55, 00014 University of Helsinki, Finland.*

**Contents**:

## Crystallographic data

**Table S1.** Crystallographic data for **2c**, **3a**, **4b** and **4c**.

| | **2c** | **3a** | **4b** | **4c** |
|---|---|---|---|---|
| empirical formula | $C_{20}H_{30}ClFeN_2P$ | $C_{16}H_{26}BrFeN_2PSi_2$ | $C_{22}H_{38}Cl_4FeN_2P_2Si_2$ | $C_{20}H_{30}Cl_4FeN_2P_2$ |
| Formula weight ($g \cdot mol^{-1}$) | 420.73 | 469.30 | 646.31 | 558.05 |
| $T$ (K) | 100(2) | 110(2) | 130(2) | 100(2) |
| crystal size (mm) | 0.35 x 0.24 x 0.09 | 0.453 x 0.298 x 0.268 | 0.697 x 0.495 x 0.216 | 0.203 x 0.160 x 0.126 |
| space group | $P\,2_1/n$ | $P$ b c a | $P$-1 | $P\,2_1/n$ |
| $a$ (Å) | 11.0280(5) | 12.0271(8) | 9.6569(6) | 6.1281(6) |
| $b$ (Å) | 11.9843(6) | 11.9819(9) | 12.0446(8) | 11.3691(11) |
| $c$ (Å) | 16.0493(8) | 28.0180(19) | 14.3274(9) | 17.4983(17) |
| $\alpha$ (°) | 90 | 90 | 104.877(3) | 90 |
| $\beta$ (°) | 106.938(2) | 90 | 105.010(3) | 97.226(6) |
| $\gamma$ (°) | 90 | 90 | 96.568(4) | 90 |
| $V$ ($Å^3$) | 2029.11(17) | 4037.6(5) | 1526.17(17) | 1209.4(2) |
| Z | 4 | 8 | 2 | 2 |
| $D_c$ ($Mg \cdot m^{-3}$) | 1.377 | 1.544 | 1.406 | 1.532 |
| $\mu$ ($mm^{-1}$) | 0.959 | 2.924 | 1.043 | 1.209 |
| $F$ (000) | 888 | 1920 | 672 | 576 |
| $\Theta$ range (°) | 1.998 - 30.658 | 2.232 - 30.604 | 1.542 - 30.558 | 2.141 - 30.554 |
| reflections collected | 30685 | 41645 | 41017 | 14384 |
| unique reflections | 6236 | 6187 | 9268 | 3703 |
| observed reflections with [I > 2σ(I)] | 5181 | 4839 | 7965 | 2740 |
| $R_{int}$ | 0.0344 | 0.0387 | 0.0222 | 0.0567 |
| max./min transmission | 0.7461/0.6748 | 0.5176/0.4011 | 0.7461/0.6256 | 0.7461/0.6920 |
| data/restraints/ parameters | 6236/198/217 | 6187/0/209 | 9268/0/298 | 3703/0/133 |
| G.o.F. on $F^2$ | 1.022 | 1.014 | 1.054 | 1.026 |
| $R1$ [I > 2σ(I)] | 0.0347 | 0.0313 | 0.0267 | 0.0366 |
| w$R2$ ($F^2$) | 0.0774 | 0.0555 | 0.0656 | 0.0645 |
| largest diff. peak/ hole (e $Å^{-3}$) | 0.921/-0.619 | 0.414/-0.352 | 0.666/-0.392 | 0.475/-0.425 |
| CSD Number | CCDC-1587526 | CCDC-1587523 | CCDC-1587527 | CCDC-1587525 |

Table S2. Crystallographic data for **5b**, **5c** and **6c**.

| | **5b** | **5c** | **6c** |
|---|---|---|---|
| empirical formula | $C_{44}H_{76}Fe_2N_4P_4Si_4 – C_6H_{14}$ | $C_{40}H_{60}Fe_2N_4P_4 – C_6H_{14}$ | $C_{26}H_{44}FeN_3P$ |
| formula weight ($g \cdot mol^{-1}$) | 1095.19 | 918.67 | 485.46 |
| $T$ (K) | 100(2) | 100(2) | 100(2) |
| crystal size (mm) | 0.310 x 0.130 x 0.080 | 0.171 x 0.134 x 0.125 | 0.780 x 0.546 x 0.268 |
| space group | $P$-1 | $C$ 2/c | $P$ $2_1$/c |
| $a$ (Å) | 9.8345(6) | 15.3428(7) | 15.6619(11) |
| $b$ (Å) | 12.3291(7) | 17.1185(9) | 9.3742(6) |
| $c$ (Å) | 12.8154(8) | 18.4549(10) | 18.7966(13) |
| $\alpha$ (°) | 107.355(4) | 90 | 90 |
| $\beta$ (°) | 102.966(4) | 93.314(3) | 108.622(2) |
| $\gamma$ (°) | 98.309(4) | 90 | 90 |
| $V$ (Å$^3$) | 1407.48(15) | 4839.0(4) | 2615.2(3) |
| Z | 1 | 4 | 4 |
| $D_c$ ($Mg \cdot m^{-3}$) | 1.292 | 1.261 | 1.233 |
| $\mu$ ($mm^{-1}$) | 0.751 | 0.767 | 0.655 |
| $F$ (000) | 586 | 1960 | 1048 |
| $\Theta$ range (°) | 1.736 - 28.457 | 1.784 - 28.284 | 2.260 - 30.642 |
| reflections collected | 24921 | 42472 | 29203 |
| unique reflections | 7025 | 6013 | 8022 |
| observed reflections with [I > 2σ(I)] | 5269 | 4053 | 6784 |
| $R_{int}$ | 0.0447 | 0.0934 | 0.0256 |
| max./min transmission | 0.7357/0.6755 | 0.9320/0.8890 | 0.7461/0.7016 |
| data/restraints/ parameters | 7025/0/289 | 6013/109/274 | 8022/0/285 |
| G.o.F. on $F^2$ | 1.016 | 1.006 | 1.081 |
| $R1$ [I > 2σ(I)] | 0.0368 | 0.0417 | 0.0282 |
| w$R2$ ($F^2$) | 0.0773 | 0.0741 | 0.0670 |
| largest diff. peak/hole (e Å$^{-3}$) | 0.514/-0.367 | 0.384/-0.358 | 0.484/-0.369 |
| CSD Number | CCDC-1587521 | CCDC-1587522 | CCDC-1587524 |

**NMR spectra**

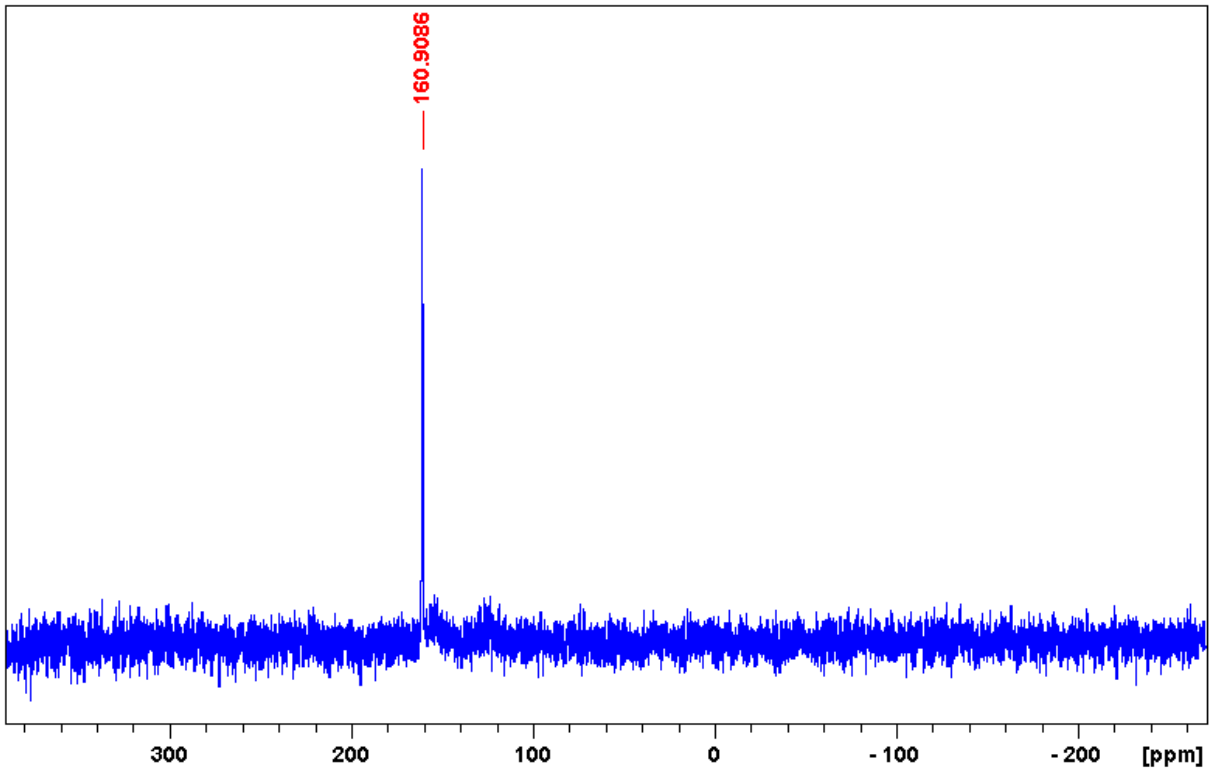


**Figure S1:** $^{31}P\{^{1}H\}$ NMR spectrum of **2a** (THF).

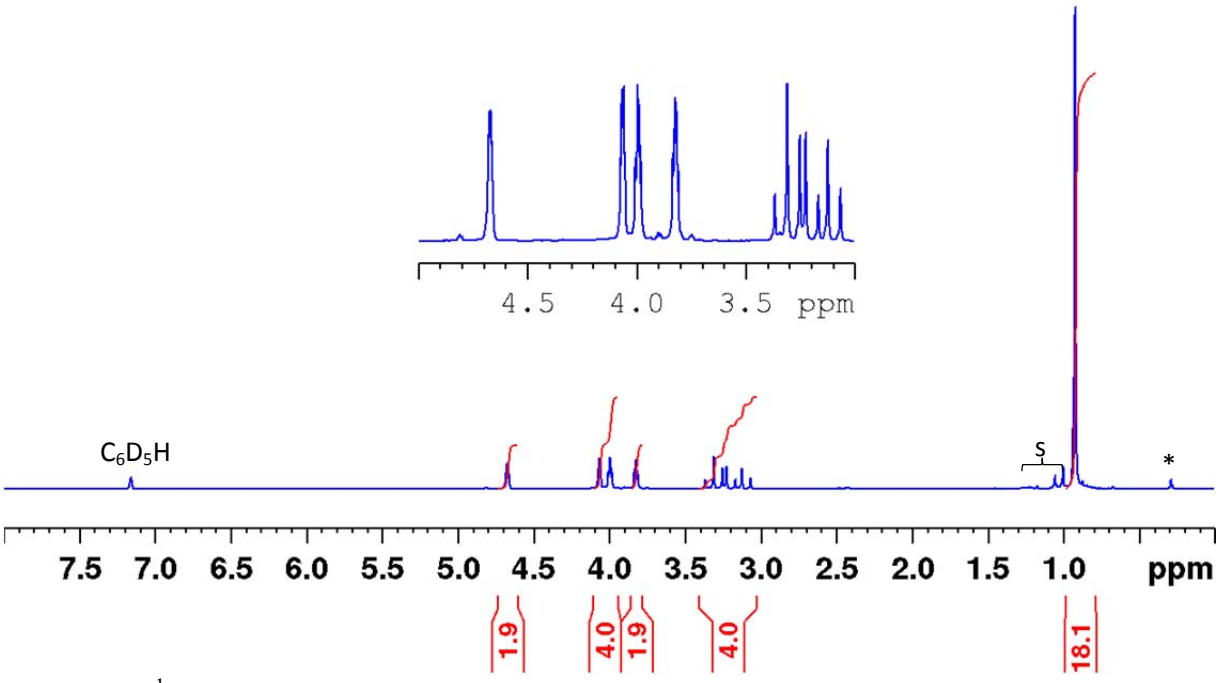


**Figure S2:** $^{1}H$ NMR spectrum of **2c** ($C_6D_6$; s and *denote signals of residual solvents and impurities, respectively).

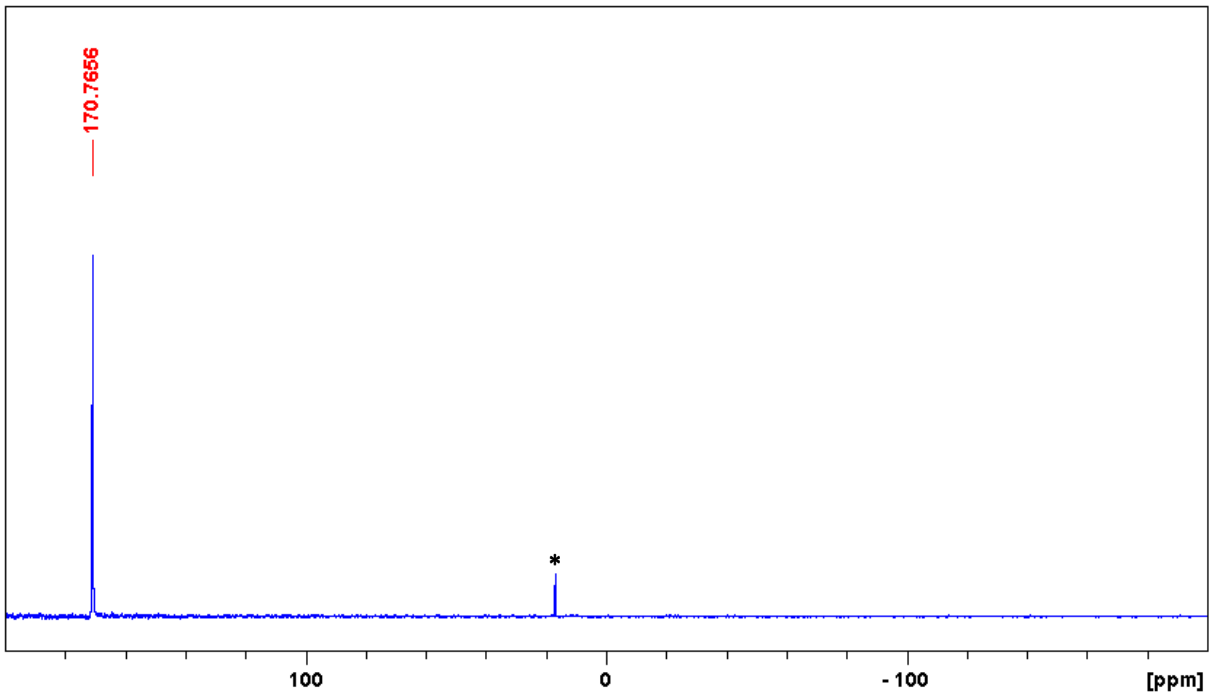


**Figure S3:** $^{31}P\{^{1}H\}$ NMR spectrum of **2c** ($C_6D_6$; * denotes the signal of a species formed by hydrolysis of **2c** by adventitious moisture).

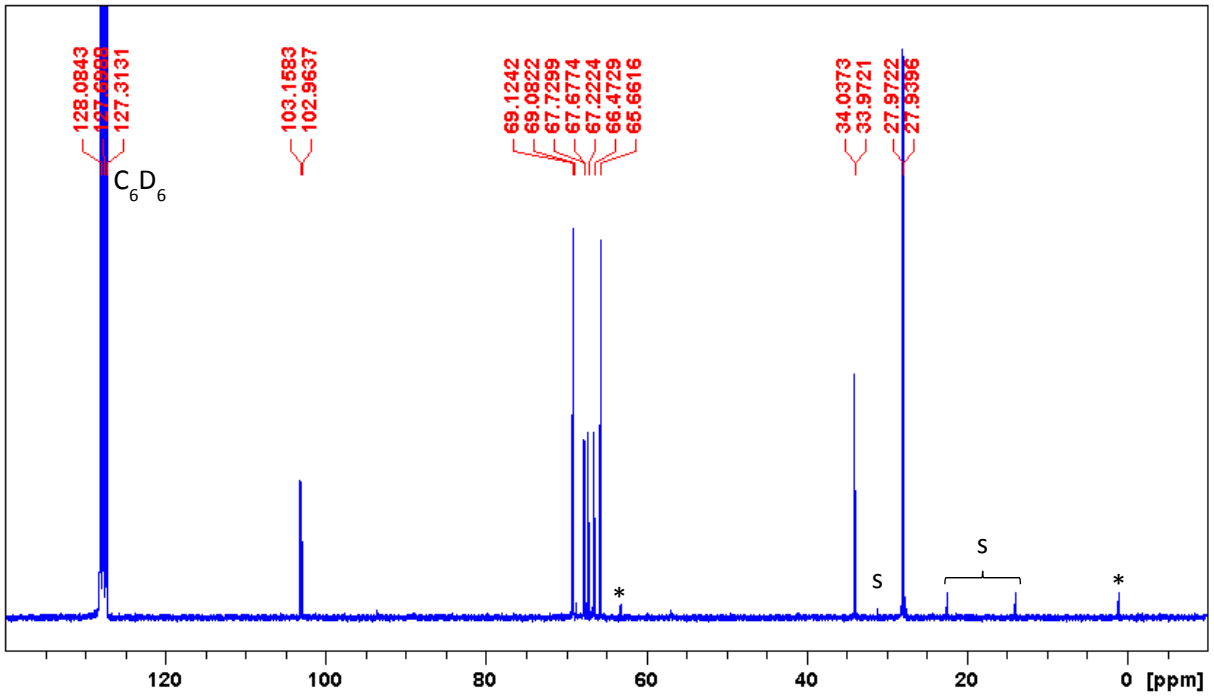


**Figure S4:** $^{13}C\{^{1}H\}$ NMR spectrum of **2c** ($C_6D_6$; s and *denote signals of residual solvents and impurities, respectively).

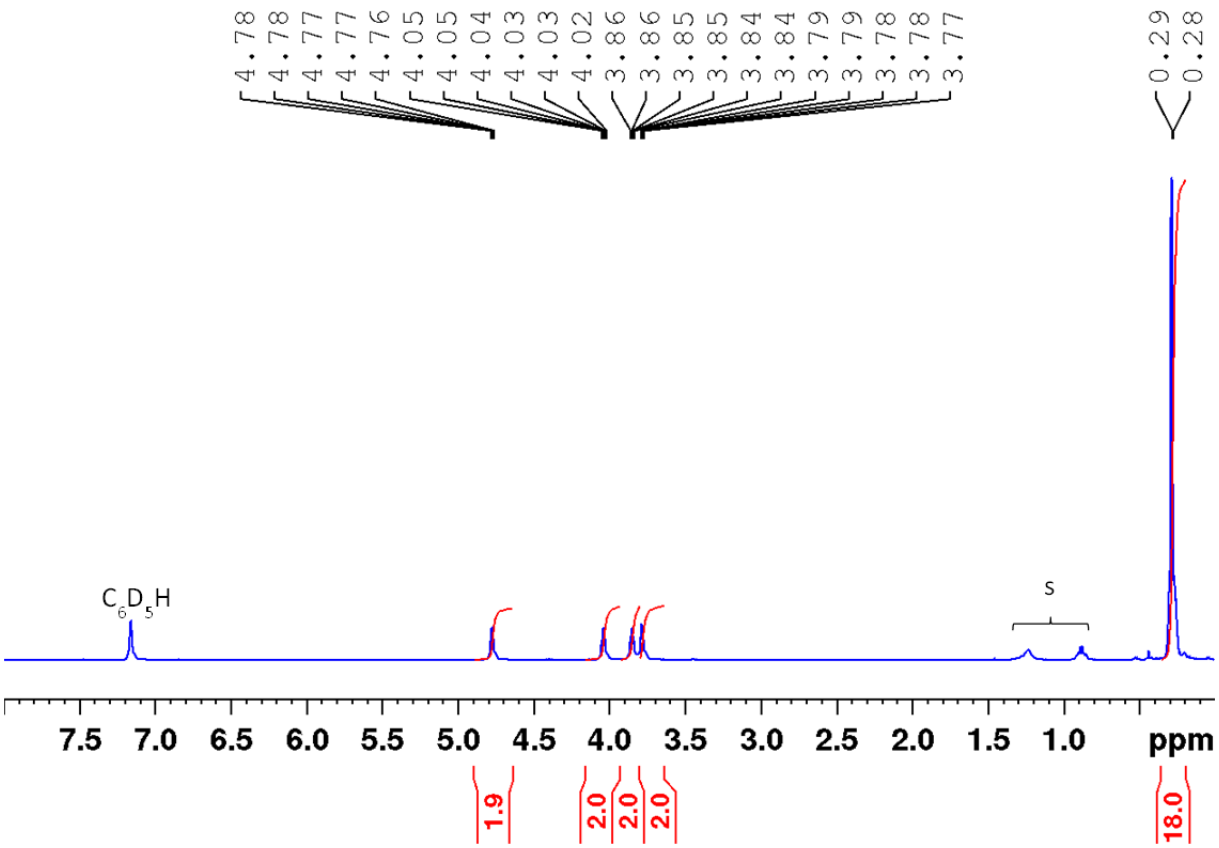


**Figure S5:** $^{1}$H NMR spectrum of **3a** ($C_6D_6$; s denotes signals of residual solvents).

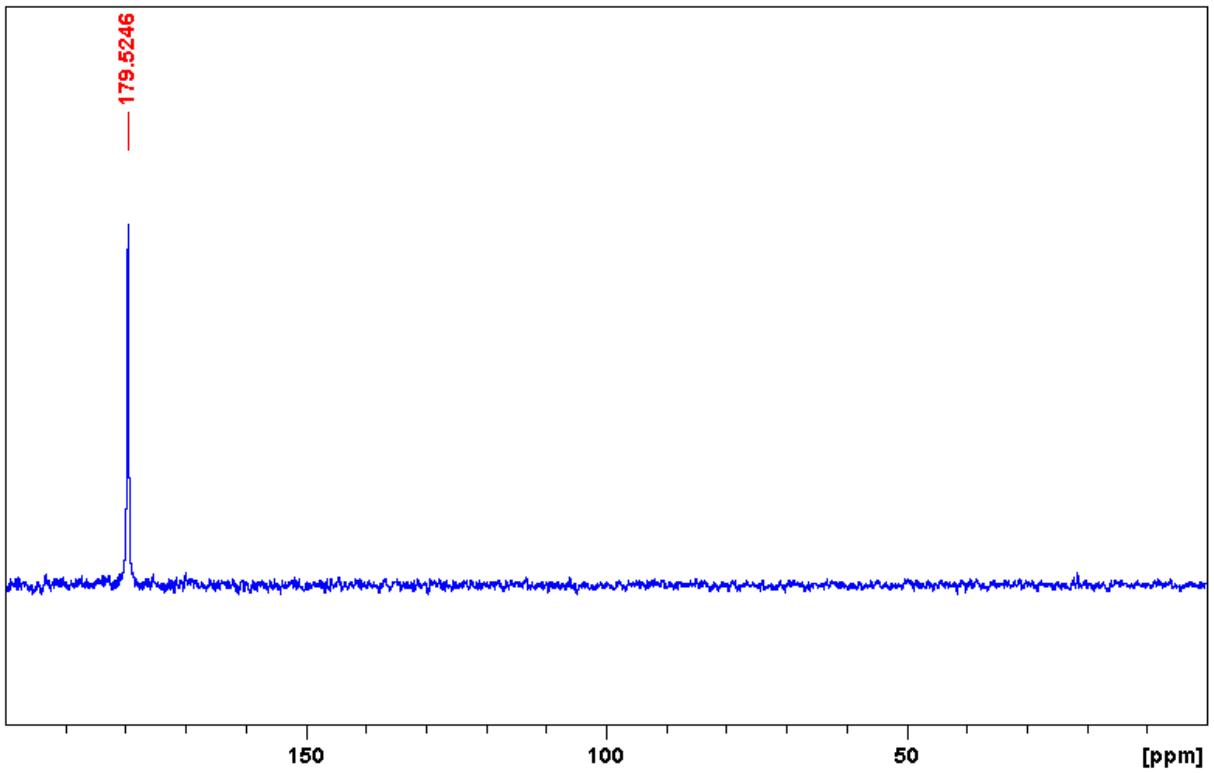


**Figure S6**: $^{31}$P{$^{1}$H} NMR spectrum of **3a** ($C_6D_6$).

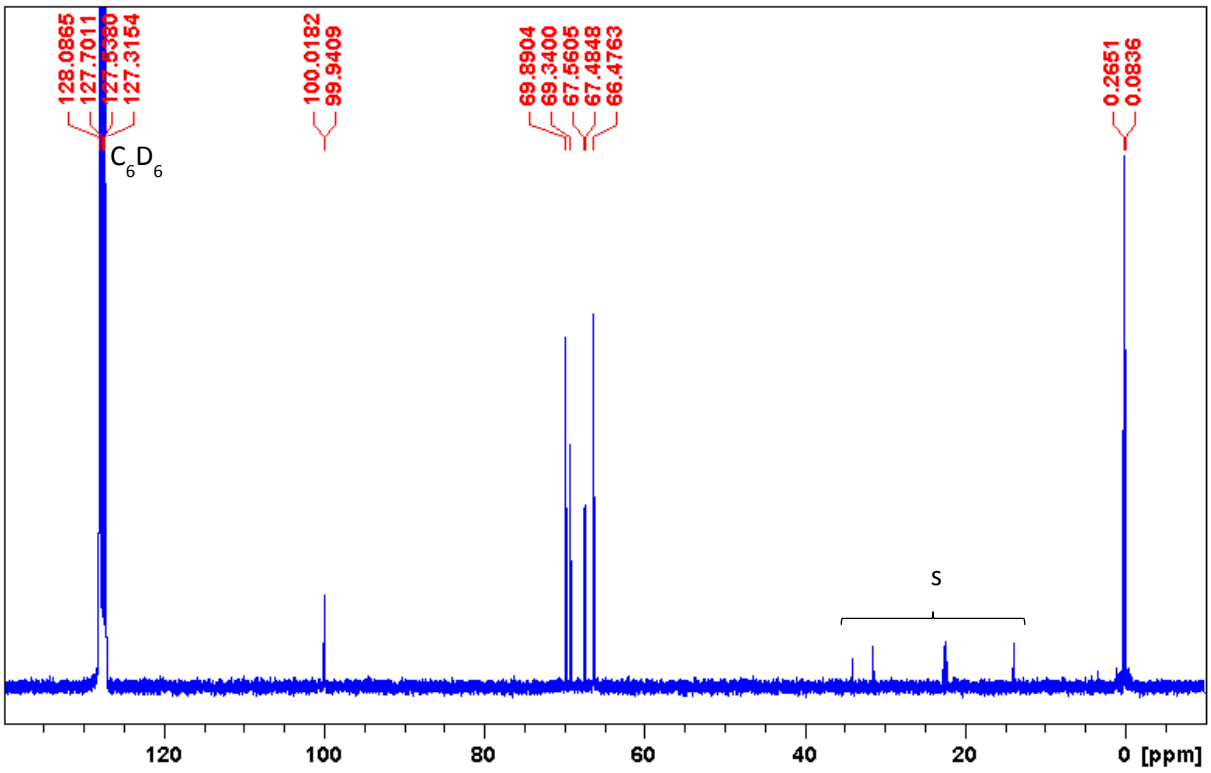


**Figure S7:** $^{13}C\{^{1}H\}$ NMR spectrum of **3a** ($C_6D_6$; s denotes signals of residual solvents).

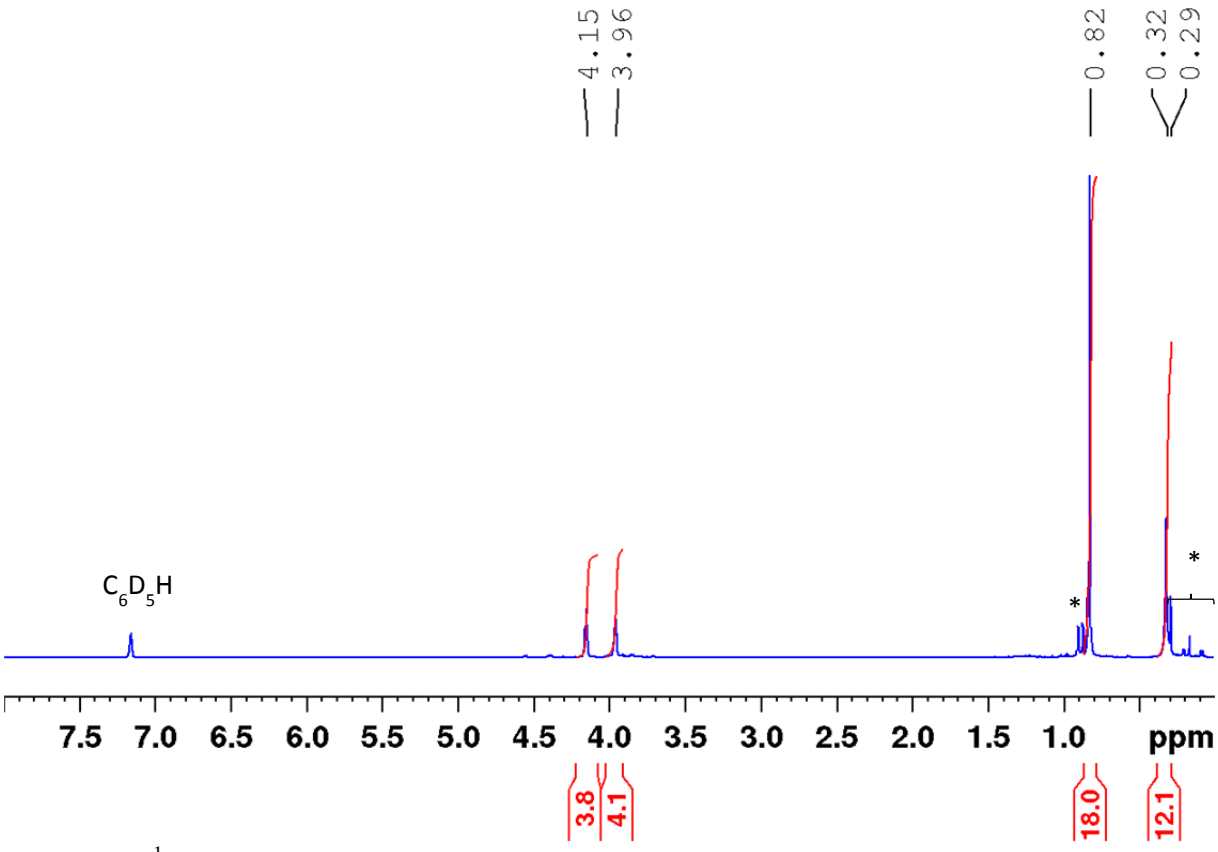


**Figure S8**: $^{1}H$ NMR spectrum of **4b** ($C_6D_6$; * denotes signals of impurities).

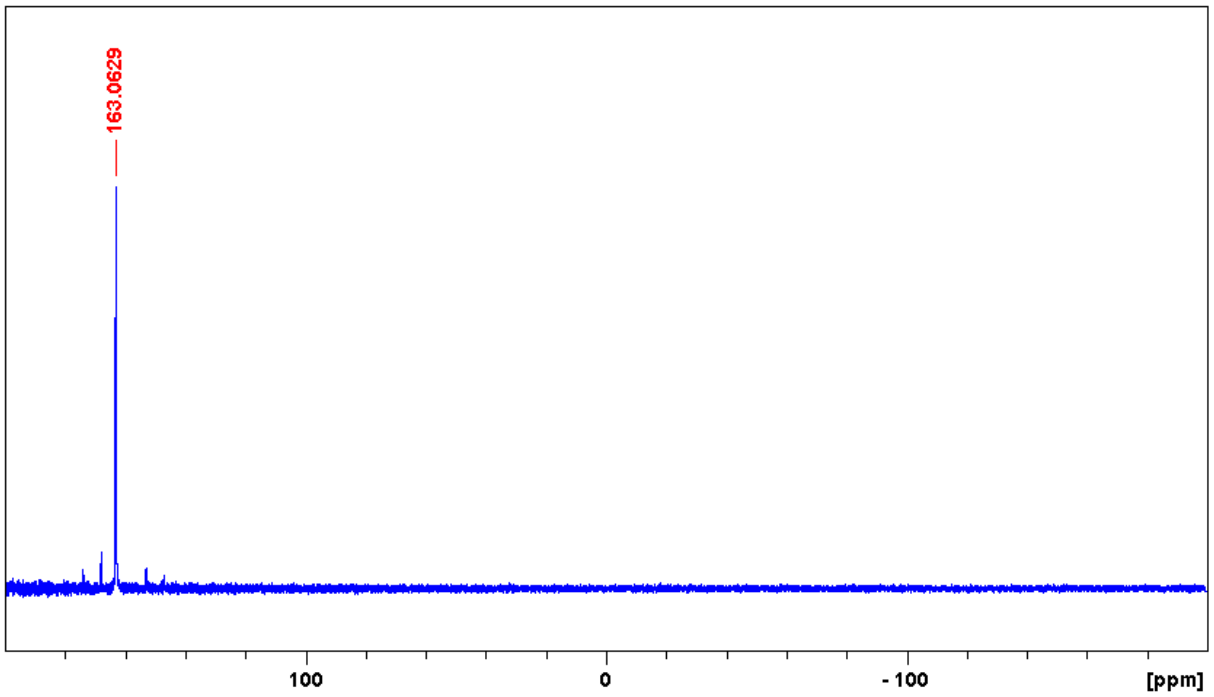


**Figure S9:** $^{31}P\{^{1}H\}$ NMR spectrum of **4b** ($C_6D_6$). Extra signals are due to a decomposition product arising from cleavage of $ClSiMe_3$.

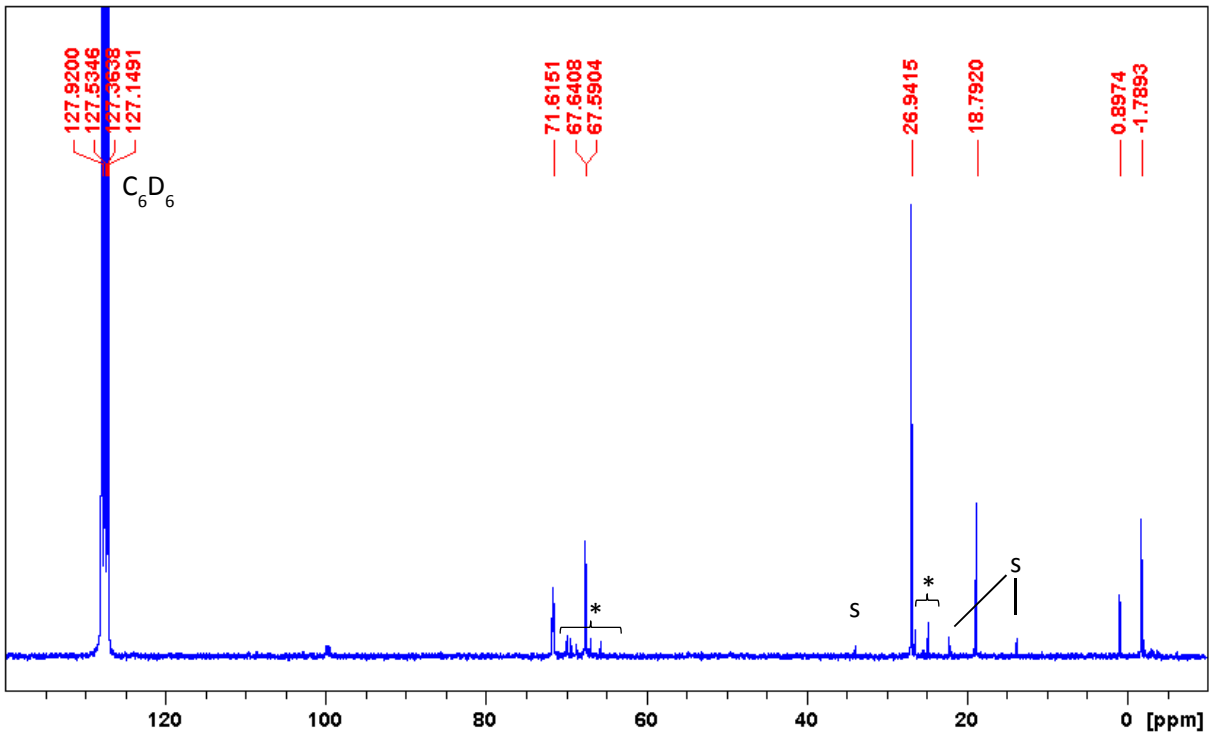


**Figure S10:** $^{13}C\{^{1}H\}$ NMR spectrum of **4b** ($C_6D_6$; s and * denote signals of residual solvents and a decomposition product arising from cleavage of $ClSiMe_3$).

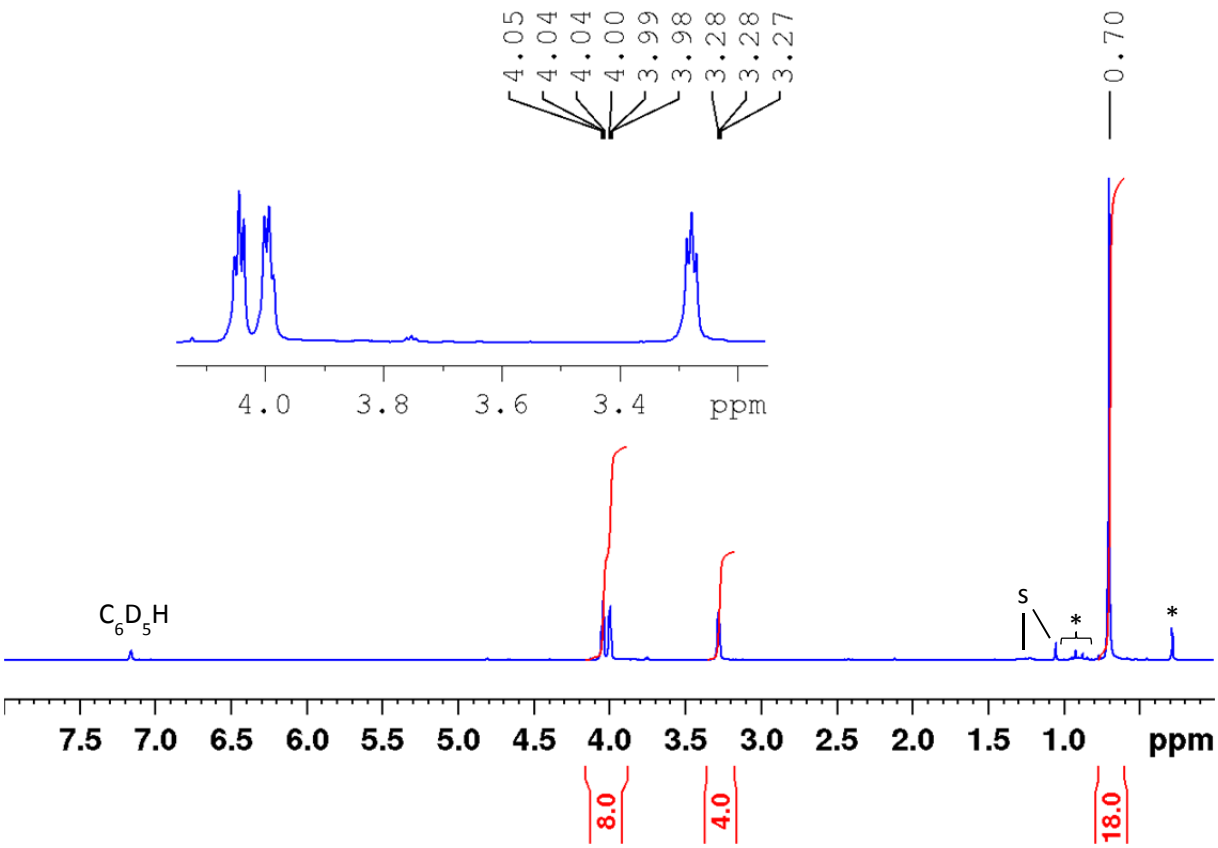


**Figure S11**: $^{1}$H NMR spectrum of **4c** ($C_6D_6$; s and * denote signals of residual solvents and decomposition products).

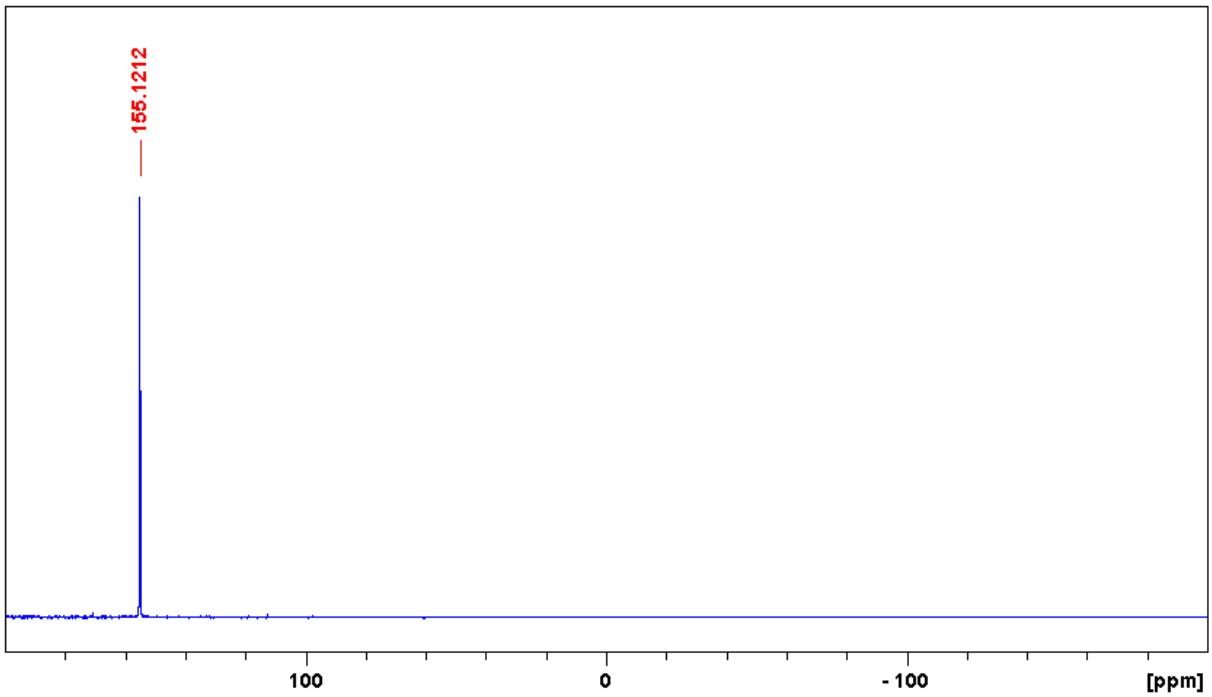


**Figure S12:** $^{31}$P{$^{1}$H} NMR spectrum of **4c** ($C_6D_6$).

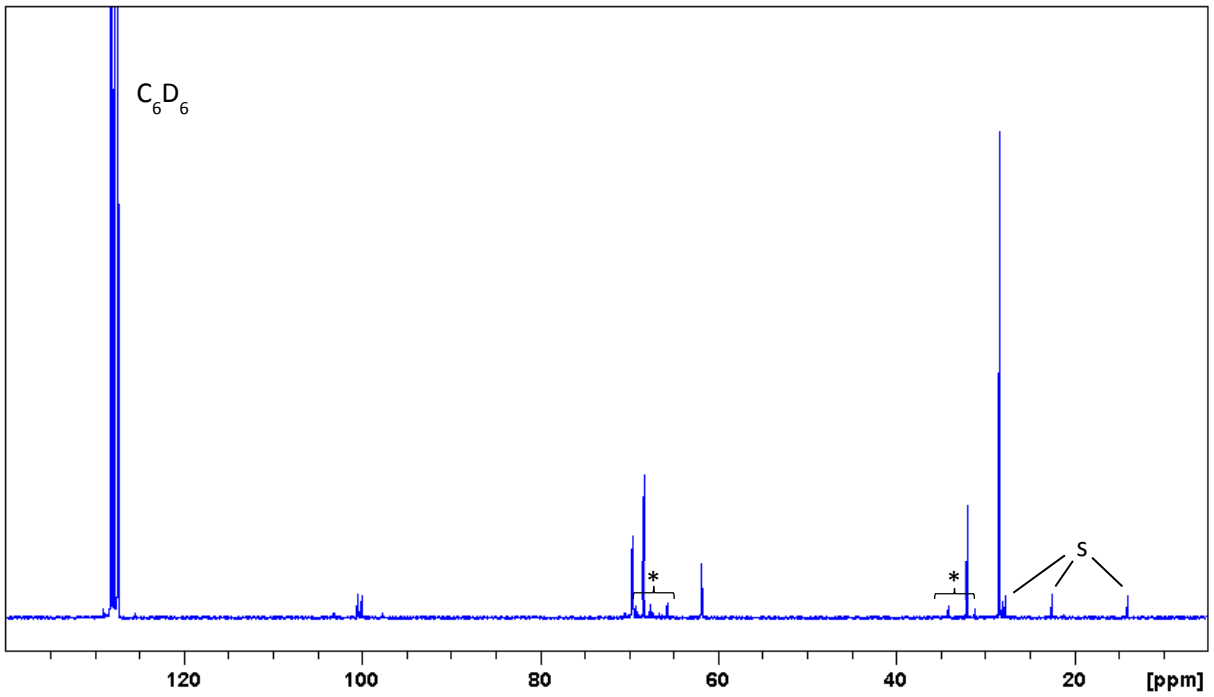


**Figure S13**: $^{13}C\{^{1}H\}$ NMR spectrum of **4c** ($C_6D_6$; s and * denote signals of residual solvents and impurities).

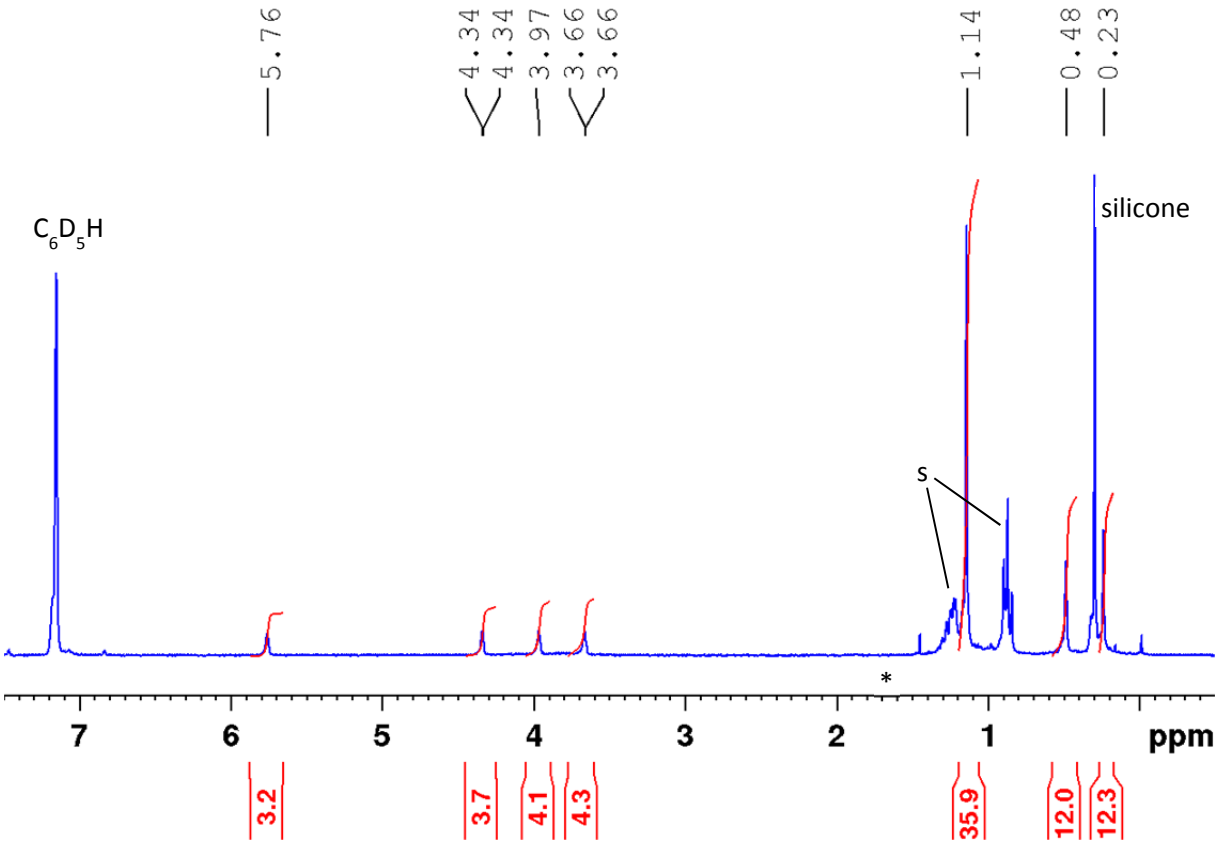


**Figure S14:** $^{1}H$ NMR spectrum of **5b** ($C_6D_6$; extra signals arising from residual solvent pentane and silicone sticking to the crystals are labelled).

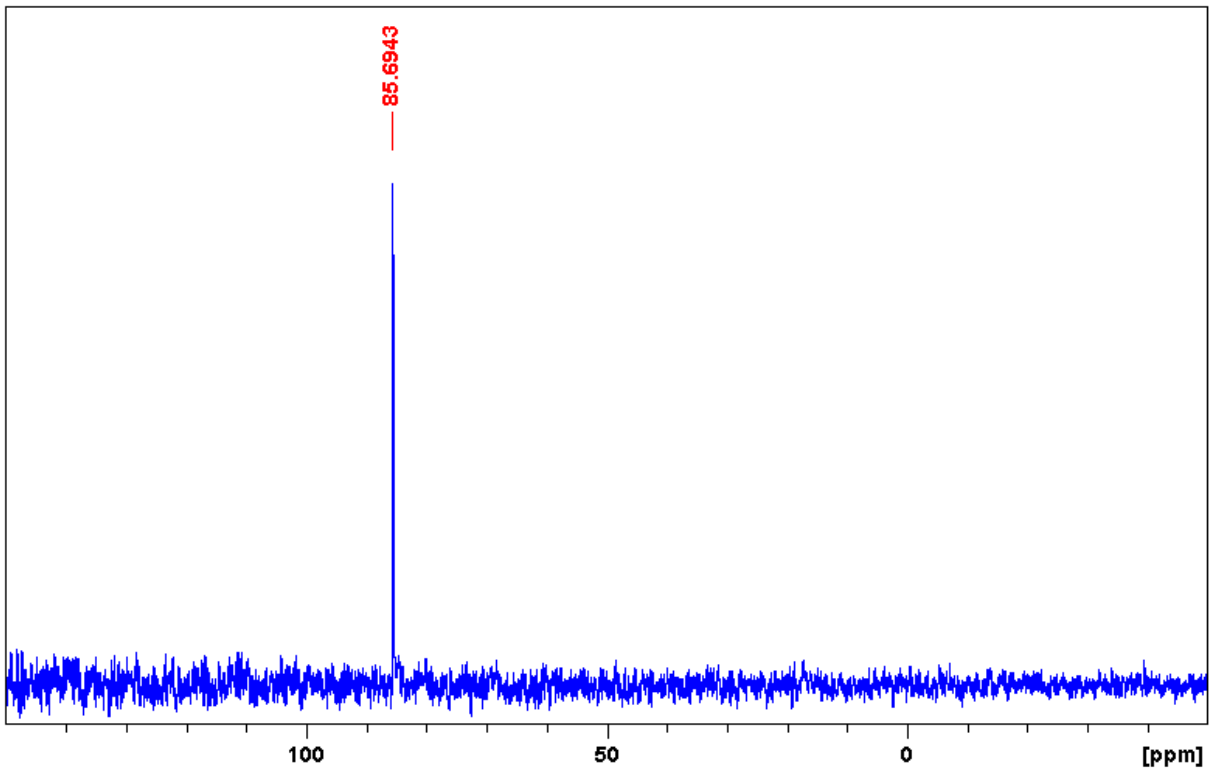


**Figure S15**: $^{31}P\{^{1}H\}$ NMR spectrum of **5b** ($C_6D_6$).

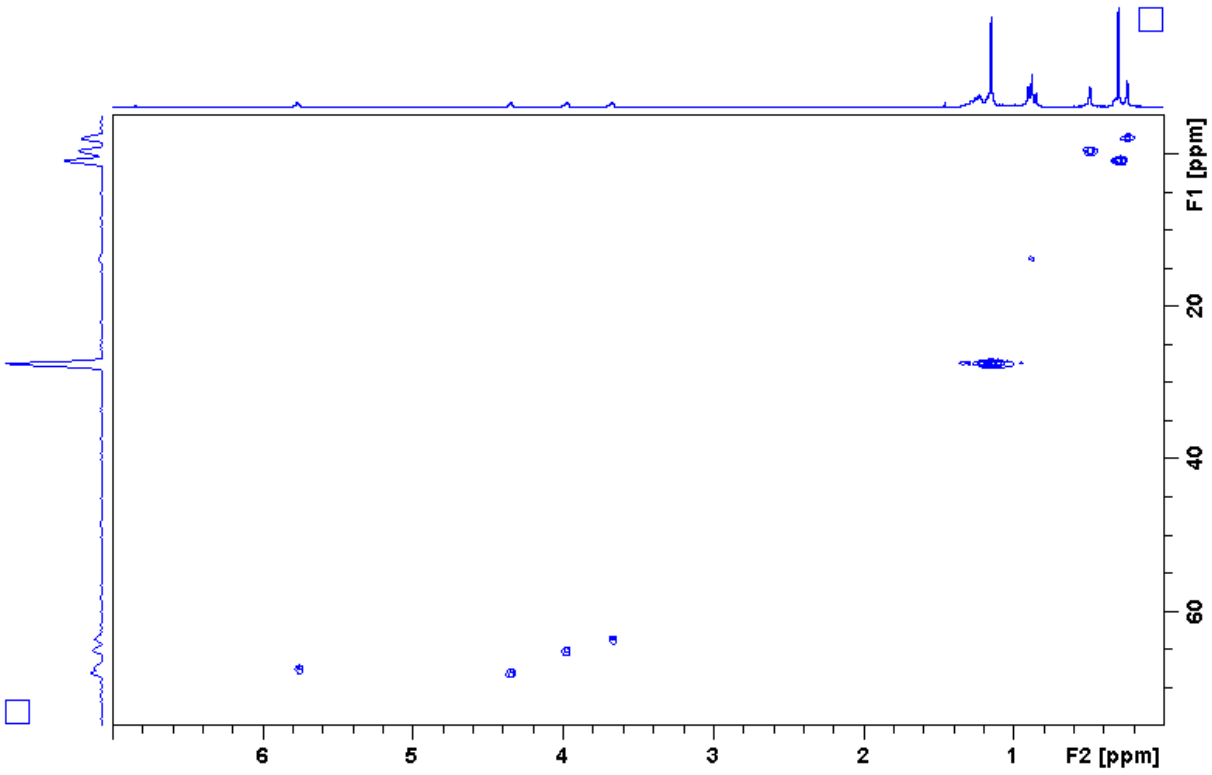


**Figure S16:** $^{1}H,^{13}C$ HSQC NMR spectrum of **5b** ($C_6D_6$).

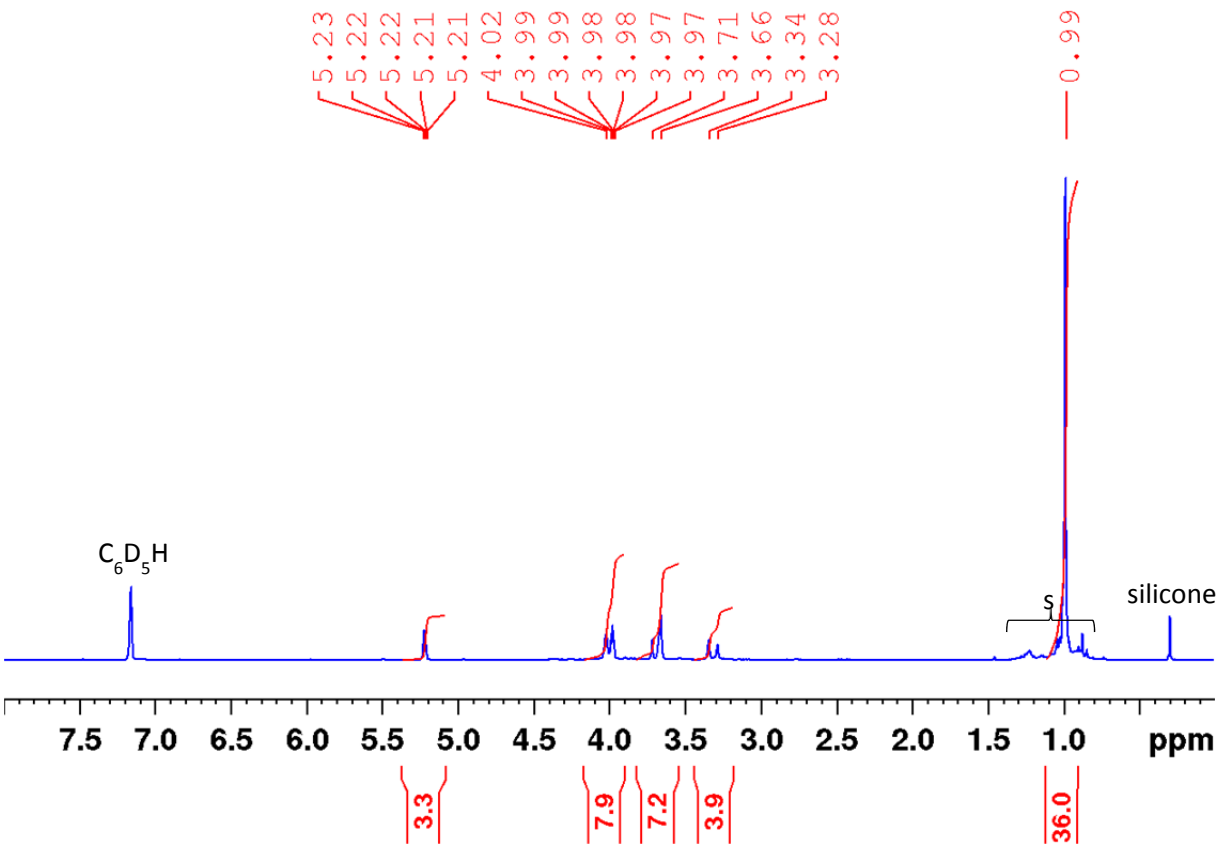


**Figure S17:** $^{1}$H NMR spectrum of **5c** ($C_6D_6$; extra signals arising from residual solvent pentane and silicone sticking to the crystals are labelled).

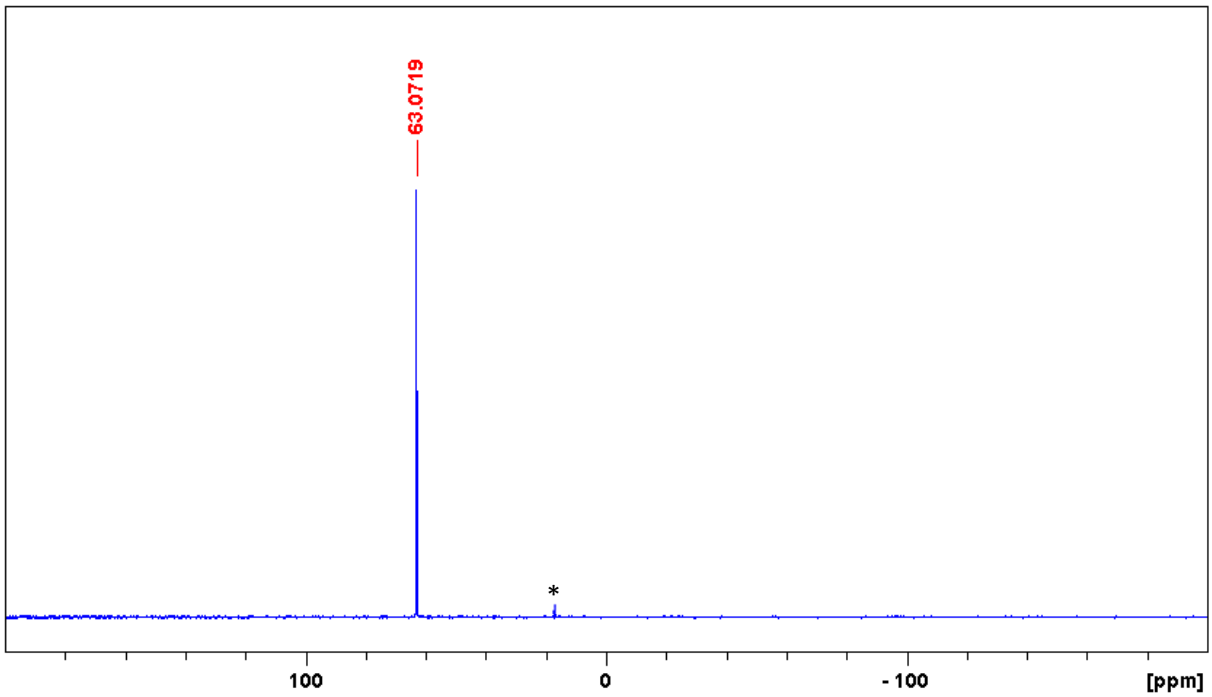


**Figure S18:** $^{31}$P{$^{1}$H} NMR spectrum of **5c** ($C_6D_6$; * denotes signal of a hydrolysis product).

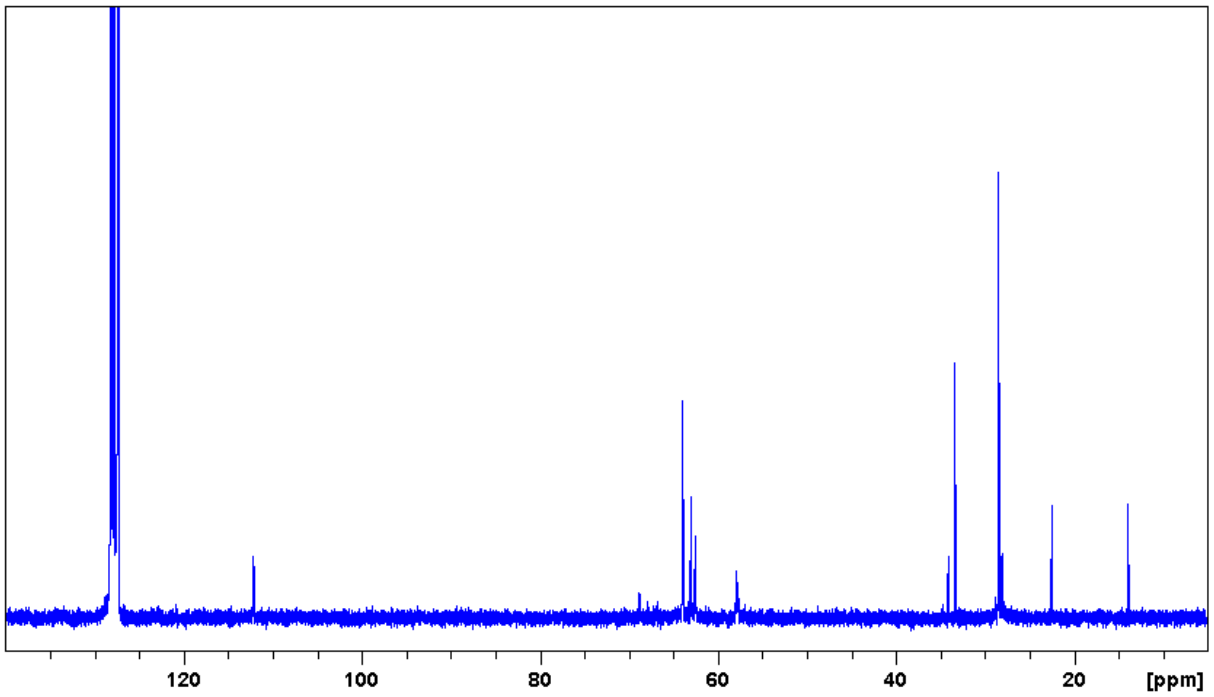


**Figure S19:** $^{13}C\{^{1}H\}$ NMR spectrum of **5c** ($C_6D_6$).

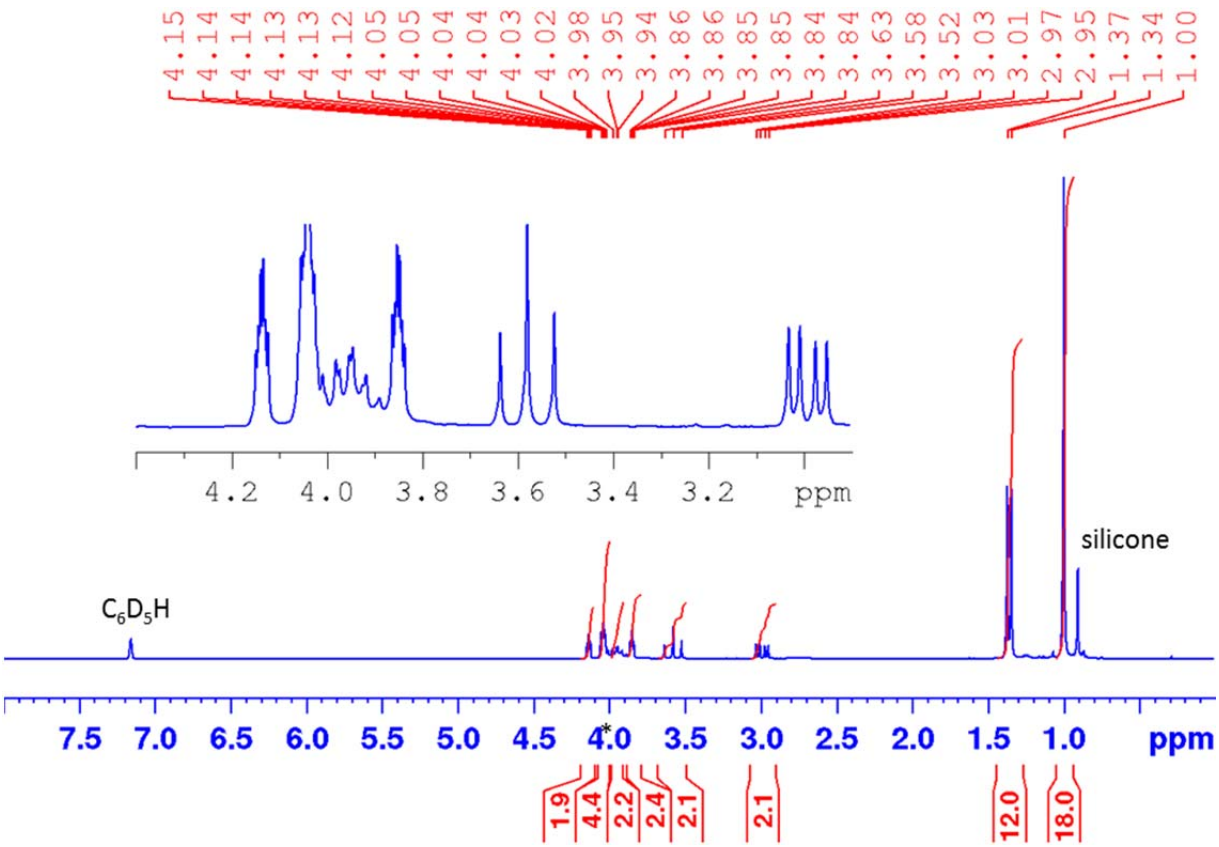


**Figure S20:** $^{1}H$ NMR spectrum of **6c** ($C_6D_6$).

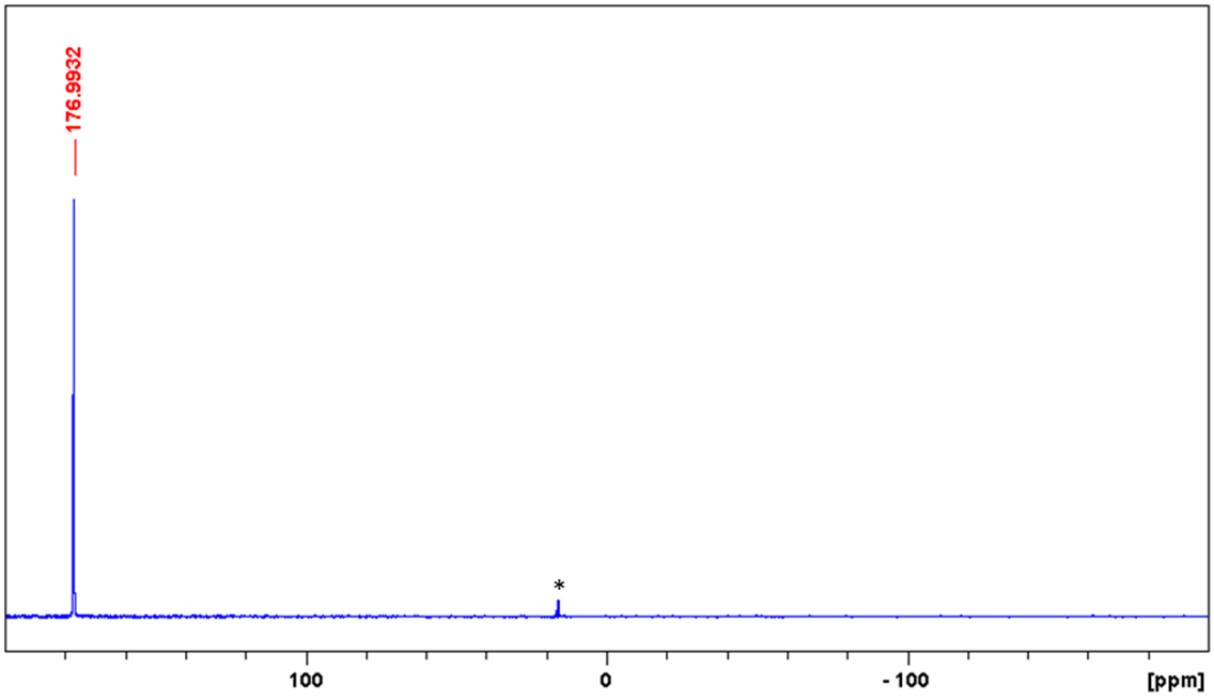


**Figure S21**: $^{31}P\{^{1}H\}$ NMR spectrum of **6c** ($C_6D_6$; * denotes signal of a hydrolysis product.

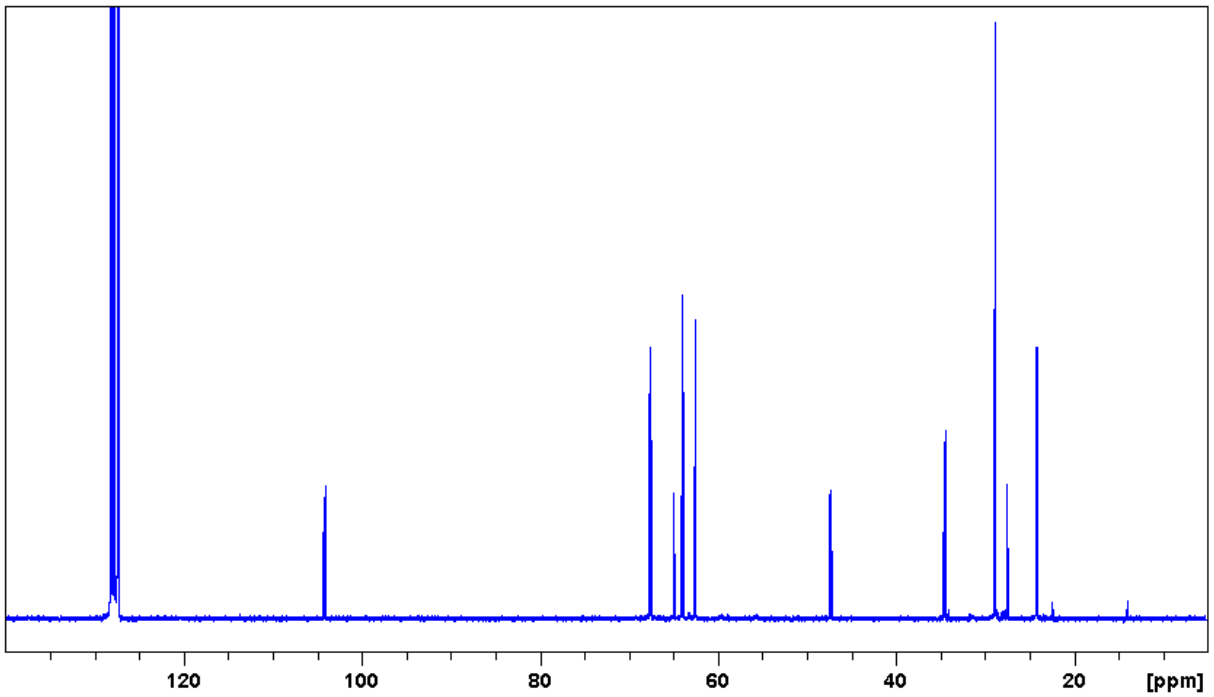


**Figure S22:** $^{13}C\{^{1}H\}$ NMR spectrum of **6c** ($C_6D_6$).

## Mass spectra

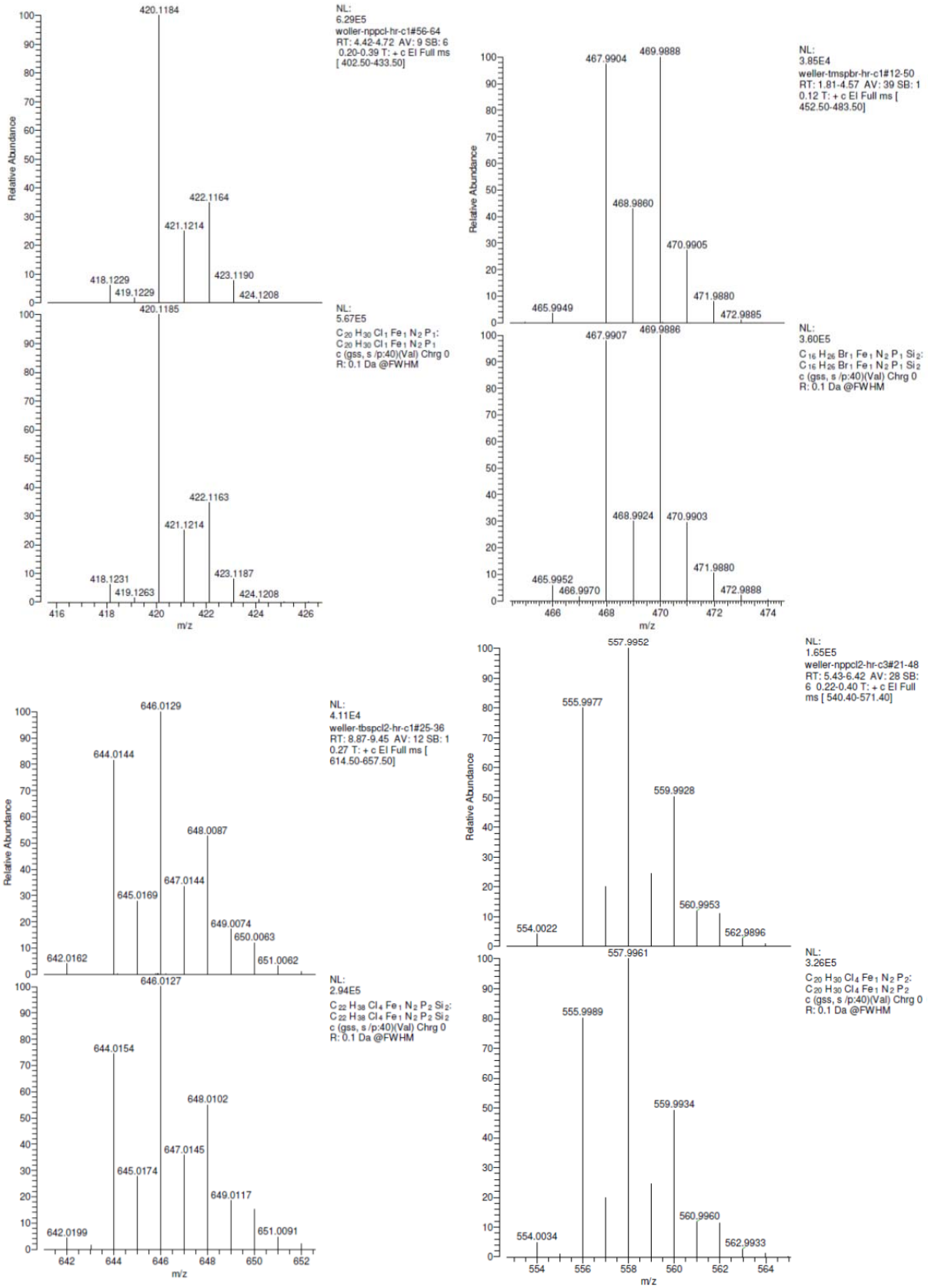


**Figure S23:** High resolution mass spectra (EI, 70 eV) of **2c**, **3a**, **4b**,**c** (from top left to bottom right; measured and simulated isotope patterns shown).

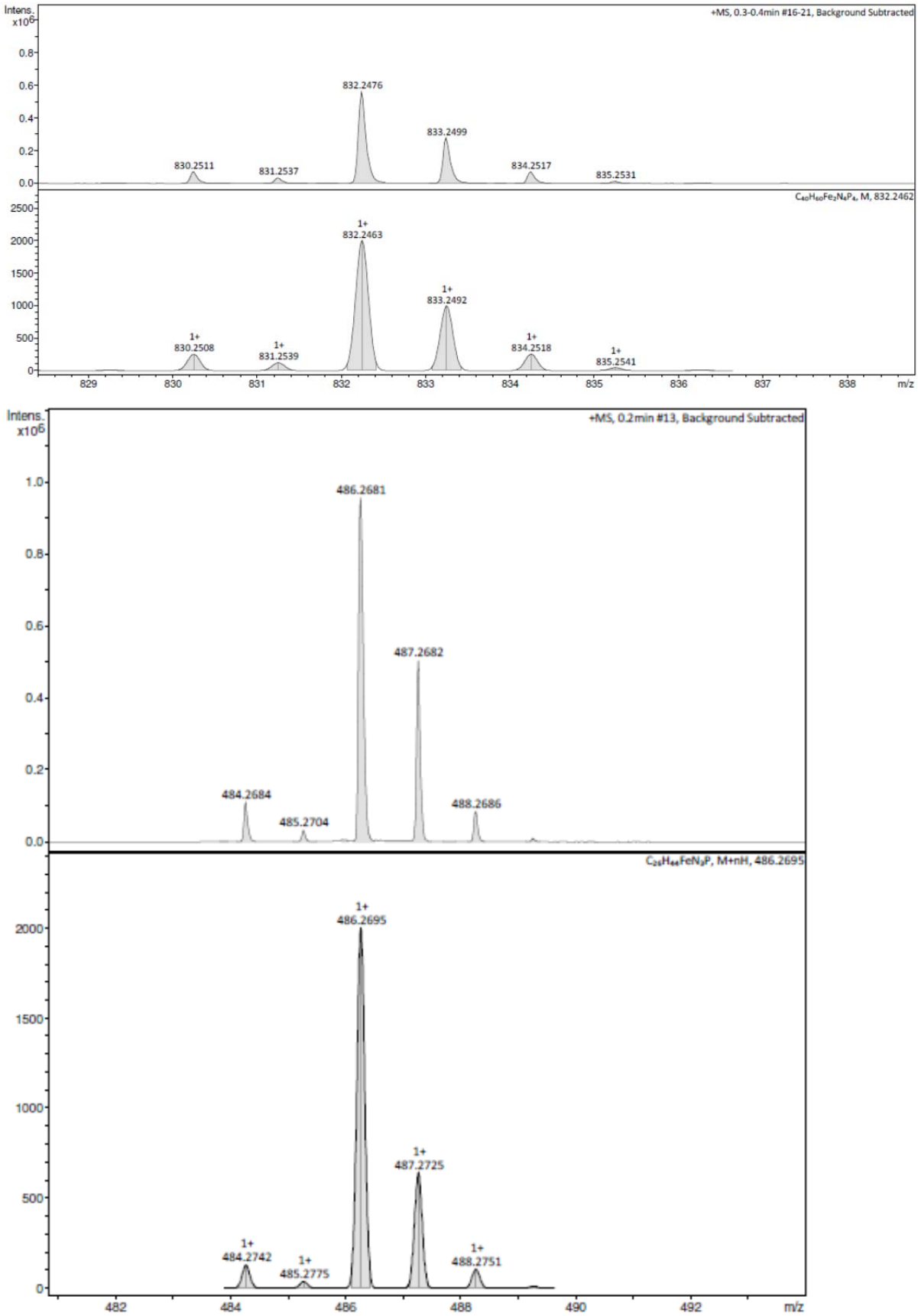


**Figure S24:** High resolution mass spectra (ESI) of **5c** (top) and **6c** (bottom). Simulated isotope patterns are shown below the observed spectra.

**Electrochemical Measurements**

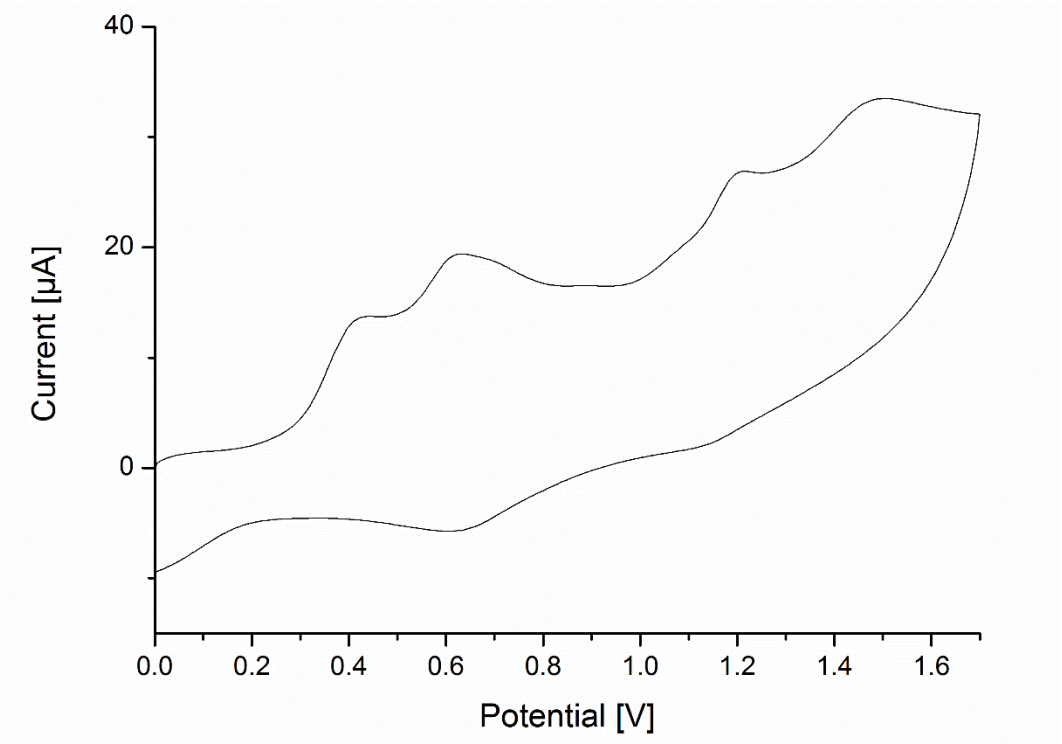


**Figure S25.** Cyclic voltammogram of **5b**.

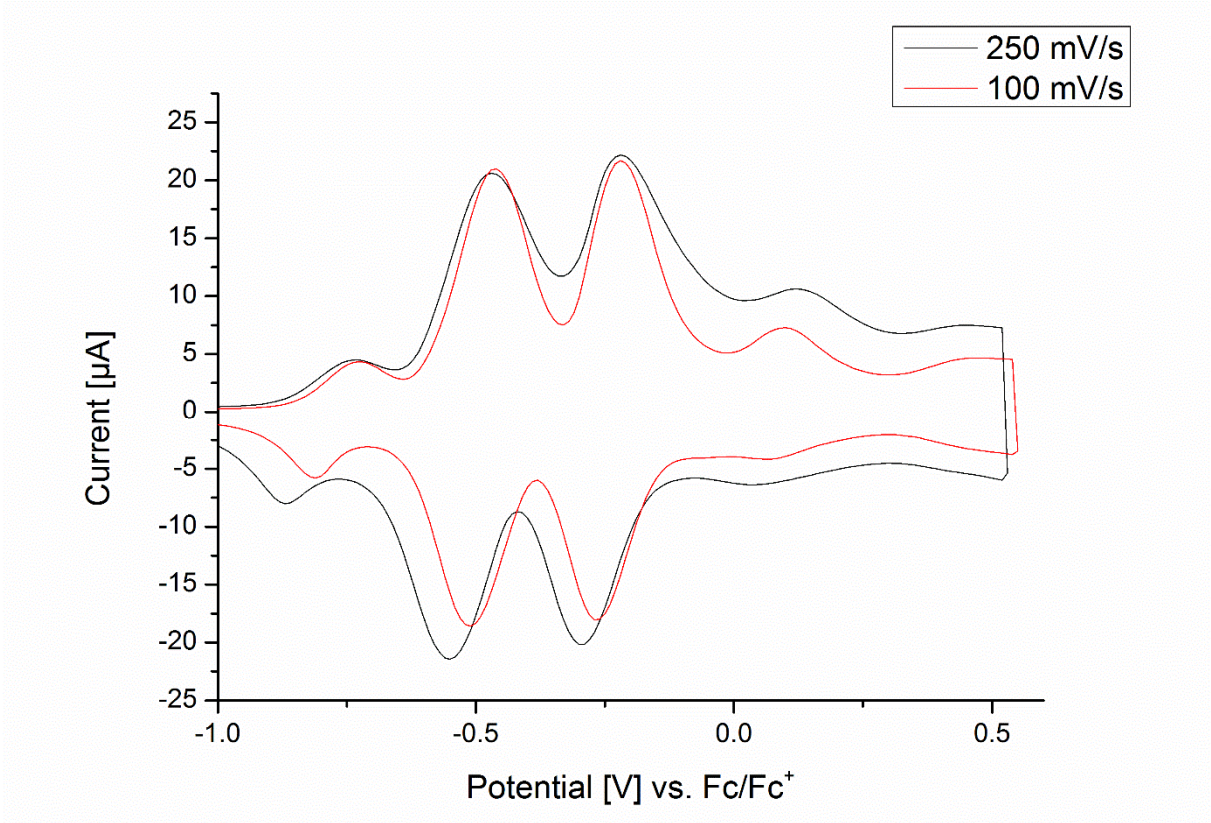


**Figure S26.** Comparison of square-wave cyclic voltammograms of **5c** at potential sweep rates of 100 and 250 mV/s (amplitude 25 mV, period 40 ms (black) resp. 100 ms (red), increment 10 mV, sampling width 1ms).

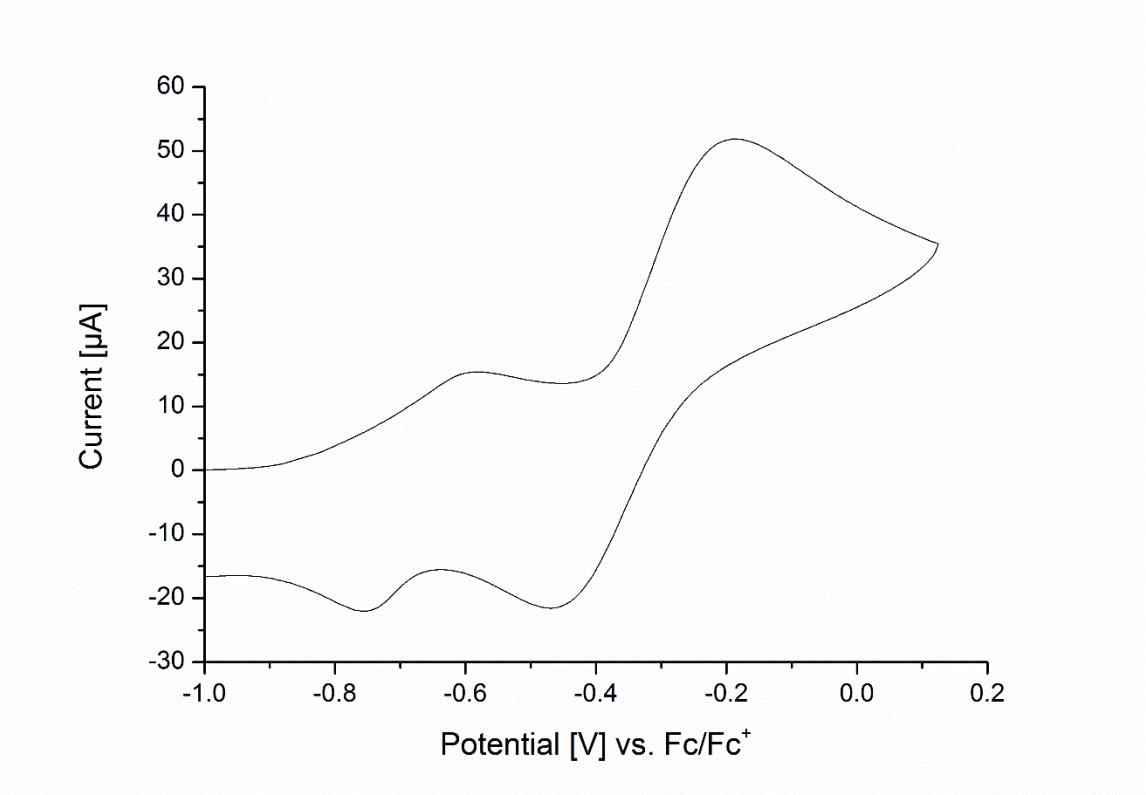


**Figure S27.** Cyclic voltammogram of **6c**. The potential sweep was reversed after ferrocene oxidation. The 1st oxidation event is due to decamethyl ferrocene used as internal reference.

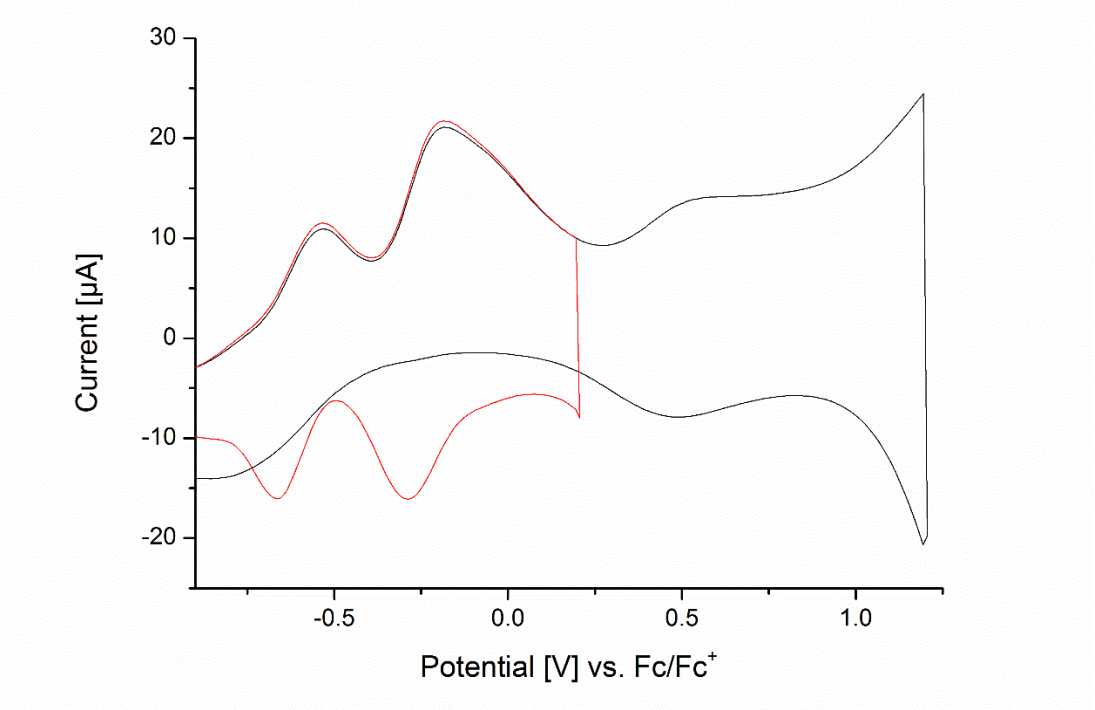


**Figure S28.** Square-wave cyclic voltammograms of **6c**. The red trace reveals that the ferrocene oxidation (2nd oxidation event) is partially reversible when the potential sweep is reversed immediately after the oxidation. The 1st oxidation event is due to decamethyl ferrocene used as internal reference.

**Computational Results**

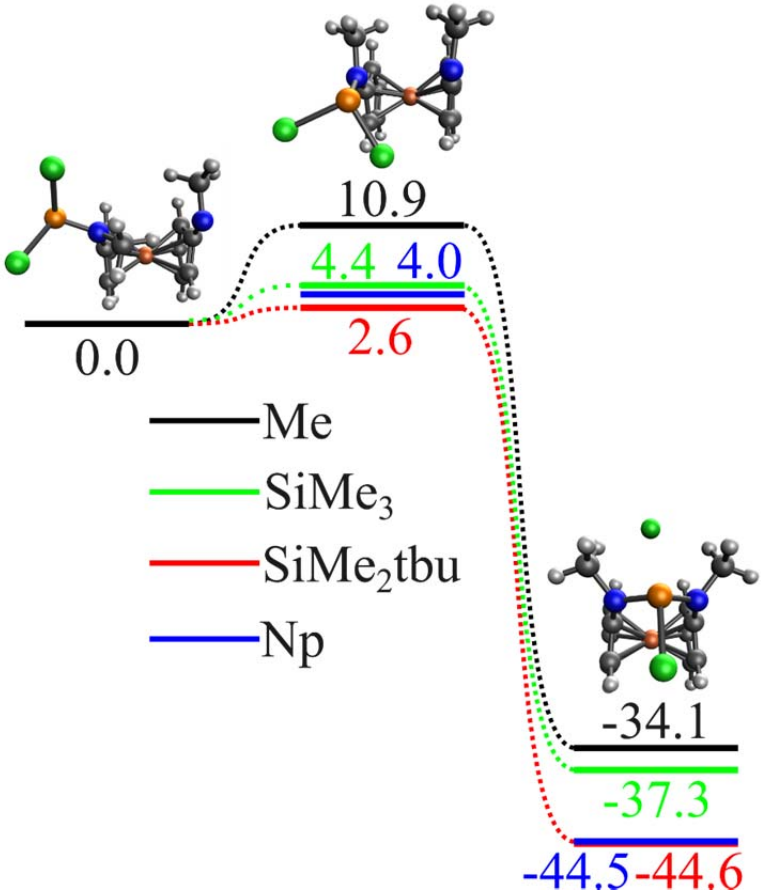


**Figure S29.** Gibbs free energy profiles for the reaction *(2⁻)* (drawn structures for species with N-Me substituents) in Scheme **3** calculated at the B3LYP-D3/6-31+G* level of theory.

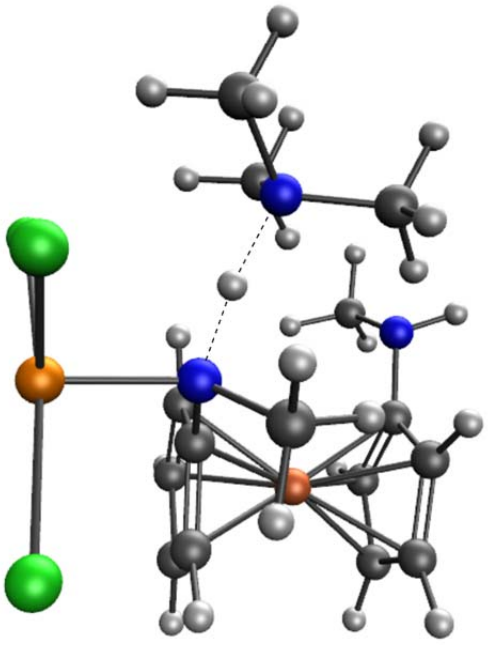

**Figure S30.** Transition state geometry for reaction *(1)* in Scheme **3** (with N-Me substituents) calculated at the B3LYP-D3/6-31+G* level of theory.

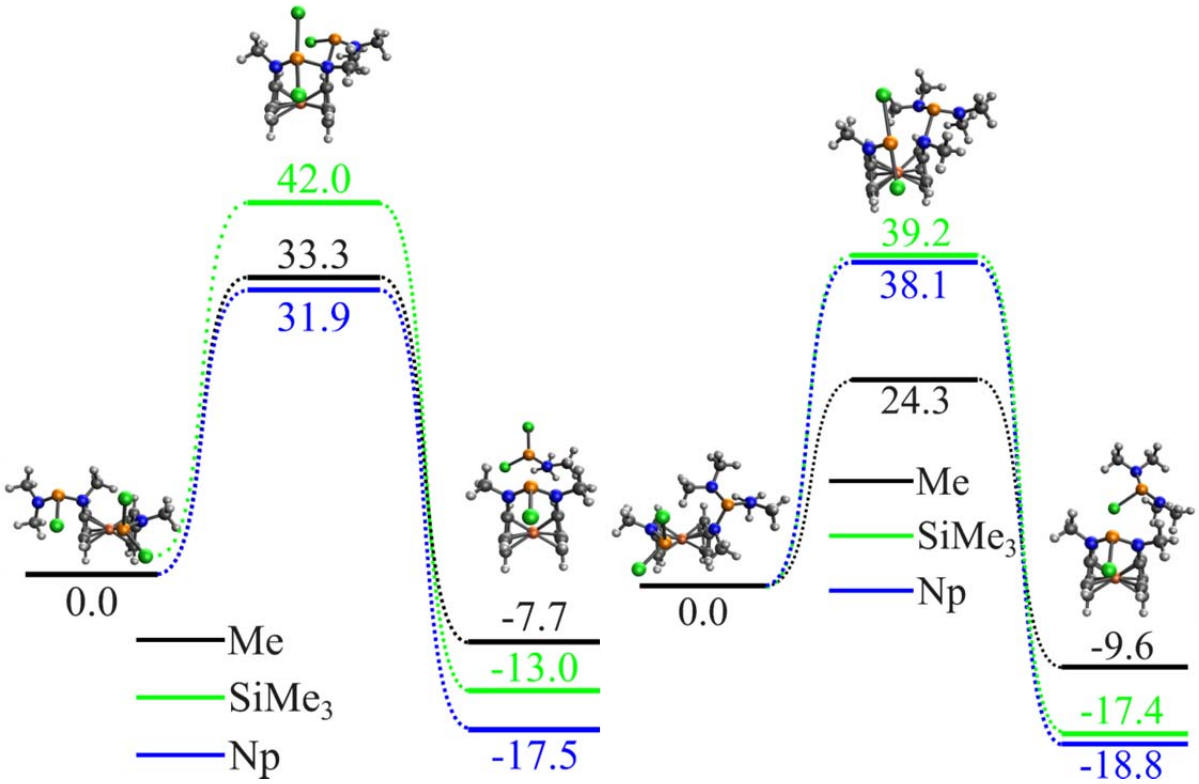


**Figure S31.** Gibbs free energy profiles for reaction *(iii)* in Scheme 5 (left) and the formation of **2b-d** from an unsymmetrically diamino-substituted ferrocenylidene-bisphosphine (right) calculated at the PCM($Et_2O$)-B3LYP-D3/6-31+G* level of theory. Molecular structures drawn refer to species with N-Me substituents.

**Table S3.** B3LYP-D3/6-31+G* Energies (E) and Gibbs free energies (G, in italics), as well as M06-2X/6-31+G* Gibbs Free energies (G, underlined) for educts, transition states, and products of reaction ($2^-$) in Scheme **3**

| R | E (*G*) (G) | E (*G*) (G) | E (*G*) (G) |
|---|---|---|---|
| $SiMe_3$ | 0.0 | 1.6 *(2.6)* (1.6) | -47.2 *(-44.6)* (-50.4) |
| $SiMe_2tBu$ | 0.0 | 2.2 *(4.4)* (2.0) | -40.5 *(-37.3)* (-40.3) |
| neopentyl | 0.0 | 2.4 *(4.0)* (3.3) | -46.9 *(-44.5)* (-46.4) |
| Me | 0.0 | 8.9 *(10.9)* (9.0) | -38.6 *(-34.1)* (-43.3) |

**Table S4.** Relative Gibbs free energies for different stereoisomers of [3]ferrocenophanes **2d**, **3d**, **6d, 6$^{Me}$d** in the gas phase and including a correction for solvation effects according to the PCM model (solvent $Et_2O$) in kcal/mol computed at the B3LYP-D3/6-31+G* level.

| | *trans, trans* | *cis, cis* | *cis, trans* |
|---|---|---|---|
| **2a** | 0.0 | 15.0 (15.9) | -* |
| **2b** | 0.0 | 20.0 (20.9) | -* |
| **2c** | 0.0 | 8.0 (9.0) | -* |
| **2d** | 0.0 | 9.7 (13.1) | 11.9 (12.5) |
| **3d** | 0.0 | 12.8 (13.3) | 14.9 (15.5) |
| **6c** | 0.0 | 9.5 (9.7) | -* |
| **6$^{Me}$d** | 0.0 | 5.3 (5.1) | -* |
| **6d** | 0.0 | 2.4 (1.2) | -* |

*Does not exist as a minimum after full geometry optimization.

**Table S5.** Relative Gibbs free energies of *transoid*- and *gauche*-conformers of **4a-d**, **10a-d** in the gas phase and with a correction for solvation effects according to the PCM model (solvent $Et_2O$, in parentheses) in kcal/mol computed at the B3LYP-D3/6-31+G* level.

| | *transoid* | *gauche* |
|---|---|---|
| **4a** | 0.0 (0.0) | 0.8 (0.9) |
| **4b** | 0.0 (0.0) | 0.3 (0.1) |
| **4c** | 0.0 (0.0) | 2.1 (2.0) |
| **4d** | 0.0 (0.0) | 3.4 (3.1) |
| **10a** | 0.8 (0.0) | 0.0 (0.0) |
| **10b** | 0.0 (0.0) | 1.7 (2.0) |
| **10c** | 0.0 (0.0) | 1.4 (1.8) |
| **10d** | 0.0 (0.0) | 0.9 (0.9) |

**Table S6.** Relative energies of the conformers of ferrocenophane-tetraphosphetanes **5a-d** with *trans*- and *cis*-fused rings computed at the B3LYP-D3/6-31+G* level (the figure in parentheses includes a PCM($Et_2O$) correction for solvation effects).

| **5a** | | **5b** | | **5c** | | **5d** | |
|---|---|---|---|---|---|---|---|
| *trans* | *cis* | *trans* | *cis* | *trans* | *cis* | *trans* | *cis* |
| 1.1 | 0.0 | 2.9 | 0.0 | 0.0 | 1.8 (1.5) | 6.0 | 0.0 |

**Table S7.** Single and double ionization energies of **5c** computed at the B3LYP-D3/6-31+G* level of theory.

| | gas phase | PCM($CH_2Cl_2$) |
|---|---|---|
| (**5c**) | 0.00 eV | 0.00 eV |
| $^{2}$(**5c**)$^{+\bullet}$ | 5.44 eV | 4.28 eV |
| $^{3}$(**5c**)$^{2+\bullet\bullet}$ | 13.00 eV | 8.87 eV |

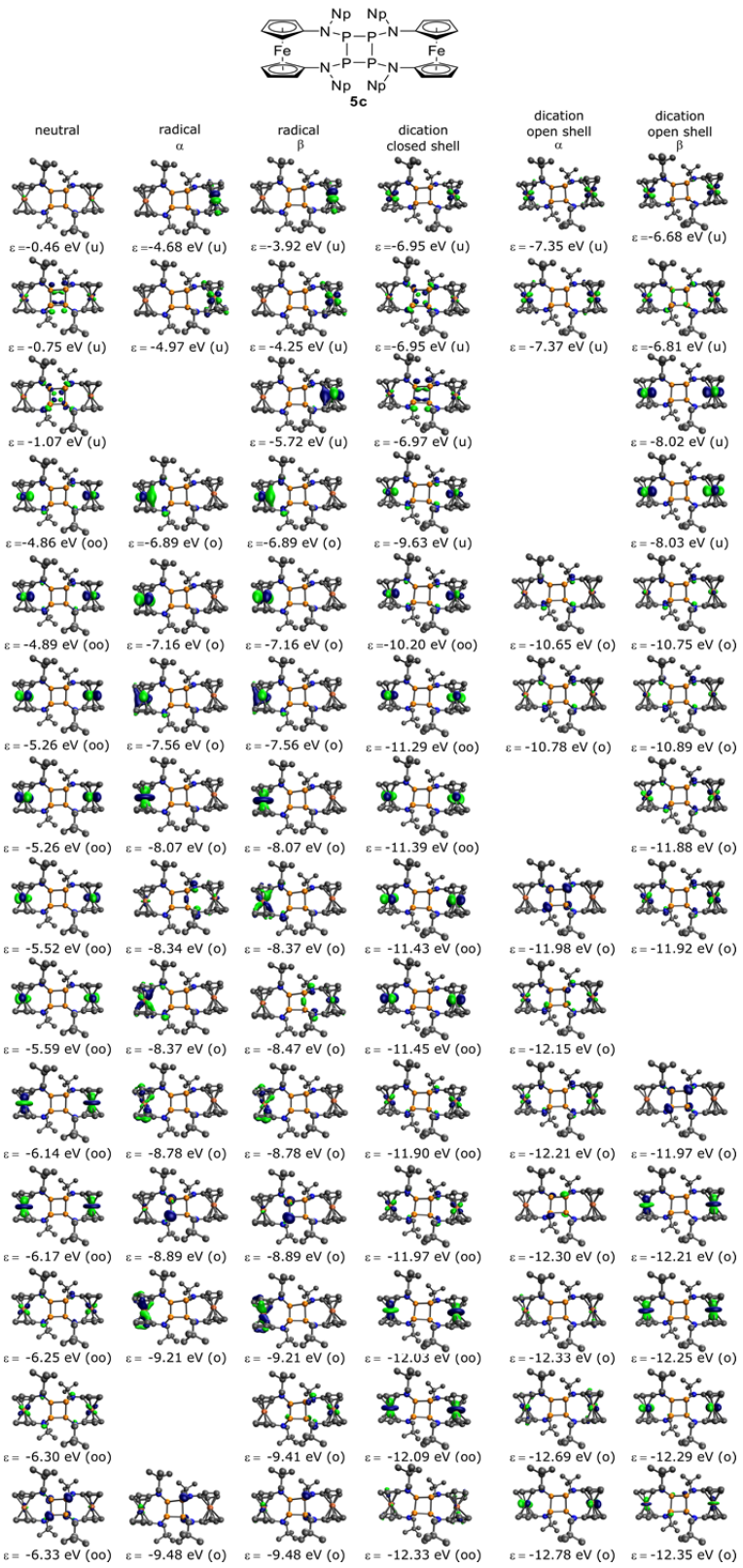


**Figure S32.** High energy singly (o) and doubly (oo) occupied, and low energy unoccupied (u) Kohn-Sham orbitals of **5c** (*trans*) and the corresponding mono- and dications calculated at the B3LYP-D3/6-31+G* level of theory. Hydrogen atoms are omitted for clarity.

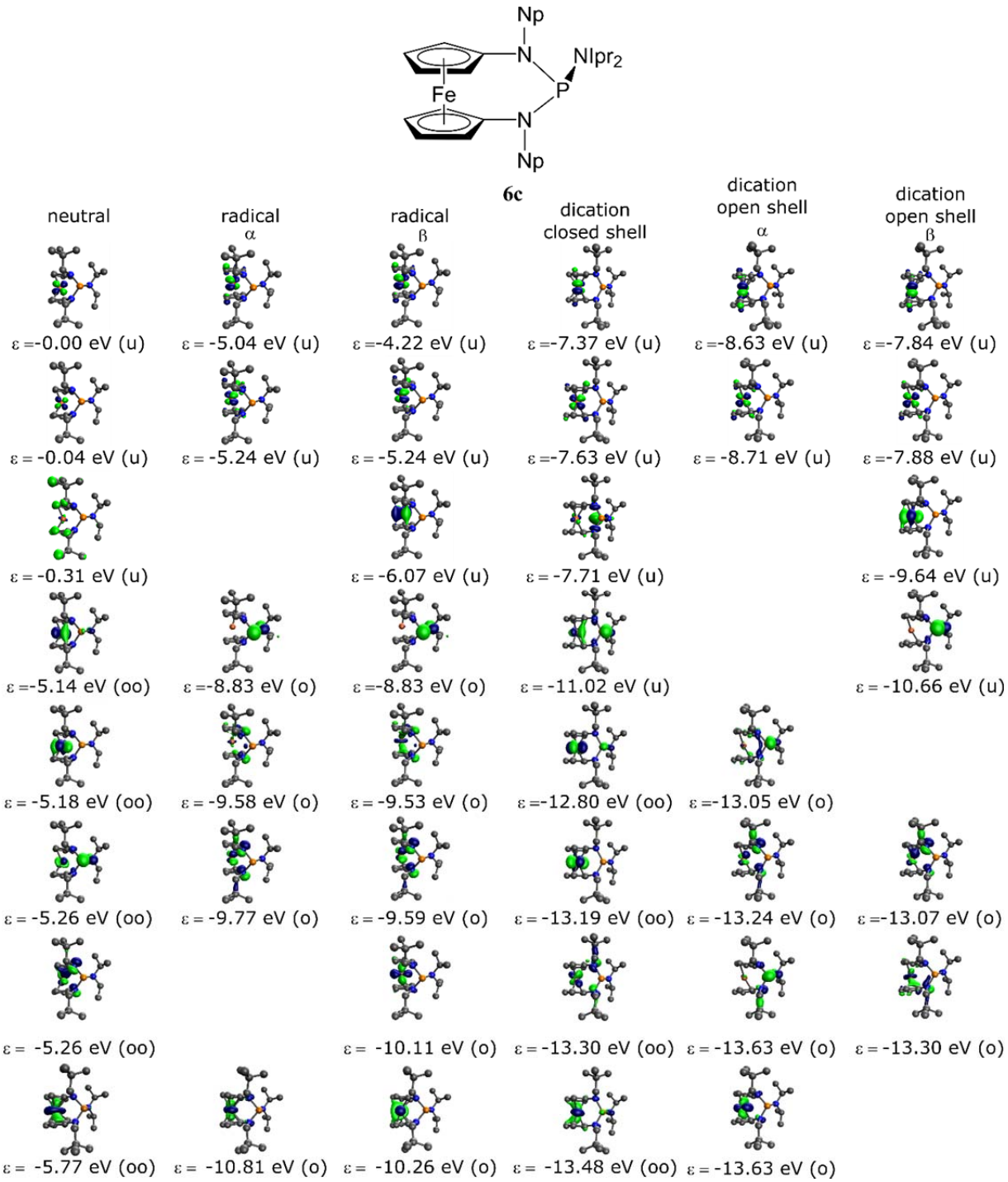


**Figure S33.** High energy singly (o) and doubly (oo) occupied and low energy unoccupied (u) Kohn-Sham orbitals for **6c** and the corresponding mono- and dications. Hydrogen atoms are omitted for clarity.

**Table S8.** Total energies and XYZ coordinates of the optimized structures

**1a**

E(B3LYP-D3/6-31+G*) = -2578.89648875
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2578.89624893
Sum of electronic and zero-point Energies= -2578.490351
Sum of electronic and thermal Energies= -2578.463261
Sum of electronic and thermal Enthalpies= -2578.462316
Sum of electronic and thermal Free energies=-2578.547315
C -0.239878011547 -0.167345857379 -0.365454923208
C -0.460700207654 -0.176446387255 1.043823464640
C 0.813384640001 -0.200165458981 1.704521849299
C 1.821924525231 -0.189202542358 0.679294135549
C 1.173316750543 -0.172067965271 -0.591359541151
Fe 0.615335306305 -1.841072349602 0.492109407784
C -0.248693174523 -3.541197860853 -0.268320231539
C -0.457429749706 -3.475881362500 1.146402275294
C 0.818723922581 -3.470243784048 1.794641930677
C 1.817896327921 -3.489015469636 0.768078608444
C 1.158471699940 -3.551241943812 -0.502131945466
N 1.037199903626 -3.416924604870 3.180688582427
Si 2.519823270626 -3.864176127199 4.036918644768
N 1.023967574976 -0.261130029961 3.103081904501
H 1.073357089789 -1.217108313337 3.453180484231
Si 1.619106830492 1.066187492698 4.067334754928
H 1.662187571539 -0.190531424910 -1.557397534938
H -1.004864447827 -0.181321526967 -1.131666009056
H 2.888790309791 -0.227994231287 0.859730045750
H -1.417490826528 -0.203521963747 1.549699310597
H 2.887570753715 -3.446631003336 0.921037919417
H 1.648697805986 -3.573998927990 -1.466984559319
H -1.024431682903 -3.556713236529 -1.023074762206
H -1.415029421784 -3.424888163037 1.650852965154
C 0.395862781487 2.500323096060 3.973563487603
C 3.305434498197 1.681189269662 3.463406904267
C 1.776144939668 0.394654494813 5.826295306263
C 3.058872337423 -5.614706060584 3.585647714230
C 2.056776246226 -3.737426832917 5.859978981085
C 3.898621836445 -2.648119249599 3.604938065768
H 0.173941015253 -3.473302732291 3.710684237866
H 3.660003935478 2.532264577713 4.060167147955
H 4.063090710751 0.889257609188 3.523064257219
H 3.249230418708 2.009852437446 2.417872235280
H 0.767605320600 3.389104080952 4.499840730601
H 0.216891770086 2.782337705499 2.927882612156
H -0.570924702832 2.221363181626 4.410718727499
H 2.071955320054 1.189088962072 6.523094730214
H 0.825720386658 -0.023127280915 6.181676525300
H 2.537826816113 -0.393162564485 5.885716776051
H 2.913898380510 -3.994547816600 6.494892648670
H 1.740056012368 -2.722029618879 6.126661332787
H 1.241681104184 -4.426518525903 6.116489396771
H 4.709155428641 -2.710768051782 4.343100076910
H 4.337086394913 -2.854874834997 2.621596882360
H 3.526672952509 -1.618115912420 3.590466237300
H 4.022622398808 -5.868029491637 4.046534410915
H 2.319617470078 -6.354499162108 3.916840607300
H 3.169332272112 -5.720547237974 2.499375276787

**1b**

E(B3LYP-D3/6-31+G*) = -2814.79361655
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2814.79202884
Sum of electronic and zero-point Energies= -2814.215678
Sum of electronic and thermal Energies= -2814.180996
Sum of electronic and thermal Enthalpies= -2814.180052
Sum of electronic and thermal Free energies=-2814.282599
C -0.004377785826 0.001162671742 -0.605025832779
C -0.162036729167 0.033791048552 0.813965397791
C 1.139392883891 -0.018769567239 1.416503458802
C 2.098246167070 -0.090817509806 0.351454746826
C 1.393559972669 -0.086683822168 -0.891600215244
Fe 0.810385631645 -1.690791053239 0.262136169680
C -0.195068769313 -3.384215284541 -0.329396184880
C -0.230623433404 -3.263372456546 1.095755859577
C 1.115860955205 -3.262248395856 1.584617123540
C 1.982695962751 -3.365421129226 0.447364605890
C 1.173672421270 -3.460088199205 -0.728710187863
N 1.520147169455 -3.137983168812 2.926795135559
Si 2.665862602745 -4.159416207308 3.793151888476
N 1.403064778819 -0.047838920167 2.802089516973
H 2.028695357950 -0.808447513168 3.057164395254
Si 1.193704137874 1.273015987993 3.933169650362
H 1.838591878541 -0.159979010708 -1.875963411364
H -0.804864085927 0.006108783252 -1.333750852656
H 3.169958825408 -0.173376408032 0.484394006053
H -1.096371166318 0.056709529324 1.359458798067
H 3.063168852872 -3.341702983395 0.477620741074
H 1.540070118201 -3.537247969961 -1.744311214040
H -1.055001503180 -3.398172453831 -0.986984523644
H -1.117583177545 -3.162443183062 1.709551782830
C -0.568560582770 1.933371149884 3.780274785543
C 2.448787694134 2.692846033140 3.617515642688
C 1.486650711395 0.506202191910 5.635498578639
C 2.005128803383 -5.950746907089 3.982650550604
C 2.838371952586 -3.329288693650 5.480439160936
C 4.325978615097 -4.170960443661 2.893948934522
H 0.802861066531 -2.697019968524 3.495272018950
C 2.333715286063 3.771672655950 4.714593316068
C 3.879494339182 2.115487045391 3.620906022863
C 2.172254105756 3.338042957278 2.241713035979
H -0.744088803427 2.774598038222 4.462361636225
H -0.777946609270 2.279947106149 2.761826148733
H -1.294958351797 1.147371161102 4.021083170477
H 1.396394429944 1.253568825680 6.432872809443
H 0.753036716755 -0.284428467578 5.835665815797
H 2.485713809390 0.059943784911 5.714342437047
H 3.445845258438 -3.936273116149 6.162365758969
H 3.323396943100 -2.350420812255 5.385000998186
H 1.864351130023 -3.171099661629 5.959571229318
H 5.102607684762 -4.600809419783 3.539060496387
H 4.296906996258 -4.764875450944 1.973748522718
H 4.635520686976 -3.152216684504 2.631023164311
C 3.017276339877 -6.817372677883 4.761829950643
C 0.666090861615 -5.917671741893 4.748410662389
C 1.769905438721 -6.575969953135 2.590090897939
H 4.615551586141 2.908920034307 3.419933469669

H 4.139672301549 1.668353744562 4.589475272803
H 4.004489525590 1.345625205008 2.849091323871
H 3.045984478505 4.589452966113 4.525022207652
H 1.331233978752 4.217528637796 4.748556131878
H 2.557661833999 3.370835878572 5.711471967598
H 2.906107820833 4.133833645959 2.039905757361
H 2.242027979144 2.609819569115 1.425051033277
H 1.176096730800 3.796147118420 2.197721520934
H 0.256505739857 -6.934101886152 4.850231262435
H 0.780774101907 -5.510436483049 5.761514534550
H -0.084733651484 -5.314032596573 4.222386249744
H 1.376686193028 -7.598707503263 2.696061311872
H 1.046946147384 -6.003270565117 1.997889078323
H 2.698172814822 -6.644084995916 2.009087137980
H 2.633920503987 -7.842756382772 4.876332946424
H 3.981541572453 -6.888101323158 4.242320378221
H 3.205448923845 -6.427632416143 5.770747477395

**1c**

E(B3LYP-D3/6-31+G*) = -2154.63415477
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2154.63304318
Sum of electronic and zero-point Energies= -2154.147120
Sum of electronic and thermal Energies= -2154.122505
Sum of electronic and thermal Enthalpies= -2154.121561
Sum of electronic and thermal Free energies=-2154.203446
C 0.208501780033 0.038146471881 -0.454696681782
C 0.037017581398 0.057747017714 0.963783915040
C 1.330495790961 -0.022357944466 1.575401752460
C 2.297925121046 -0.114271864238 0.523105860821
C 1.605537105576 -0.083316046613 -0.728898553739
Fe 0.972852337743 -1.682834183863 0.397958467131
C -0.177900539197 -3.322694493922 -0.065886957120
C -0.002038843972 -3.223266357027 1.350800717179
C 1.400500968315 -3.281355478236 1.635926552339
C 2.088011695157 -3.409743946171 0.385138352468
C 1.114907188800 -3.452941513433 -0.660337162359
N 2.032171279177 -3.174343383372 2.892052371281
C 2.786142302826 -4.315270497735 3.415409284178
N 1.560171516953 -0.061123188917 2.966094832849
H 2.470785814649 -0.455006382827 3.179238207245
C 1.237394396567 1.113090132814 3.779261653046
H 2.059384212999 -0.160317611403 -1.708895178891
H -0.585519874237 0.066683582595 -1.189870191845
H 3.366104568122 -0.226181074525 0.664558546906
H -0.904227001175 0.097282515718 1.496990451132
H 3.163327257910 -3.439171066054 0.264105707769
H 1.325054926210 -3.527653155010 -1.719592904127
H -1.122311094765 -3.283931012845 -0.593988399008
H -0.784300285189 -3.088315343432 2.087948663271
H 0.179406380485 1.353442282641 3.613541831008
C 2.080463474194 2.409413028856 3.596437485838
H 1.324999104847 0.791819627225 4.826153729763
C 2.013146512944 -5.602842667975 3.826839193086
H 3.327594074743 -3.944141726378 4.296307304026
H 3.546776972095 -4.582678702257 2.670735615450
H 1.416533733497 -2.753891480430 3.580553348418
C 3.006084441929 -6.507399707213 4.582921194084
C 0.839643797221 -5.242259417503 4.753708566234
C 1.486712353325 -6.362332022902 2.593545253687
H 2.529325943169 -7.451859042035 4.873823777378
H 3.874569959848 -6.752138217432 3.956925330239
H 3.375338321866 -6.023144122501 5.496591036043
H 0.335364225034 -6.148527545620 5.111817656549
H 1.182544304642 -4.681162733698 5.634022772531
H 0.091929245055 -4.634335892332 4.230574991254
H 1.006144733160 -7.300735384355 2.900458479980
H 0.753356912477 -5.776053257176 2.033421183193
H 2.306005635689 -6.614130535453 1.908078424162
C 1.706440099976 3.361581058039 4.749380385145
C 3.581138483843 2.079551431771 3.669975075553
C 1.765860935954 3.101971594568 2.256152060928
H 2.245518986639 4.313033478833 4.659635517925
H 0.631534967671 3.586495948994 4.744380608849
H 1.954895424386 2.926594081205 5.726468055896
H 2.318141219472 4.047750416633 2.177157497025
H 2.038976724308 2.480099511682 1.399445406955
H 0.695698788248 3.331148532517 2.174116919729
H 4.182739579734 2.995811469703 3.620932903341
H 3.832516057828 1.565150702166 4.607837885811
H 3.888839998241 1.438622303101 2.835205434881

**1d**

E(B3LYP-D3/6-31+G*) = -1840.08719687
E(PCM-B3LYP-D3/6-31+G* (ether)) = -1840.08816311
Sum of electronic and zero-point Energies= -1839.826429
Sum of electronic and thermal Energies= -1839.812398
Sum of electronic and thermal Enthalpies= -1839.811454
Sum of electronic and thermal Free energies=-1839.866649
C -0.342322385472 -0.095481332771 -0.063418641592
C -0.452649475547 -0.119562810032 1.362624473170
C 0.846004347343 0.095384760595 1.921281186620
C 1.764888283542 0.234791668311 0.828336504844
C 1.028316688382 0.129065108747 -0.393947098105
Fe 0.825201146855 -1.598650952409 0.708056879829
C 0.343957790557 -3.402671024962 -0.152874372600
C -0.079277368297 -3.374345339340 1.214058334495
C 1.076419571030 -3.189177080583 2.039528431842
C 2.208989169438 -3.063179021360 1.174350286542
C 1.756491929407 -3.204574761113 -0.178524665644
N 1.059869465789 -3.085625019612 3.449327183614
C 2.310240397302 -3.382617950934 4.146379344720
N 1.136683479945 0.118328288191 3.297476033476
H 0.767488894636 -0.726202467426 3.735955467939
C 2.535229585253 0.310462638676 3.657320051390
H 1.444784473217 0.187548799905 -1.391389093035
H -1.153969247266 -0.242159243115 -0.764765660408
H 2.834286258790 0.374267761704 0.910623622453
H -1.355495107020 -0.295372168535 1.934266608475
H 3.228798559516 -2.876660099687 1.482627561418
H 2.381732148016 -3.154007518834 -1.060735615887
H -0.302464451673 -3.525670275118 -1.012318703826
H -1.098698698079 -3.459764021520 1.571256578654
H 2.866424795279 1.302873817828 3.332232887450
H 3.215727382338 -0.437881155736 3.213434754009
H 2.629860156620 0.261861945398 4.746445038469
H 2.727839569948 -4.369949599690 3.890328230520
H 2.132675207158 -3.338678527169 5.225195395341
H 3.057730143385 -2.622362834199 3.901448628079
H 0.284324944212 -3.614157561249 3.835347483009

**van der Waals complex of 1a and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -2753.39998970
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2753.40565893
Sum of electronic and zero-point Energies= -2752.870621
Sum of electronic and thermal Energies= -2752.836581
Sum of electronic and thermal Enthalpies= -2752.835637
Sum of electronic and thermal Free energies=-2752.935734
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C 0.020252707994 -0.065492314840 1.441266522393
C 1.340914258911 -0.190561360270 1.985389091666
C 2.250117019919 -0.184337819054 0.878421856610
C 1.501728948132 0.002907712125 -0.328275126048
Fe 0.901848519038 -1.726075470364 0.588144711283
C -0.185118986759 -3.201589653849 -0.323312953810
C -0.250719850410 -3.336032234071 1.094854684996
C 1.083178615019 -3.526550345624 1.580915958705
C 1.972679316732 -3.553446702716 0.459716869068
C 1.189615668731 -3.313887940438 -0.713642122442
N 3.350055755696 -3.799881652450 0.517152846624
Si 4.537548791274 -3.709938162764 -0.775085472804
C 4.566915742722 -1.964507516592 -1.490945346312
N 1.687771681645 -0.295019634437 3.331495382297
Si 0.596683034928 -0.307155965978 4.700472316017
C -0.585804816129 -1.783892130163 4.643789221155
C 1.678859195523 -0.422087867249 6.243741112222
C -0.406278211617 1.292748238597 4.760366791392
C 4.154640256714 -4.944757317871 -2.151660170195
C 6.181969228165 -4.147783327691 0.041335672094
N 4.551104076913 -1.336870885865 3.886406816467
C 5.292384058506 -1.302158991004 2.628186758257
C 4.272252147708 -2.712004709754 4.289759182644
C 5.252793164579 -0.601156876950 4.935772494512
H 2.665721838879 -0.558475987253 3.492635523173
H 3.664972881151 -4.100290803519 1.430614699540
H 5.392062084459 0.439222103214 4.623197823319
H 4.657096511531 -0.606488411252 5.853528719823
H 6.247031302022 -1.033833657478 5.161483018472
H 4.727567412088 -1.831101235184 1.855463515908
H 6.291363133646 -1.772259233069 2.718652620091
H 5.430182133215 -0.263657603584 2.307963385360
H 3.648224709629 -3.194336801465 3.531053235962
H 3.718517712670 -2.718272060252 5.233495625812
H 5.194081987699 -3.310696732951 4.425364263263
H -1.143527476459 -3.276722835294 1.703742264183
H -1.018493662546 -3.020553553479 -0.990099107169
H 1.375613843170 -3.625954701203 2.619362463872
H 1.564208792783 -3.236223176846 -1.725280075940
H -0.904459874014 -0.084624156420 2.001580043066
H -0.707823962917 0.198689530796 -0.665827773401
H 1.913168022278 0.060506940497 -1.327838700032
H 3.322697330815 -0.292022006979 0.949444481987
H 0.258341610790 2.156666604021 4.885310246664
H -0.984161275161 1.454048274566 3.843393527751
H -1.111683980203 1.281980238179 5.601877994016
H -1.265457410289 -1.784123500322 5.506272679992
H -1.197890817681 -1.773704925118 3.734593688030
H -0.029706922829 -2.729897652869 4.651033154519
H 1.059321874778 -0.331840803679 7.145102735692
H 2.209302964702 -1.379305640346 6.305819324071
H 2.421986591482 0.383852691239 6.268541348863
H 3.188527253792 -4.744368720525 -2.629168840398
H 4.924965506144 -4.906411335251 -2.933472411737
H 4.121806893158 -5.968388765604 -1.758556532978
H 5.189528846912 -1.906456973637 -2.392893546738
H 3.553004482608 -1.644329481418 -1.755875383379
H 4.955403693583 -1.243116633048 -0.761966615366
H 6.991427327719 -4.136554657653 -0.699486882633
H 6.448476706918 -3.436359270221 0.831904756337
H 6.155970292395 -5.152606507471 0.482318839223

**van der Waals complex of 1a and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -2871.35722421
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2871.36248742
Sum of electronic and zero-point Energies= -2870.741440
Sum of electronic and thermal Energies= -2870.703710
Sum of electronic and thermal Enthalpies= -2870.702766
Sum of electronic and thermal Free energies=-2870.810204
C 0.020990328197 -0.011798368999 -0.088461026990
C 0.247492380898 -0.042513766846 1.324935984294
C 1.661854220807 0.013361183646 1.532946751060
C 2.302492311198 0.129680509440 0.257017640608
C 1.288786565301 0.115170296368 -0.745529722299
Fe 1.246655660061 -1.621009020240 0.345343585341
C 1.903520498935 -3.329517923168 1.411508355588
C 2.581091418874 -3.185046489552 0.155134258916
C 1.606591761363 -3.210717381194 -0.895579232398
C 0.320100323037 -3.328496445139 -0.293431006076
C 0.501740481085 -3.381578437691 1.126112276597
N 2.482383877365 -3.410673722913 2.680286431780
N -0.722133673199 -0.099520529183 2.332503138659
H -0.322664227986 -0.153967285253 3.260617903680
Si -2.461673525253 -0.263411360936 2.154802187887
C -3.168552984467 1.228338905797 1.239686457303
C -2.903946823754 -1.839895374966 1.210994980822
C -3.151012204893 -0.330879694897 3.911707917190
Si 4.199450480172 -3.332422317884 3.029647252251
C 4.925670105044 -1.662881938028 2.514376461177
C 4.415124997400 -3.559291017355 4.890332394125
C 5.108092815296 -4.729657660375 2.140015126060
N 0.319857462790 -3.284507756968 5.060898902732
C -0.943566896636 -3.802170386038 4.507452546055
C -2.080608612436 -4.068044518334 5.507189877255
C 0.168893657459 -1.921513810026 5.593571628308
C 1.473462363686 -1.120792204280 5.601911518922
C 0.957470814203 -4.185072818883 6.035383897779
C 1.238028914611 -5.584404254729 5.483702379033
H 1.803842403356 -3.330138769526 3.442879438303
H 0.321241371458 -6.169409152892 5.351218626589
H 1.749890921190 -5.527538794330 4.516886860918
H 1.878384675193 -6.134264878808 6.183043236763
H -2.344161139937 -3.165559974488 6.070709374016
H -1.816997483931 -4.850729585831 6.227118678538
H -2.976870251697 -4.399552725266 4.969188008362
H -4.245873530757 -0.258200051070 3.887802657463
H -2.781465167447 0.501859792195 4.523680421166
H -2.898825898190 -1.267770658300 4.421716072643
H -4.254993097470 1.131748493525 1.113004069339
H -2.971888209294 2.152680912666 1.796696776139
H -2.726466992015 1.345574313102 0.243395593353
H -3.969767714414 -1.861510055311 0.948915603963

H -2.325355964727 -1.916563864311 0.283632140362
H 1.907314653080 -3.726950521368 6.324673390716
H 0.356266605978 -4.263010968719 6.961469037730
H -1.281581597166 -3.073028498834 3.763521534805
H -0.720458807890 -4.719303405296 3.952276213424
H -0.556362459019 -1.405944069471 4.956448108562
H -0.266667191932 -1.928894273054 6.610284223880
H 3.369619358763 0.195989718921 0.088040488845
H 1.443739134861 0.164047800176 -1.815759384541
H 2.157503164377 -0.036325032520 2.494461617047
H -0.938608224374 -0.075355881075 -0.583412140134
H 3.646306238600 -3.067925114201 0.012386841962
H 1.815378441177 -3.126243257695 -1.954450049684
H -0.630020415252 -3.353574029225 -0.811850898800
H -0.281870848911 -3.441051286181 1.866310506629
H 1.271733620323 -0.077429295251 5.873642615643
H 2.194031466393 -1.510250329304 6.328035810707
H 1.941609890353 -1.140567267056 4.611996682067
H 5.485456777625 -3.565073816770 5.133906385798
H 3.954106980297 -2.745982085987 5.460250224376
H 3.991473186694 -4.508658547740 5.236970857196
H 6.019591968508 -1.651269696687 2.606841289994
H 4.669624322337 -1.421172818304 1.476693420039
H 4.526766846097 -0.856476650878 3.143029621019
H 6.184446427035 -4.690015680532 2.354037833988
H 4.730985877977 -5.702583042474 2.479454546865
H 4.982625696195 -4.691326933758 1.052580421117
H -2.684920589027 -2.735490438740 1.804756173898

**van der Waals complex of 1b and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -2989.29604127
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2989.30104272
Sum of electronic and zero-point Energies= -2988.594481
Sum of electronic and thermal Energies= -2988.553092
Sum of electronic and thermal Enthalpies= -2988.552148
Sum of electronic and thermal Free energies=-2988.668343
C -0.007086403435 -0.025803427018 -0.023313714365
C 0.114243167437 -0.021392141448 1.404787089517
C 1.495794202767 -0.160956151861 1.728387333132
C 2.226735592420 -0.258197691589 0.499913425873
C 1.296553792757 -0.205799422019 -0.586152669756
Fe 1.201902801282 1.525880603745 0.608185849334
C 0.389634110447 3.273318800353 -0.067078146197
C 0.521590832193 3.309582684933 1.352549576851
C 1.911311662206 3.159379757183 1.670428313855
C 2.652194170820 3.059577528369 0.448905710229
C 1.698444377936 3.094609292792 -0.621588056791
N 4.032241267871 2.944129291427 0.283822307243
Si 5.297697534927 2.653672237494 1.458986115509
C 4.734257791162 1.467135331800 2.816556398214
N 1.634992868179 -0.315498536064 -1.939784526920
Si 0.640872556891 -0.232022705892 -3.386377288767
C 1.881953866213 0.044525776617 -4.786683295449
C -0.575792746756 1.212948119953 -3.306621161675
C -0.306798412149 -1.875048787889 -3.678905014429
C -1.211659995532 -2.205926067607 -2.473335323241
C 6.716782590569 1.861469715362 0.492875593036
C 5.899521295529 4.298094608520 2.249523034318
C 4.721682760971 5.011229708826 2.946593451051
C 7.009219349467 4.022704986974 3.286123397477
C 6.452663439423 5.224713637164 1.146952397689
C -1.182663047188 -1.755321861528 -4.945300765763
C 0.707279753644 -3.022590286442 -3.867737502613
C 6.241134606326 3.914512733955 -2.737765192456
N 4.793228454599 3.798501585937 -2.579258236497
C 4.161778656114 5.117466502085 -2.528290278364
C 4.212958045547 2.970298876521 -3.632288876174
H 2.637927452823 -0.333124561764 -2.084857373154
H 4.326039026705 3.080629643351 -0.689371676175
H 3.089223109634 5.008288918669 -2.342694619496
H 4.588370553305 5.695429561440 -1.702644645847
H 4.304487646570 5.687979222596 -3.466278423194
H 4.651159949517 1.966888117768 -3.599664203380
H 4.379300314237 3.391305367671 -4.643057345237
H 3.134372580791 2.875740798225 -3.476104000168
H 6.694984329966 2.917822482127 -2.736820333768
H 6.658698574700 4.485187071808 -1.902004325548
H 6.521656560157 4.422430154186 -3.680984103514
H 1.921523097463 -0.165204252002 2.723445511202
H -0.700467461926 0.097137150185 2.107517353187
H 3.302104038499 -0.335301037871 0.390611336620
H -0.928034938988 0.088629105833 -0.576009965880
H 2.327444253162 3.129685363713 2.666941602220
H -0.283845212435 3.408322837095 2.069141651951
H -0.534866995606 3.334394008844 -0.627078605034
H 1.938186379960 2.970891690813 -1.668888533976
H 5.608506401100 1.091607376112 3.363329270224
H 4.064719939265 1.932495194845 3.547321374767
H 4.208820585185 0.609172129521 2.386685074848
H 7.595778659858 1.715869709134 1.132617378443
H 6.417688795972 0.878791031048 0.107384522280
H 7.025845821547 2.475410864196 -0.359998784507
H -0.963655120849 1.438459634556 -4.308235434636
H -1.436670410400 1.007079715236 -2.661266941464
H -0.083134232092 2.112733561226 -2.921181828437
H 1.409518116471 -0.102211613770 -5.765259217506
H 2.286761018722 1.062743712017 -4.766039378247
H 2.724789065790 -0.655096488985 -4.722994882768
H 7.356480016072 4.965430425947 3.736222837561
H 6.654841156174 3.383312899057 4.104808341188
H 7.884919680205 3.537265383091 2.835627311657
H 6.774550614400 6.185896526637 1.576141850392
H 7.322981844062 4.788210831486 0.639604431996
H 5.689812486128 5.441482237279 0.389001540336
H 5.055688160967 5.967358919420 3.378277770657
H 3.905994699700 5.228286741620 2.247174639511
H 4.308607729803 4.413087264421 3.768983261119
H -1.749348350876 -3.149904166141 -2.651111870903
H -0.635352018449 -2.321502547537 -1.548750316256
H -1.969651341767 -1.430621657009 -2.302571963459
H -1.722013616741 -2.697676808501 -5.124732452609
H -1.935940634512 -0.962700826916 -4.850986182972
H -0.587017254670 -1.548732195624 -5.844189346875
H 0.180636604723 -3.977505248059 -4.016379849389
H 1.347533912280 -2.864395297394 -4.745216204312
H 1.355279677271 -3.134509627517 -2.989622907123

**van der Waals complex of 1b and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -3107.25060774
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3107.25544964

Sum of electronic and zero-point Energies= -3106.462942
Sum of electronic and thermal Energies= -3106.417691
Sum of electronic and thermal Enthalpies= -3106.416747
Sum of electronic and thermal Free energies=-3106.539847
C 0.091117470822 -0.575502230818 0.802256941798
C 0.164039715361 0.156655361050 2.030467810860
C 1.541366582044 0.294966523418 2.397181783938
C 2.320064539544 -0.305112099982 1.356750983589
C 1.425306592390 -0.857248596645 0.382535340030
Fe 1.120928793214 1.164372910719 0.514747884864
C 1.532629895342 3.179407588564 0.672311300943
C 2.312590660786 2.576518469527 -0.367629781990
C 1.412235282907 2.024634998649 -1.325442361132
C 0.076262025230 2.281031891666 -0.873590639984
C 0.148283997954 3.023917111954 0.348329773636
N -0.920031712732 3.523170977714 1.099974804145
Si -2.640605978612 3.333499755990 0.809377987884
C -3.094059906979 4.114888635530 -0.848213518174
N 1.989027315426 0.903146927620 3.574801539628
Si 3.611362421130 1.380339959719 4.051825239820
C 3.396607259129 2.791978578269 5.288422943261
C 4.567420892579 -0.063051509618 4.884159028243
C 6.045136339221 0.333347139214 5.092893776583
C 4.600789966214 1.993266115996 2.564836519107
C 3.940789296410 -0.392698482314 6.254690979186
C 4.503113861365 -1.321738818522 3.993446002016
H -0.627073123049 3.872959099854 2.004197185787
C -3.143407291080 1.509562266994 0.778703546835
C -3.507270143230 4.242665781237 2.259005111974
C -5.036206525316 4.190237665223 2.044059017481
C -3.063351343032 5.720097824412 2.321392891967
C -3.172562743439 3.555467707499 3.599238367482
N -0.930397750513 0.337530109620 5.441710099274
C -1.348436639916 1.498644548805 6.241332923022
C -0.234214201605 2.528941300080 6.435141712187
C -0.107512388872 -0.596234139308 6.227217652186
C 0.412558282908 -1.791209541860 5.426194122875
C -2.065400407084 -0.304877424536 4.758379359693
C -3.118430700122 -0.980644338737 5.652574587143
H 1.220492580341 1.074083953074 4.219167079387
H -0.387907989962 -2.488018776259 5.155480638235
H 0.908290302667 -1.461237087434 4.508147332836
H 1.138224683178 -2.348682768302 6.029228818156
H -3.567426520861 -0.271334572523 6.357449137153
H -2.689767337721 -1.806827275602 6.231129314375
H -3.923926640571 -1.392235354170 5.032277875003
H -4.156055901202 3.967323981163 -1.081286643987
H -2.890223455848 5.191984733243 -0.846745097176
H -2.511087145933 3.675322499632 -1.665852648008
H -4.213086042901 1.393544547739 0.562059525304
H -2.586730713234 0.965482950477 0.007334653342
H 0.750062951791 -0.031163131690 6.607344237921
H -0.655158082054 -0.958185306378 7.119780744562
H -2.551295714986 0.469411992997 4.152626221786
H -1.665313274177 -1.033659386315 4.047310325901
H -2.179603154832 1.980323339374 5.716107140640
H -1.738863813927 1.190682430875 7.230332116838
H 3.393085934768 2.527469614386 -0.405924644023
H 1.683081075873 1.481770729847 -2.221806488516
H 1.908002857554 3.662378744487 1.566816541967
H -0.827532032386 1.954727888531 -1.369951818355
H 3.398470653616 -0.341979942710 1.310493587900
H 1.718228167252 -1.375142968469 -0.521876788752
H -0.815940634447 -0.837921026627 0.273256992242
H -0.662270761589 0.561411695448 2.595920795872
H -0.617883691413 3.405165461985 6.971655598920
H 0.600922905207 2.129104326035 7.019839749985
H 0.155959872117 2.862776955904 5.466727828832
H 4.364428517047 3.084042334828 5.714826154080
H 2.966418915536 3.674902347472 4.799849940417
H 2.739097950963 2.517816891225 6.120162975327
H 5.454901142679 2.586315942004 2.915334800775
H 4.998639933724 1.178754812772 1.950325778028
H 3.987479387708 2.626796764731 1.919139745353
H -2.934390272126 1.016063483548 1.734529200142
H -3.656080616516 4.085160783908 4.434261381864
H -3.528234146334 2.518702734993 3.621948728943
H -2.095016535052 3.540368647325 3.806868009590
H -5.554522363391 4.695588792154 2.872792065442
H -5.336877934699 4.693568361957 1.116709641478
H -5.411450424221 3.159656548138 2.005747874842
H -3.581140035377 6.237709117194 3.143221439532
H -1.985579144019 5.824062327674 2.496590855397
H -3.299281670590 6.258382742778 1.395328574742
H 4.463684254002 -1.242033705854 6.720635733732
H 4.006769851087 0.451652328678 6.952808375246
H 2.886612263220 -0.672940143716 6.158702685328
H 6.593472941822 -0.484771067907 5.584489504713
H 6.553455136866 0.541454146150 4.143190437444
H 6.148822359885 1.220866528503 5.731369719653
H 5.021317813737 -2.160975165512 4.482329372558
H 3.470035526478 -1.632396766541 3.800569014361
H 4.991299310817 -1.163883382034 3.023119480804

**van der Waals complex of 1c and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -2329.14352260
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2329.1480485
Sum of electronic and zero-point Energies= -2328.532880
Sum of electronic and thermal Energies= -2328.501470
Sum of electronic and thermal Enthalpies= -2328.500526
Sum of electronic and thermal Free energies=-2328.595697
C -0.014766747235 -0.095723939545 0.404490049779
C 0.087475064456 -0.342070264702 1.811731589131
C 1.473182417810 -0.438386598831 2.158452162004
C 2.221900005399 -0.300913427257 0.943992603867
C 1.306606763128 -0.065115767108 -0.131614454771
Fe 0.925935122880 -1.890604680335 0.715106805070
C 0.790493939126 -3.338898120169 -0.755442287555
C -0.304264411905 -3.448084405571 0.157439338968
C 0.229752586254 -3.681320779463 1.461626677448
C 1.654961739011 -3.699498482075 1.361325306151
C 2.008140893828 -3.497129329370 -0.013290556622
N 3.344373441443 -3.473503809337 -0.497050313486
C 3.507275887330 -2.922793183769 -1.843724125781
C 4.979060015442 -2.762413678161 -2.283694769329
C 5.690936003636 -4.129463253975 -2.303953834150
N 2.021270564727 -0.620026128700 3.421674710082
C 1.275429516703 -1.332374033839 4.455162650846
C 0.973789604850 -0.481243427989 5.713392015180
C 0.120523245596 0.737652757741 5.324412581677

C 0.207467648734 -1.359063902410 6.717979448746
C 2.297409302373 -0.009096073000 6.340927134511
C 4.974256509680 -2.176642285141 -3.708998958689
C 5.724130815920 -1.804342180796 -1.338669564709
N 4.834736831168 -1.719429526023 3.689278569554
C 5.680723275642 -0.809729998423 4.457659783666
C 5.330136831414 -1.897932455096 2.325840831608
C 4.683050721082 -3.003614750567 4.367616852156
H 3.007467838328 -0.892131138515 3.406214643426
H 3.746497037226 -4.405902469022 -0.434019121310
H 5.727470385777 0.161893994105 3.954586681213
H 5.249797023903 -0.657893914263 5.452538457159
H 6.713439593949 -1.192289512672 4.576157551395
H 4.617608737512 -2.484388311646 1.736818016377
H 6.316289008641 -2.401951861203 2.299421967230
H 5.438312341539 -0.920227464106 1.844869012159
H 3.997491509017 -3.642396654009 3.801354789512
H 4.262411131217 -2.848405784276 5.366791876399
H 5.646315459279 -3.539966522729 4.475130644494
H 1.853311180447 -2.216792634640 4.762982090919
H 0.334383100074 -1.711821654915 4.038941604469
H -0.342823782818 -3.781483415459 2.374991343480
H -1.352414238915 -3.342540285452 -0.092896728733
H 2.357105509034 -3.806684416041 2.177503839052
H 0.711707511578 -3.134745360013 -1.814688993964
H -0.744906848081 -0.436661512526 2.495327569325
H -0.935896600614 0.025875912229 -0.151078988998
H 1.572287411097 0.085913413035 -1.170478818376
H 3.297351740566 -0.385715376476 0.861441104011
H 3.025703403667 -1.937373640338 -1.838119478106
H 2.981865743589 -3.532397874550 -2.602118571309
H -0.070459581349 1.375617556929 6.196873520317
H 0.628979313583 1.337279006803 4.561866960839
H -0.851291788909 0.426444767081 4.919204425935
H 2.113302689077 0.591389923430 7.240787496077
H 2.921434863288 -0.865707226192 6.631723726740
H 2.865916990213 0.601369805961 5.630796426769
H -0.028213791537 -0.795929816979 7.629698134939
H -0.739545352532 -1.716787854753 6.292339008140
H 0.797217021100 -2.237962664912 7.011687389549
H 6.705225510124 -4.030540848362 -2.710443954256
H 5.788396100203 -4.553116599512 -1.296672975241
H 5.148599706090 -4.850478291589 -2.929883162357
H 6.754149597844 -1.643751954530 -1.682069523484
H 5.225733215770 -0.827287697224 -1.295900814578
H 5.758777840884 -2.207698495897 -0.323928358706
H 5.999391975620 -2.031133931648 -4.071529227606
H 4.460353203691 -2.842782598125 -4.413969914124
H 4.468351875832 -1.202756576012 -3.735189148396

**van der Waals complex of 1c and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -2447.10082171
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2447.10588122
Sum of electronic and zero-point Energies= -2446.403596
Sum of electronic and thermal Energies= -2446.368506
Sum of electronic and thermal Enthalpies= -2446.367562
Sum of electronic and thermal Free energies=-2446.470233
C -0.003507450965 -0.021685509379 -0.025581976466
C 0.003321602699 -0.058211668136 1.407095402147
C 1.362014547210 -0.057783512795 1.840491351416
C 2.194705162319 -0.014822965892 0.676009296819
C 1.352245063488 -0.021527209837 -0.482015754510
Fe 0.954326985162 1.638457407518 0.764171431566
C -0.056901850803 3.302189750975 0.124618222924
C 1.296004636458 3.346573613994 -0.344755931852
C 2.164821054339 3.359939009359 0.792267355195
C 1.346441549808 3.284977859191 1.962594880724
C -0.024999348278 3.261897044040 1.549305869613
N 3.560040956401 3.497752973402 0.743150717767
C 4.386420344471 2.759711001263 1.699573904489
C 5.586773649672 3.571254438517 2.236999613108
C 6.490481958204 4.015666891421 1.072442555640
N 1.807545986196 -0.047278972102 -1.802506249972
C 1.067859134211 0.696726353565 -2.823909314050
C 0.455543320701 -0.170823591842 -3.951127488945
C -0.521634733149 -1.199821813895 -3.359090461535
C 1.575596937891 -0.901627227787 -4.710279145257
C -0.293953823704 0.766259878770 -4.915420742396
C 6.386372654762 2.661348727302 3.186910977373
C 5.075682336565 4.805671936928 2.999618538723
N 5.037637367503 0.041855569260 -1.820435833839
C 5.518967983835 1.410810750433 -2.060366165047
C 4.503760067326 2.288943382713 -2.795516341883
C 5.692066949172 -0.579463418904 -0.656361995397
C 7.196520101618 -0.869558835416 -0.785461990533
C 5.092148834898 -0.779395157626 -3.043175709283
C 4.585968317426 -2.209649451083 -2.846599299802
H 3.901354302515 3.404215318778 -0.206388682534
H 2.818675661760 0.080771925372 -1.839709460806
H -0.872424023529 -0.062296857947 2.043661957080
H 1.705805882520 -0.060139325558 2.867317402051
H 3.274463251033 0.011324796908 0.655678595698
H 1.612585579356 3.371892160925 -1.379868156907
H 3.754591259819 2.457992563629 2.539807383854
H 5.766040797217 2.318598959428 4.025425450252
H 5.530813859245 0.090003522845 0.196694364237
H 5.155196876033 -1.503194358754 -0.417972622488
H 7.768866749641 0.044848720043 -0.979820211891
H 7.572357908228 -1.307654009732 0.146951136095
H 7.407398229559 -1.577968823322 -1.594500806193
H 6.116011079547 -0.801421905305 -3.463101136911
H 4.462808785027 -0.288369330182 -3.792640051220
H 5.726196867403 1.861782889996 -1.083605264525
H 6.477179008877 1.413630044493 -2.613192235276
H 0.271757957198 1.274368858834 -2.337099205933
H 1.740611075363 1.431883621362 -3.288524072646
H -0.942926605433 3.274453911313 -0.496876172013
H -0.881886346678 3.198151561348 2.207787783336
H 1.697942489719 3.254974651446 2.985312249581
H -0.883605882113 0.000901012605 -0.652697339244
H 4.753783697005 1.824391390512 1.247521625203
H 4.890229863466 3.310483120012 -2.895726628885
H 4.287419563451 1.920614195878 -3.803951196521
H 3.560186615286 2.325661743977 -2.241757602995
H 4.466434414601 -2.692212781005 -3.822974384410
H 5.283128211622 -2.819775184670 -2.262200849981
H 3.614256265446 -2.212728721530 -2.341280829436
H -0.920352998404 -1.854378010757 -4.144627295173
H -0.021276768259 -1.823668997126 -2.610604869772
H -1.373442362845 -0.703973707202 -2.876091224906

H -0.746952030825 0.198625534788 -5.737787644497
H -1.098255814973 1.307505764887 -4.400040281600
H 0.383125714902 1.510167665246 -5.356588282284
H 1.164916564667 -1.498839350611 -5.534209528473
H 2.292387756503 -0.188072455311 -5.140010168284
H 2.120521037479 -1.574308477244 -4.041684583180
H 5.913382606479 5.405943026130 3.376649622351
H 4.461309258023 5.435664011234 2.347853957227
H 4.461533156273 4.509200340858 3.860352759303
H 7.354876717783 4.579359055093 1.444717892884
H 6.875152427701 3.150020227317 0.516248395531
H 5.947076431032 4.663266914849 0.374359256089
H 7.247885928514 3.196027409261 3.605623227437
H 6.765772363596 1.773438118280 2.663669807065

**van der Waals complex of 1d and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -2014.59089961
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2014.59612025
Sum of electronic and zero-point Energies= -2014.207572
Sum of electronic and thermal Energies= -2014.186375
Sum of electronic and thermal Enthalpies= -2014.185431
Sum of electronic and thermal Free energies=-2014.257799
Fe -0.061838878692 -0.012906839730 -0.043324551796
C -0.156555111242 0.051065742553 2.079458932771
C 1.193297635249 0.006109238317 1.603534543423
H 1.955519313156 0.750998380126 1.788983988750
C 1.362444664740 -1.191687866859 0.833727771936
H 2.275839685511 -1.506955337048 0.345404152503
C 0.108181993555 -1.869858883712 0.797719045220
H -0.103951106062 -2.795365143862 0.276957046298
C -0.834687577876 -1.089609517385 1.541733844097
H -1.883295394743 -1.312413501832 1.687818363896
C 0.574042361947 0.451587088816 -1.945946980857
H 1.511309894349 0.119356957216 -2.374496855784
C -0.670409555597 -0.251071971996 -2.005224136785
H -0.837554256294 -1.205614533500 -2.486025088009
C 0.373794407772 1.643913076183 -1.186988589941
H 1.133343354501 2.374916594037 -0.940491875234
C -0.991599793802 1.677176678375 -0.762158444044
H -1.460351946926 2.435807250264 -0.149156867304
C -1.643063796329 0.509492966155 -1.275400883586
N -3.018875538455 0.217874829026 -1.068676828834
H -3.598288219756 0.861076096180 -1.603649676213
C -3.421118294783 -1.165402131742 -1.305521618675
H -2.843995983192 -1.815010432591 -0.639270647155
H -3.263325956572 -1.510905040148 -2.341063227006
H -4.483605309017 -1.275574047634 -1.063366184357
N -0.723171445441 1.003174751883 2.917230400659
C -0.103714956225 2.317675675526 2.958463563587
H 0.892421616395 2.260685104559 3.413400765344
H 0.003685063646 2.772582875712 1.958083193749
H -0.716356079802 2.976253463203 3.582094999010
H -1.744848821108 1.052105027457 2.828142675043
N -3.726401962515 1.336183775692 2.756515517312
C -4.108598164568 1.725100441221 4.110446054826
C -3.986186474411 2.401113438154 1.791106596823
C -4.367443415273 0.087077976029 2.350766858182
H -5.060169355197 2.668840590864 1.737660354346
H -3.423027814395 3.298917178538 2.070817943260
H -3.657876424459 2.071660375037 0.801595048672
H -5.472740687224 0.165610288898 2.346602139498
H -4.083632189423 -0.713887195220 3.042948552682
H -4.030888119846 -0.175997901892 1.343964143484
H -3.571767590989 2.635665530282 4.398881960067
H -5.195449634967 1.918189549162 4.203839935490
H -3.835360465211 0.930762768464 4.813248441809

**van der Waals complex of 1d and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -2132.54691564
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2132.55177377
Sum of electronic and zero-point Energies= -2132.076671
Sum of electronic and thermal Energies= -2132.052022
Sum of electronic and thermal Enthalpies= -2132.051078
Sum of electronic and thermal Free energies=-2132.130205
C 0.065429717179 -0.054678965639 0.000286292794
C 0.136822842684 -0.099773851218 1.432274858147
C 1.515798988084 -0.042319660347 1.807525934643
C 2.296615759526 0.032475336115 0.614405972504
C 1.403916238975 0.035449896317 -0.502740781052
Fe 1.006956358273 1.636046513495 0.726578175182
C -0.049662735449 3.258149051774 0.016906058611
C 1.308973095132 3.400227977248 -0.413841442161
C 2.129561251945 3.377214486400 0.760210916823
C 1.276868204615 3.287785060020 1.908928191815
C -0.070923043464 3.216514466126 1.448352930972
N 1.732130317119 3.552685646463 -1.729057819840
C 3.123503222763 3.255072627875 -2.024286127035
N -1.088452645263 -0.083901697766 -0.829296151222
C -2.350078979307 0.267586194129 -0.184272971436
N -0.047154737599 2.454792216956 -3.943021803970
C -1.423962566355 2.727898176574 -3.497375221505
C 0.391113538746 3.260218385403 -5.094534683405
C 0.146977904969 1.004738263629 -4.098820032682
H 3.210399173246 3.415061913456 0.778579208790
H 1.604839560046 3.253802742575 2.940098990504
H -0.954190193917 3.117498082468 2.067078917191
H -0.906866067447 3.189474937443 -0.637698629603
H 1.897639678678 -0.025407292889 2.820629237306
H -0.704507589400 -0.133073983295 2.111533606763
H 3.375025793586 0.114481661662 0.565848004067
H 1.673308204111 0.113870295003 -1.547385610966
H -1.159589247822 -0.981170354900 -1.304080306823
H -2.257011822361 1.274732500916 0.234734121845
H -2.647687783295 -0.414513086515 0.630126761954
H -3.146141688887 0.275518411262 -0.936479681055
H 3.784224211619 3.977871535041 -1.531026087446
H 3.425348361088 2.242556533784 -1.702055490540
H 3.280660471677 3.342565398884 -3.103514599657
H 1.088188464953 3.140685870676 -2.415312040414
H -0.522424702718 0.590340157120 -4.877696236877
C 1.589187055090 0.596985671909 -4.403399424187
H -0.162650275327 0.555055654277 -3.149645585897
H -2.166189345981 2.350659631582 -4.227357973418
C -1.700490643739 4.205726404240 -3.209938218857
H -1.568390336448 2.141172743234 -2.582680806461
H 1.455130139376 3.055497056288 -5.253618940704
C -0.373672082304 3.052039924666 -6.411825353505
H 0.336650227131 4.312803352951 -4.798871074844
H 1.688900123583 -0.491456934001 -4.317435517266
H 1.900203599194 0.873284437812 -5.417140766587

H 2.285964142840 1.059574282855 -3.695701904909
H -2.656207615652 4.304267704881 -2.681992251808
H -0.915896111833 4.641349841809 -2.581687973802
H -1.772093618485 4.800485712915 -4.127381905625
H 0.041331898668 3.703045717609 -7.190775703193
H -0.299154537346 2.017801220305 -6.767004444285
H -1.437111191796 3.295538499880 -6.305614620475

**2a *(trans,trans)***
E(B3LYP-D3/6-31+G*) = -3379.29996362
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3379.30478128
Sum of electronic and zero-point Energies= -3378.910957
Sum of electronic and thermal Energies= -3378.882868
Sum of electronic and thermal Enthalpies= -3378.881924
Sum of electronic and thermal Free energies=-3378.968953
C -0.098491646707 -0.137302049132 0.352511358388
C 0.027225897803 0.068517645122 1.762786456715
C 1.416592587617 0.160300921443 2.074634861286
C 2.156337417530 0.027149438857 0.849221359718
C 1.209808910503 -0.178330862362 -0.213828133123
Fe 0.937722427287 1.615745723655 0.731300880948
C 0.094809135917 3.278301157574 -0.171825700080
C 0.220891184407 3.491030908551 1.237393588785
C 1.596757434842 3.344145934893 1.585884809366
C 2.325853339147 3.022388154718 0.389425163794
C 1.389896588377 3.003638499271 -0.702292265795
N 3.734586938082 2.785784579474 0.328636101307
Si 4.701372177663 4.294227501242 0.107337497879
N 3.581335589100 0.077946718141 0.744268508688
Si 4.372098453210 -1.524652552020 1.000334996489
P 4.489232270146 1.299810948619 -0.017343820654
Cl 3.889214902470 1.003685478976 -2.168126754792
H 1.467222729716 -0.274816131763 -1.259166735950
H 1.638580552172 2.754137258594 -1.724157434096
H -0.829203426659 3.294159600256 -0.735614355576
H -0.588796632139 3.698595037953 1.925054554884
H 2.028722486843 3.409743839249 2.575745118051
H -1.028038433608 -0.219081473101 -0.196270994568
H -0.788672916383 0.166637842399 2.467227493808
H 1.855366192931 0.346412151665 3.046003658845
C 6.537417810962 3.873649443270 0.082083724999
C 4.182720218664 5.100296568673 -1.512409932886
C 4.318288857406 5.429962371053 1.561434241956
C 3.741636963425 -2.715187288216 -0.313993585656
C 6.242686165792 -1.335572121525 0.883117469580
C 3.889481108914 -2.125067398551 2.720103099508
H 7.105937531692 4.812301535017 0.030754326797
H 6.853388568621 3.339648478812 0.985567216739
H 6.818677666552 3.266096416456 -0.784967810443
H 4.901801828745 6.356325849770 1.478882176101
H 3.257841908504 5.703533237660 1.592666330907
H 4.574871384809 4.954073377646 2.515882648180
H 4.741308653026 6.029275176223 -1.686239349417
H 4.368148310508 4.425939347108 -2.357104261842
H 3.114274882549 5.345669658006 -1.507435544897
H 4.366229236822 -3.091930210290 2.928284934371
H 4.211883601505 -1.416999197930 3.493388007249
H 2.806011523861 -2.258824516877 2.812647155618
H 6.703353777013 -2.303142991632 1.125003742606
H 6.575236432985 -1.050091149097 -0.120834272915
H 6.630088547784 -0.593845870027 1.590957975758
H 4.190572614013 -3.709605401889 -0.192226652143
H 2.652731813618 -2.827815713123 -0.255582167620
H 3.987639109224 -2.348881053632 -1.317962923216

**2a *(cis,cis)***
E(B3LYP-D3/6-31+G*) = -3379.27676869
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3379.28017696
Sum of electronic and zero-point Energies= -3378.888085
Sum of electronic and thermal Energies= -3378.860053
Sum of electronic and thermal Enthalpies= -3378.859108
Sum of electronic and thermal Free energies=-3378.945011
C -0.273612806855 0.421862860181 -0.606320989709
C -0.374841834660 0.005921603070 0.757963829415
C 0.941067505679 -0.275551667472 1.233296677344
C 1.868060350505 -0.051107838521 0.158896033615
C 1.100396488322 0.377478627124 -0.982189805582
Fe 0.849005255197 1.659397756947 0.623662249037
C 0.300367756865 3.658429985211 0.536518580915
C 0.183967161673 3.159579430448 1.871474476392
C 1.462986460429 2.670921163553 2.274101493656
C 2.387488682091 2.879127092018 1.194294039686
C 1.654112317572 3.498978695368 0.120503390470
N 3.751383765177 2.455309239195 1.175278132270
P 4.000781581538 1.392802713613 -0.202834787922
Cl 6.080990112085 0.938157930925 0.040614981011
N 3.289879544507 -0.148336393427 0.254922481340
Si 4.026942685975 -1.753011614893 0.571602230797
Si 4.905752073748 3.206212273271 2.324905841203
C 2.618451980916 -3.000326884182 0.734907580680
C 3.938315447631 4.447089882286 3.369270533384
C 6.232826987400 4.179267240177 1.400732148679
C 5.669080544366 1.905710317658 3.455223977355
C 5.023882307118 -1.729539273648 2.170698090470
C 5.084769961934 -2.303988212520 -0.891094271214
H 1.513250274353 0.659592920671 -1.941783799625
H -1.094306250193 0.732034319369 -1.240308833568
H -1.286045340945 -0.056476918183 1.338808528697
H 1.215612613394 -0.574037902826 2.236257402600
H 2.062380198082 3.752790774729 -0.848901739716
H -0.501915636302 4.071183331006 -0.061533490818
H -0.721659092279 3.129771719307 2.463517652448
H 1.705077114313 2.191810008839 3.213370942776
H 6.877620969922 4.702847421184 2.119686393031
H 6.868635586077 3.546164951429 0.775712020710
H 5.769612561949 4.937257093441 0.756211510262
H 4.658531806097 5.045352501608 3.943489469688
H 3.349196913411 5.133700490069 2.750732863664
H 3.256429142479 3.972250734016 4.082376582015
H 6.253186530999 2.391502261010 4.248470976182
H 4.890061432161 1.299564849862 3.933860387010
H 6.333237710672 1.228095529018 2.910972439097
H 3.054130181976 -4.008535410737 0.743099969393
H 2.039906483923 -2.880120320320 1.656736916659
H 1.919667487028 -2.943435043297 -0.107444605435
H 5.451716086518 -3.325205719027 -0.720086229919
H 4.486196349439 -2.315509513761 -1.810936270920
H 5.950736342943 -1.657712778771 -1.058873585986
H 5.340725703218 -2.748068636931 2.432642485243
H 5.918979817470 -1.106448507291 2.086815677231

H 4.420679922359 -1.340676312318 3.000338404972

**2b** ***(trans,trans)***

E(B3LYP-D3/6-31+G*) = -3615.19767277

E(PCM-B3LYP-D3/6-31+G* (ether)) = -3615.20204853

Sum of electronic and zero-point Energies= -3614.635847

Sum of electronic and thermal Energies= -3614.600645

Sum of electronic and thermal Enthalpies= -3614.599700

Sum of electronic and thermal Free energies=-3614.699316

C -0.290538475938 -0.128240410092 -0.298923375633
C -0.333174080820 0.192256621270 1.093828925462
C 1.007674650755 0.378627525255 1.545595710504
C 1.888516608639 0.180314895903 0.426070441348
C 1.073914732916 -0.144964942661 -0.713914158006
Fe 0.621279628247 1.698750571076 0.043708051316
C -0.181570503915 3.237426589714 -1.090982735522
C -0.238902787593 3.565160993368 0.299407175939
C 1.089177632322 3.523196338549 0.818716929850
C 1.974803830910 3.150877371014 -0.251075507473
C 1.180357510636 2.998497452873 -1.439101111918
N 3.386195338234 2.971714707349 -0.131666261311
Si 4.408842447498 4.458128848208 -0.047111255506
N 3.312848722311 0.291139466637 0.473709539463
Si 4.187451995593 -1.073638488670 1.270492496973
P 4.227005873422 1.498013951980 -0.315880511151
Cl 3.834905099711 1.042541188936 -2.453438167726
H 1.444352153029 -0.310864572464 -1.714973407488
H 1.560675854709 2.685327218276 -2.400711594460
H -1.028303496835 3.156398110546 -1.760568245195
H -1.135149806040 3.779514719226 0.867417137093
H 1.385408186603 3.693716688920 1.844085876875
H -1.146823249623 -0.300510175556 -0.938227905686
H -1.226204688788 0.304020940469 1.695020145769
H 1.322498876153 0.667646793131 2.539039661376
C 5.808838358425 4.332471992503 -1.305029915532
C 3.285229283153 5.900972008800 -0.497874243271
C 5.110373164840 4.683960841849 1.724958470610
C 3.877954402407 -2.719086238661 0.335848315030
C 6.033242710797 -0.681614939498 1.294921286777
C 3.579752563442 -1.206862865365 3.052576610138
H 6.366091351399 5.277430729025 -1.343607957955
H 6.519396573666 3.532077987520 -1.074109342732
H 5.403579521565 4.136028532303 -2.304533563980
C 5.794250226878 6.068519925899 1.805247239419
C 3.976941140563 4.620082834476 2.769153009001
C 6.149983358067 3.596133054056 2.066043097272
H 3.878278258514 6.817378754298 -0.604495290336
H 2.778756154883 5.712684702495 -1.451427570050
H 2.510475255687 6.080667826159 0.254728156130
H 4.134395811606 -1.997172974340 3.574863725406
H 3.749466172192 -0.267560860224 3.593285791513
H 2.514464956781 -1.449948693427 3.115476775143
H 6.539449918223 -1.455114510492 1.886442822845
H 6.484756947784 -0.673962094995 0.297020586932
H 6.244137423941 0.285004623702 1.764351171322
C 4.883432526911 -3.775428461626 0.852933092930
C 2.448701391637 -3.252161991855 0.579962585306
C 4.100171605913 -2.515342260280 -1.176838119932
H 6.554466914863 3.764815657712 3.075592198407
H 5.708024899046 2.593109052120 2.054986325679
H 6.996461223713 3.595344774870 1.368940969624
H 6.224434271849 6.220252734185 2.806454376697
H 6.614727435951 6.165534495996 1.082505508791
H 5.087900006061 6.888766540410 1.627106249181
H 4.378394461921 4.806213949519 3.776683663184
H 3.197553124655 5.370339303954 2.585024468190
H 3.501841395917 3.632169466614 2.781814440071
H 4.698063440541 -4.739693339401 0.356826649265
H 5.922791800761 -3.496739418232 0.642265522921
H 4.789333800349 -3.945626619436 1.933925226260
H 2.308583741109 -4.201847340496 0.041500199567
H 2.263651244220 -3.451285577685 1.642939716131
H 1.678541141719 -2.558676505755 0.229207495691
H 3.968302788303 -3.469284126126 -1.709288195281
H 3.397108994624 -1.793181937004 -1.601965079589
H 5.111720853724 -2.153168656959 -1.400938934226

**2b** ***(cis,cis)***

E(B3LYP-D3/6-31+G*) = -3615.16584233

E(PCM-B3LYP-D3/6-31+G* (ether)) = -3615.16909237

Sum of electronic and zero-point Energies= -3614.604231

Sum of electronic and thermal Energies= -3614.569163

Sum of electronic and thermal Enthalpies= -3614.568219

Sum of electronic and thermal Free energies=-3614.667129

C -0.377307987963 -0.062664058746 0.015010384630
C -0.327685577768 -0.512594370079 1.371920895518
C 1.041610927204 -0.554727231187 1.774285469192
C 1.853922321236 -0.156215785927 0.658262646846
C 0.958575699156 0.153984055859 -0.427452253906
Fe 0.564814252935 1.336413736678 1.228111603946
C -0.309463955642 3.222354608202 1.222821580746
C -0.346584222558 2.648509189739 2.530650726651
C 0.993249914875 2.355643540081 2.925054440906
C 1.876827006827 2.763423679044 1.866296426511
C 1.052513257761 3.307874177985 0.815708022387
N 3.292184636111 2.543027001148 1.821444157668
P 3.629964237874 1.683743551410 0.321723690898
Cl 5.766001107505 1.693657787562 0.301884105920
N 3.276090269631 -0.015186462524 0.665375704221
Si 4.352849991363 -1.453967722897 0.545051810984
Si 4.318221331269 3.389331885359 3.031055439024
C 3.412739550883 -3.143557043069 0.661586997075
C 4.724569754471 5.154770164221 2.396505920045
C 5.880576166989 2.416325657344 3.447870488696
C 3.359552668699 3.550051638831 4.654783038430
C 5.597707934727 -1.382465362104 1.964340043407
C 5.213775137926 -1.436158294606 -1.141677755745
H 1.264811188841 0.517704387428 -1.399490736832
H -1.274312108225 0.102054134228 -0.567975283535
H -1.179853926621 -0.746521195734 1.997040416991
H 1.418262324904 -0.796442529040 2.758317480555
H 1.413430577901 3.673050193788 -0.136368166036
H -1.166274118590 3.527464043778 0.635943282419
H -1.236327015367 2.439341397200 3.110441543051
H 1.299323531645 1.870607716300 3.840469377240
H 6.171131605341 2.652931428025 4.479789985225
H 5.705420994097 1.337312056291 3.385212895966
H 6.724486177531 2.653946313804 2.794763256930
C 5.717918811238 5.828142441116 3.370370108054
C 5.358589584621 5.116068278115 0.991720421775

C 3.431110822390 5.997576456920 2.330799516275
H 3.973775636222 4.134143905521 5.352408094972
H 2.393128027476 4.052218700334 4.557364516289
H 3.191873946329 2.569019941508 5.115645472660
C 4.451172525028 -4.221712858524 0.248766433254
C 2.951500907273 -3.472516124364 2.097154060925
C 2.214727065487 -3.257709528057 -0.305403194982
H 6.084669580166 -2.103439580421 -1.141955691548
H 4.529510480477 -1.782896948381 -1.926324074742
H 5.563552514892 -0.438700887381 -1.418264358150
H 6.145132877860 -2.328465062276 2.058029271634
H 6.329488944705 -0.583416811035 1.816471556925
H 5.083894982874 -1.196564940034 2.915284510326
H 5.586311269284 6.138902466217 0.654847166025
H 6.293629161211 4.545254814838 0.972751206500
H 4.684849105939 4.669345715823 0.251172977642
H 3.657363177071 7.006683926964 1.953918672833
H 2.687499489618 5.553641975198 1.658536459841
H 2.962792777364 6.115737355911 3.315678897367
H 5.947782032223 6.849147902072 3.030245714117
H 5.312780215704 5.910548931222 4.386970117187
H 6.668168596854 5.282302915977 3.428780480193
H 4.008144731722 -5.220532264794 0.373901960887
H 4.750284219535 -4.129631766921 -0.800979069761
H 5.359091338578 -4.193995324327 0.864077374315
H 2.532607983760 -4.489743236793 2.131847823361
H 3.781883116253 -3.437973158419 2.813033059951
H 2.171283923459 -2.793157843024 2.448179898238
H 1.842177830792 -4.293491692183 -0.312588018659
H 1.382210097419 -2.611592434972 -0.018027016207
H 2.493721528189 -3.007630004422 -1.336879908607

**2c *(trans,trans)***

E(B3LYP-D3/6-31+G*) = -2955.03551592
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2955.04051012
Sum of electronic and zero-point Energies= -2954.566492
Sum of electronic and thermal Energies= -2954.540645
Sum of electronic and thermal Enthalpies= -2954.539700
Sum of electronic and thermal Free energies=-2954.621132
C -0.070862224471 0.098013986589 0.624324404100
C -0.345592591645 0.133824375944 2.036833879999
C 0.903452519017 0.125678536343 2.723701152345
C 1.950831452423 0.057597170690 1.751938974479
C 1.354415162676 0.025733237778 0.456530279578
Fe 0.775858623707 1.728222776716 1.409734559959
C -0.145168778009 3.110068095383 0.299064222328
C -0.425121667302 3.363204757346 1.688131712047
C 0.818469935154 3.578533467308 2.350748065561
C 1.866302421502 3.488567127288 1.381258966439
C 1.275754433590 3.214171669507 0.112102605320
N -1.106363780611 2.824111692039 -0.719331297499
P -2.059436400330 1.416426223936 -0.829917251213
Cl -3.372685157340 1.582715124846 1.009441809715
N -1.039402365028 0.112972652454 -0.426636482528
C -1.677319366606 -1.207752713652 -0.698029184744
C -1.229805568879 -1.923732324551 -1.995601438119
C 0.286690468008 -2.176883079088 -1.990901487742
C -1.806627497825 4.023831155925 -1.262636274231
C -1.387908384482 4.467620393492 -2.685420365405
C -1.715025784178 3.376809660002 -3.719910070213
C -2.198996559480 5.738670522987 -3.008137683105
C 0.114351013365 4.789808290970 -2.742838695321
C -1.976027973489 -3.272493813411 -2.035545858018
C -1.604412588469 -1.095975141566 -3.237184137750
H -1.330116394562 0.227809443599 2.473347780081
H 1.036441165341 0.192419772256 3.795886101125
H 3.013088814949 0.061307406649 1.960101816289
H 1.874633751628 0.011421478093 -0.490751529713
H -1.406143504234 3.316708272230 2.139904718310
H 0.948997992521 3.748684852718 3.411753235060
H 2.926388804682 3.581055584455 1.579751633447
H 1.799524589065 3.051312240283 -0.819197175150
H -2.889892569815 3.842230160856 -1.255427354280
H -1.628489122600 4.843731955770 -0.557960548048
H -1.955922628310 6.105730744351 -4.012586646765
H -3.278682646400 5.543234635721 -2.976168733442
H -1.980232855405 6.544478619560 -2.295425114366
H -1.464162007971 3.722252103886 -4.730731317730
H -1.141833905342 2.462921765421 -3.528401509302
H -2.780389448175 3.115936069600 -3.705641004060
H 0.378465999508 5.206049556989 -3.723008352237
H 0.400296108005 5.519484591936 -1.975049829737
H 0.712489408573 3.886512345875 -2.591881016237
H -2.768179807213 -1.081926664040 -0.724152303982
H -1.463170781165 -1.848829867494 0.164350459010
H -1.331533358057 -1.636300617329 -4.152394467541
H -2.681337947206 -0.890573449443 -3.273306169982
H -1.077706675439 -0.135306773312 -3.247968377748
H -1.710106823055 -3.832903531171 -2.939957814002
H -1.721728273195 -3.896131539029 -1.168626625146
H -3.064136489437 -3.127806041689 -2.040123262064
H 0.576013796727 -2.779195534850 -2.861106863783
H 0.839133912487 -1.234030342237 -2.039276434863
H 0.603936295428 -2.711102374188 -1.086660929542

**2c *(cis,cis)***

E(B3LYP-D3/6-31+G*) = -2955.02353804
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2955.02688084
Sum of electronic and zero-point Energies= -2954.554696
Sum of electronic and thermal Energies= -2954.529024
Sum of electronic and thermal Enthalpies= -2954.528080
Sum of electronic and thermal Free energies=-2954.608378
C 0.640489359047 -0.046302283521 -0.134231266092
C 0.115676718115 0.072417114660 1.199177361682
C 1.212529734004 0.088152136810 2.114280113600
C 2.420847450747 0.009276142665 1.358304204598
C 2.073145595833 -0.080489532955 -0.021619604787
Fe 1.318359682518 1.670656560071 0.798759314403
C 0.577328694915 3.124753519032 -0.471708393331
C 0.052949781701 3.269394872329 0.859318868105
C 1.146509416199 3.489503029111 1.751805124594
C 2.353391118024 3.454255555181 0.990272011094
C 2.007138660334 3.237652844777 -0.375833413064
N -0.149438435521 2.797269158585 -1.653108270352
P 0.528406213591 1.321648997614 -2.332358045709
Cl -0.634052897106 1.111395219195 -4.088895838063
N -0.093118639064 -0.004085959282 -1.355370698925
C -1.493166486723 -0.456611004075 -1.326199403266
C -1.671401599244 -1.983054481910 -1.533776390714
C -0.970600126876 -2.787172108784 -0.423815812242

C -1.566537467177 3.189550517022 -1.713258591883
C -1.805022038195 4.629554934007 -2.237121407188
C -1.248752883577 4.762089250075 -3.665245389517
C -3.328547843206 4.858847551485 -2.250239541899
C -1.140975152304 5.676944211592 -1.325136080107
C -3.184487231394 -2.270803722697 -1.492781619960
C -1.103254305787 -2.391298923184 -2.903826874031
H -0.927582758997 0.143959656291 1.471948368925
H 1.134225528088 0.165603054098 3.191000276115
H 3.427178079804 0.022557423788 1.756287957817
H 2.764133784586 -0.125002358642 -0.852698815521
H -0.987633237525 3.216312736203 1.146155411495
H 1.067680931072 3.637754341912 2.821043085542
H 3.358131608422 3.564269126418 1.377129070465
H 2.698719689054 3.132966201345 -1.200991355326
H -2.082154816726 2.499479775244 -2.384807750916
H -2.039763408103 3.072586834558 -0.728546690424
H -3.564405109259 5.860605089617 -2.629545687612
H -3.837272854359 4.130027335799 -2.894727210135
H -3.754679230072 4.775454398308 -1.241506276627
H -1.419166228699 5.775053678534 -4.050815887973
H -0.171816996059 4.564100206916 -3.683323166736
H -1.730608145056 4.051257772933 -4.346861585081
H -1.375637560707 6.688923545818 -1.678871911078
H -1.494708341321 5.590615318715 -0.290229711156
H -0.051659825703 5.568997314989 -1.315281222236
H -2.032611803878 0.055131857056 -2.126290796193
H -1.975462470688 -0.153673039573 -0.386583520846
H -1.231277342948 -3.468756061072 -3.066586787421
H -1.609659440770 -1.859932067155 -3.718245480542
H -0.034978887465 -2.158672880810 -2.967082055714
H -3.378287093427 -3.338669461102 -1.651305915607
H -3.618625158362 -1.993596914380 -0.522850618639
H -3.718670734563 -1.715344719476 -2.274735806120
H -1.163095046466 -3.859537931142 -0.555251876586
H 0.113489703094 -2.636163523253 -0.440992392319
H -1.332459856783 -2.498711642364 0.570904577410

**2d** ***(trans,trans)***

E(B3LYP-D3/6-31+G*) = -2640.48477953
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2640.48972305
Sum of electronic and zero-point Energies= -2640.243123
Sum of electronic and thermal Energies= -2640.227435
Sum of electronic and thermal Enthalpies= -2640.226491
Sum of electronic and thermal Free energies=-2640.285325
C -0.023987499851 -0.005415992862 -0.079859055825
C -0.263856948323 -0.067135929470 1.322355146701
C 1.008553210544 -0.118023740062 1.981888217890
C 2.032730159340 -0.036844234289 0.978497692930
C 1.388489654299 0.013256906806 -0.289724740852
Fe 0.844798179212 -1.696952725798 0.767127247748
C 1.082470356442 -3.141336989868 2.128282816011
C -0.184388112684 -3.317642135673 1.479756347594
C 0.061508162685 -3.502703557986 0.089490767097
C 1.473706777511 -3.472672027031 -0.120931115680
C 2.111748733158 -3.268997437704 1.135000254959
N 1.251188802373 -2.906427932418 3.523811906780
P 1.846798448996 -1.502996466608 4.266747898071
Cl 3.995200051940 -1.485541981646 3.542453351763
N 1.185224020368 -0.208579154249 3.393177150582
C 1.378418772606 1.105665321827 4.037630998464
C 1.506730235200 -4.141312953514 4.291693002300
H 0.687660332993 -4.842677024624 4.118432055801
H 1.549251244015 -3.913622756400 5.358666044837
H 2.449888191277 -4.611091844170 3.991822910455
H 0.526528413842 1.746237259203 3.799393854562
H 2.298247915467 1.589733387799 3.691576668434
H 1.429473646643 0.984406384783 5.121499958831
H -1.221456276041 -0.124896549854 1.816762735605
H -0.778976821746 0.002816446086 -0.851030936424
H 1.884949092879 0.034867789725 -1.247847828282
H 3.092615965869 -0.082429327567 1.171180675853
H -0.690362994223 -3.622158449041 -0.675494863972
H 1.972885563709 -3.562469665056 -1.073661806257
H 3.167695113854 -3.153404005046 1.319873579236
H -1.144826625701 -3.259164360038 1.968540349002

**2d** ***(cis, trans)***

E(B3LYP-D3/6-31+G*) = -2640.46646787
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2640.47040991
Sum of electronic and zero-point Energies= -2640.224861
Sum of electronic and thermal Energies= -2640.209449
Sum of electronic and thermal Enthalpies= -2640.208505
Sum of electronic and thermal Free energies=-2640.266422
C 2.359998764005 1.766069675699 -0.777039612213
C 2.401060461407 1.740809291843 0.649408337847
C 1.064085161892 1.617087771861 1.125579529373
C 0.175816496530 1.576517737849 -0.008612421225
C 0.997492598847 1.664171590151 -1.187065322498
Fe 1.515588385599 0.009043468550 -0.069513281185
C 2.342356734787 -1.710800946783 -0.879462418987
C 2.485853363129 -1.714661408450 0.539258199177
C 1.180459445167 -1.634005228265 1.117087748330
C 0.219398596531 -1.600715978578 0.047862686151
C 0.951160418712 -1.637295294544 -1.186601129097
N -1.185876271891 -1.427986035333 0.180966284294
P -1.681914004914 -0.070144894073 -0.823718764291
Cl -3.787661964623 -0.090843847920 -0.593883728794
N -1.244752719052 1.417765530401 0.038464585732
C -1.919925825346 1.915215150656 1.248867726770
C -1.724461633589 -1.717918173534 1.516013972788
H -1.524796009336 1.500872639094 2.182464258204
H -1.413662736483 -2.728357392962 1.799180306202
H -2.813958882609 -1.693119834448 1.486649685553
H -1.374679926868 -1.018059676337 2.284020165394
H -2.981884829017 1.676763530897 1.200487362129
H -1.813393241899 3.004926185670 1.278990888991
H 0.637364102960 1.629904075580 -2.207032240578
H 3.217044481883 1.834449318074 -1.434227153433
H 3.291497638217 1.788488714896 1.262664162775
H 0.763053315948 1.543424521978 2.159556740450
H 0.519529213208 -1.599570220763 -2.177682271393
H 3.144054821159 -1.748389833405 -1.605470594089
H 3.417728178953 -1.760786778356 1.087439592029
H 0.960404764784 -1.584458199392 2.174309393777

**2d** ***(cis,cis)***

E(B3LYP-D3/6-31+G*) = -2640.47061328
E(PCM-B3LYP-D3/6-31+G* (ether)) = -2640.47465743
Sum of electronic and zero-point Energies= -2640.228631

Sum of electronic and thermal Energies= -2640.213390
Sum of electronic and thermal Enthalpies= -2640.212446
Sum of electronic and thermal Free energies=-2640.269803
C -0.037601701763 -0.017514098981 0.041927554196
C 0.026029193636 -0.028298939908 1.467055293076
C 1.408261116558 -0.017297113507 1.854373649613
C 2.187962565144 -0.015397216661 0.650789134758
C 1.296221325404 -0.020659392024 -0.459580392478
Fe 0.967621314396 -1.694746459718 0.720825171950
C 1.462216249084 -3.203607427427 2.051859527753
C 0.081209262580 -3.287123642416 1.669038362208
C 0.020951764971 -3.475897480915 0.256279671585
C 1.354953267766 -3.489709511800 -0.244571363242
C 2.244045888770 -3.327777884033 0.856084223373
N 1.959530819351 -2.926616557334 3.355614168094
P 2.987131433081 -1.500735836363 3.299324576320
Cl 3.565149878205 -1.365000285173 5.332505152731
N 1.911893994128 -0.114289751302 3.181307879289
C 0.979505707642 0.306692993494 4.231826587505
C 1.039744213944 -3.245907193628 4.452066941309
H 0.136485291029 -2.623227791077 4.450613088191
H 1.547501431742 -3.116125123928 5.405760050953
H 0.739519937410 -4.292320649030 4.361999998224
H 0.097771355001 -0.341523701680 4.309085453028
H 0.644340070780 1.323247952100 4.013864213192
H 1.489285137605 0.312862473470 5.193216155142
H -0.819107377009 -0.053075426847 2.136265211338
H -0.941451734649 -0.014559594179 -0.547572519451
H 1.586382897772 -0.028827414831 -1.498953178696
H 3.265493163634 -0.038722806866 0.603998322878
H -0.881052284599 -3.582081878673 -0.326453200405
H 1.646841641918 -3.600134888478 -1.277607491763
H 3.320271973945 -3.274081327424 0.804515491678
H -0.765676985202 -3.208438311871 2.331836208875

**3a *(trans,trans)***
E(B3LYP-D3/6-31+G*) = -5490.84240425
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5490.84692724
Sum of electronic and zero-point Energies= -5490.453690
Sum of electronic and thermal Energies= -5490.425488
Sum of electronic and thermal Enthalpies= -5490.424544
Sum of electronic and thermal Free energies=-5490.511091
C 0.096899146088 -0.004964045020 -0.046166320784
C 0.126962750099 -0.001336173419 1.380108666645
C 1.502296444712 0.012569555968 1.795995704814
C 2.317320865370 0.058369933728 0.611117696042
C 1.446909228058 0.030845915518 -0.518019630129
Fe 1.152981312972 -1.624327690630 0.696269753224
C 1.664186348081 -3.003523270639 2.055432367072
C 0.299057869259 -3.206940456833 1.655742072384
C 0.281933406639 -3.449424909316 0.250007035070
C 1.632392431522 -3.421310693938 -0.221079968028
C 2.490347072609 -3.163482630315 0.888313579793
N 2.088273966195 -2.724057029334 3.391767988103
P 2.736507740004 -1.258741045561 3.958241748172
Br 4.887882415849 -1.239700183882 2.837513265890
N 1.941520780073 0.011440139935 3.156443443792
Si 2.177645540340 1.672818829062 3.830414387591
Si 2.493318873846 -4.211759322212 4.336679404551
C 0.954254843106 -5.297462072328 4.346716994456
C 2.974929284510 -3.728127293902 6.093332545620
C 3.919870362626 -5.086976946478 3.476209549791
C 0.531949927220 2.574680577548 3.669478342805
C 3.510954056461 2.535186955550 2.820426988509
C 2.691870007791 1.549361485233 5.639283594623
H -0.721468956166 -0.053123747802 2.049676885917
H -0.791786885520 -0.054598724549 -0.662047407788
H 1.758097744257 0.011555826807 -1.554655700667
H 3.397914370162 0.043350101799 0.601239950313
H -0.601274524165 -3.600152979563 -0.357249702401
H 1.949316283959 -3.545824223862 -1.248640290452
H 3.563263655509 -3.035560918202 0.866223194639
H -0.556215035333 -3.132414506252 2.314372619808
H 3.699460742850 3.546848597083 3.202829686348
H 4.449174895524 1.969637880868 2.861223339555
H 3.217297016120 2.623185628606 1.767919831364
H 0.622152043608 3.597282796397 4.058700550603
H 0.210345302861 2.640486869761 2.624088980497
H -0.258133438927 2.066778491305 4.236126119824
H 2.742506691070 2.564381727674 6.056320675559
H 1.975737617120 0.975602871865 6.238573889292
H 3.679454429467 1.090172860707 5.758667544531
H 4.211251522480 -5.992901803687 4.023587460038
H 3.646875703284 -5.383623532757 2.456786011176
H 4.792302913101 -4.426334602834 3.411537032401
H 1.148988860372 -6.223383284837 4.903578148670
H 0.109548758986 -4.787300234106 4.825770968406
H 0.651034340153 -5.574132184028 3.330789170574
H 3.129246653953 -4.646088842674 6.676670432869
H 3.907028599054 -3.153067408407 6.123766728334
H 2.196452637556 -3.140033198412 6.592645009440

**3a *(cis,cis)***
E(B3LYP-D3/6-31+G*) = -5490.81420523
E (PCM-B3LYP-D3/6-31+G* (ether)) = -5490.81755821
Sum of electronic and zero-point Energies= -5490.425919
Sum of electronic and thermal Energies= -5490.397678
Sum of electronic and thermal Enthalpies= -5490.396734
Sum of electronic and thermal Free energies=-5490.482850
C 0.580953205288 -0.027236254646 -0.223019701649
C 0.188502606715 -0.044108935693 1.148952223138
C 1.373696767568 0.007361069678 1.959736591193
C 2.500110315711 0.049564068790 1.062041542935
C 2.009147221382 0.016359023829 -0.275080638048
Fe 1.362016617831 -1.655954238029 0.769409878737
C 1.367837269560 -3.139723878699 2.177235961891
C 0.183425798003 -3.196862926188 1.365626773966
C 0.576954587842 -3.403497955864 0.009484084292
C 2.005030604956 -3.457939583516 -0.034330984772
C 2.494788754421 -3.308359735499 1.295238171085
N 1.404100655810 -2.868911072107 3.579354092550
P 2.407585260392 -1.445542694045 3.842136001398
Br 2.364618726605 -1.286918101528 6.141964299639
N 1.410458364809 -0.067406376412 3.385786485966
Si 0.685033210238 1.270079515007 4.338205430712
Si 0.673263672239 -4.059355839655 4.706708666561
C -0.679646583906 -3.262517870752 5.750303225159
C 1.994426011575 -4.866111993231 5.786468335392
C -0.094395415573 -5.434035715043 3.664433111428
C -0.672371130799 0.629892415349 5.479267841941

C -0.074556495258 2.492360351623 3.115730425219
C 2.009599325579 2.210779117925 5.298959258005
H -0.821134499150 -0.118525156804 1.530232978824
H -0.086706372631 -0.070543557645 -1.073933723923
H 2.613933180707 0.009657386414 -1.172788064414
H 3.538859824750 0.058441187215 1.365016321401
H -0.089866433630 -3.475835762706 -0.840111813711
H 2.610661186132 -3.576610457373 -0.923610894038
H 3.533269927901 -3.278507104661 1.597775920496
H -0.826282192581 -3.067654805194 1.731750572264
H 1.526574087879 -5.586037166488 6.471934961242
H 2.711364941957 -5.417055641395 5.164104563820
H 2.552183005051 -4.142703707660 6.386214763272
H -1.218076967277 -4.035978674271 6.314761826127
H -0.284300055976 -2.535721480900 6.464595253440
H -1.406261058964 -2.744940232502 5.111716173123
H -0.377336360507 -6.253484865564 4.338854905919
H -0.995677458194 -5.116588928499 3.129987969367
H 0.608899259293 -5.834866098258 2.925840357210
H 1.545258828844 3.022452537106 5.875684647981
H 2.561003596370 1.574548973259 5.995558234174
H 2.731747327531 2.664653740579 4.608035792682
H -0.354435488260 3.398161123363 3.670286452594
H 0.631772269125 2.784226069696 2.330396141540
H -0.976509783377 2.108494646864 2.628043101473
H -1.201382457941 1.475391570151 5.939718916498
H -1.406052719346 0.041150268025 4.914661239934
H -0.281663491171 -0.002083002988 6.280927844869

**3d *(trans,trans)***
E(B3LYP-D3/6-31+G*) = -4752.02222968
E (PCM-B3LYP-D3/6-31+G* (ether)) = -4752.02697832
Sum of electronic and zero-point Energies= -4751.780757
Sum of electronic and thermal Energies= -4751.764982
Sum of electronic and thermal Enthalpies= -4751.764038
Sum of electronic and thermal Free energies=-4751.823495
C -0.292148304353 -0.092357566960 0.101456142512
C -0.038567136394 -0.025167785382 1.503002435465
C 1.377661413868 0.033812472491 1.696924622136
C 2.009847250399 0.004440642704 0.419591457080
C 0.975008204355 -0.112718585739 -0.574232520692
Fe 0.868559659104 -1.683452201961 0.643085679266
C -0.143407008436 -3.316042395086 -0.051645488507
C 1.113338538044 -3.115244905407 -0.717197648200
C 2.159185694499 -3.230456447207 0.265244266699
C 1.538427994153 -3.438735885437 1.531454269150
C 0.121881883033 -3.492131688963 1.338258275239
N 1.256798475191 -2.895852422979 -2.119561764204
C 1.647804074473 -4.119648369948 -2.849038922847
N 1.131852551491 -0.184226396197 -1.990424447097
C 1.404362878016 1.133980128039 -2.599274671376
P 1.792721273200 -1.472959654822 -2.882990312106
Br 4.106971960476 -1.399791247564 -2.179121028255
H 0.601048893138 1.823342551172 -2.320941118948
H 1.427057368413 1.044987031380 -3.689952286810
H 2.364579628406 1.540202993225 -2.253750509368
H 0.913009097527 -4.903696027235 -2.640853468035
H 2.642977212197 -4.465955862202 -2.539005177019
H 1.657612365825 -3.926188268027 -3.926301341225
H -1.113130407161 -3.268953720610 -0.530068178074
H -0.621183207982 -3.616675231483 2.115360973506
H 2.051503841318 -3.515031180752 2.481539344987
H 3.213781394409 -3.094301725669 0.070808085285
H -0.786801215051 -0.043724235542 2.284888630862
H 1.885336791641 0.066510299379 2.652397077943
H 3.071706981836 -0.015227901709 0.218108441630
H -1.255339794293 -0.182903726232 -0.383860855197

**3d *(cis,trans)***
E(B3LYP-D3/6-31+G*) = -4751.99840438
E (PCM-B3LYP-D3/6-31+G* (ether)) = -4752.00221879
Sum of electronic and zero-point Energies= -4751.757273
Sum of electronic and thermal Energies= -4751.741614
Sum of electronic and thermal Enthalpies= -4751.740669
Sum of electronic and thermal Free energies=-4751.799789
C 0.013280240333 -0.009621914454 -0.008853120850
C 0.013269218192 0.007526908151 1.420525700972
C 1.377810604183 0.007624694165 1.869683969616
C 2.213578027753 -0.003149114629 0.700208802169
C 1.368851612351 -0.026210149674 -0.450767845141
Fe 0.985990815099 -1.665126402184 0.756040165739
C -0.026956910862 -3.436731112117 0.394237120895
C 0.111688040157 -3.199159033581 1.793777551095
C 1.511696036885 -3.099915058180 2.096519629499
C 2.232728321272 -3.298548105992 0.862021762473
C 1.282267646219 -3.494833026949 -0.180801771794
N 2.053074802129 -2.824367591436 3.392823828181
C 2.590060333316 -4.029138591145 4.049364500577
N 1.813336351911 -0.107671795885 3.222226320979
C 0.734729947871 -0.007689806357 4.215479351830
P 3.045597531613 -1.344674109902 3.345975965069
Br 3.601386541237 -1.158353820762 5.554479523671
H 1.806844687503 -4.794071522755 4.047840080489
H 0.192073917207 0.927408672194 4.046673251761
H 1.166178299147 0.020594545011 5.215926611905
H 0.035871561208 -0.853488573596 4.157178693039
H 2.851979546188 -3.803772048671 5.084454036035
H 3.474566010606 -4.441965325234 3.537561950574
H 3.308648504724 -3.253622886062 0.748825498844
H 1.510496693234 -3.639365605387 -1.229046688016
H -0.961290968216 -3.531252863368 -0.144138996664
H -0.686964018639 -3.068284185464 2.512347109262
H 3.294548120575 -0.031521200872 0.694326998996
H 1.707329855886 -0.059795081465 -1.478117807812
H -0.867015208440 -0.023501184538 -0.638168566462
H -0.864745798022 -0.016347240223 2.050076002093

**3d *(cis,cis)***
E(B3LYP-D3/6-31+G*) = -4752.00222905
E (PCM-B3LYP-D3/6-31+G* (ether)) = -4752.00618638
Sum of electronic and zero-point Energies= -4751.760886
Sum of electronic and thermal Energies= -4751.745338
Sum of electronic and thermal Enthalpies= -4751.744394
Sum of electronic and thermal Free energies=-4751.803020
C 0.031966127770 -0.035062918138 -0.052623076497
C -0.054941094122 -0.034106987825 1.373678344172
C 1.273392183885 -0.018791743684 1.897334373083
C 2.183568120973 0.007477393700 0.799274745270
C 1.421791445263 0.001068323974 -0.419191906802
Fe 0.990547703528 -1.681768728192 0.702666157497

C 0.142283847540 -3.283875810604 -0.253720281802
C 1.529838987745 -3.180613456395 -0.616088217394
C 2.295360089535 -3.285569804936 0.595509954712
C 1.390054133926 -3.456283006271 1.684601851373
C 0.061558258358 -3.466362703069 1.161225612612
N 2.043550901510 -2.905459199186 -1.914634152537
C 1.148444584602 -3.250599799382 -3.022984781718
N 1.947455273743 -0.076765907555 -1.739594730697
C 1.026465324750 0.340932183188 -2.800767446401
P 3.042336450563 -1.454695547219 -1.840674423344
Br 3.737624058028 -1.297445485710 -3.999206483072
H 0.156469058763 -0.324405314052 -2.901725008325
H 1.556496394574 0.363827139024 -3.753563297286
H 0.668813833269 1.351138258586 -2.575705956953
H 0.235202395196 -2.638014597154 -3.045057283711
H 0.860570935420 -4.302583957078 -2.925315363360
H 1.674890773148 -3.120458236151 -3.969129995144
H -0.697290608863 -3.215788666883 -0.931858854495
H -0.851130667439 -3.577627025107 1.732125010502
H 1.667552038608 -3.552071466684 2.726339970128
H 3.372250757179 -3.209599622391 0.665217692481
H -0.970648508428 -0.055920097868 1.950142624585
H 1.548161453378 -0.033507394674 2.944083628099
H 3.263413748290 -0.003572548918 0.863572824518
H -0.803947652815 -0.075685200433 -0.737448754622
H -1.65399000 0.88740100 -2.10446700
H 0.58920200 2.28149000 -1.49817500
H 1.46099900 -1.00546000 2.23937600
H -0.70951800 -2.38732100 1.39517100
H -0.67979100 -2.40834600 -1.30861500
H 1.51880500 -1.05557300 -2.12327600
H 5.56047400 -2.23726200 2.54863400
H 5.03724800 -0.54673600 2.70139900
H 3.84332500 -1.86009100 2.76729600
H 4.75911300 -3.82397400 -0.12173100
H 3.05979500 -3.41414400 0.18191100
H 3.80879100 -2.99417100 -1.36770900
H 6.93717900 -1.63891200 -0.17936600
H 6.05747400 -0.85015500 -1.50496100
H 6.52456600 0.08193900 -0.07512100
H -6.75504300 1.76044600 -0.84198700
H -5.60977800 0.88265600 -1.87755400
H -6.48194000 0.02441600 -0.60029900
H -5.98784000 2.24586600 2.25284200
H -5.61903700 0.51875600 2.44262400
H -4.38040200 1.73765900 2.80106500
H -4.68426400 3.85794200 -0.07727700
H -3.06768600 3.40483500 0.49488900
H -3.53129500 3.09079000 -1.18436400
Cl 4.83624900 2.08340800 1.10297900
Cl 4.38495000 1.56703800 -2.08944400

**4a** *(transoid)*
E(B3LYP-D3/6-31+G*) = -5101.32120821
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5101.32745941
Sum of electronic and zero-point Energies= -5100.926782
Sum of electronic and thermal Energies= -5100.891083
Sum of electronic and thermal Enthalpies= -5100.890139
Sum of electronic and thermal Free Energies= -5100.997945
C -0.03338200 1.96756100 0.63475900
C -1.14802800 1.27920500 1.19212800
C -1.94422700 0.78526700 0.10960000
C -1.29749800 1.14631900 -1.11594300
C -0.12466000 1.88236700 -0.79061200
Fe -0.01380000 -0.01189300 0.03502500
C 1.18688400 -1.21737000 1.21437700
C 0.05050200 -1.94701400 0.76470200
C 0.06523800 -1.95816200 -0.66633500
C 1.21538600 -1.24199500 -1.10133300
C 1.92169000 -0.79357400 0.05978800
N 3.23749900 -0.21656100 0.08083400
Si 4.56804300 -1.41829800 0.41659900
C 4.76880500 -1.52380100 2.28484700
N -3.25855300 0.21667400 0.23857200
Si -4.62110600 1.43039000 0.34101300
C -3.89637500 3.09653300 -0.15133100
C 3.98488300 -3.06339200 -0.28787900
C 6.16627100 -0.89299400 -0.41664100
P -3.29080400 -1.44768600 -0.00872900
Cl -3.88733900 -1.65139400 -2.09162700
Cl -5.12670300 -1.97669100 0.93078300
C -5.99366600 0.96881300 -0.85535500
C -5.20807200 1.48313800 2.12734100
H 0.75998300 2.44536700 1.19314100
P 3.29484900 1.43389100 -0.23507600
H -1.37215300 1.14310700 2.24215300

**4a** (gauche)
E(B3LYP-D3/6-31+G*) = -5101.32295936
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5101.32909587
Sum of electronic and zero-point Energies= -5100.927930
Sum of electronic and thermal Energies= -5100.892516
Sum of electronic and thermal Enthalpies= -5100.891572
Sum of electronic and thermal Free energies=-5100.996701
C 0.213292993635 0.594590229456 -0.738058056267
C 0.197205548460 0.359952402710 0.671762654817
C 1.516607194010 0.011025786234 1.075020217481
C 2.351539308625 0.013407508250 -0.085212299733
C 1.542897206047 0.382765015650 -1.208183870732
Fe 1.488118635874 1.897366702851 0.206528792501
C 0.754497202389 3.695312650826 -0.448623567175
C 0.632620968823 3.615610418063 0.970181197576
C 1.949110486285 3.476023198631 1.515890491649
C 2.875889560752 3.439867845111 0.427238477952
C 2.139975589652 3.578578396642 -0.785134174551
N 2.306690105367 3.678102933137 2.891259027495
Si 2.828141817567 5.388385946034 3.238336009471
N 3.709597509123 -0.449566340805 -0.126218337974
P 4.820062603315 0.745503441177 -0.534461338042
Cl 5.470996806673 0.179689087811 -2.521839299340
Si 3.935435303478 -2.230337002628 0.180081702423
P 2.538227296375 2.541672713514 4.099540267501
Cl 0.733727119482 1.399505838603 4.040273377949
Cl 3.910213927545 1.159748433797 3.217205306040
Cl 6.551262675954 0.132374677451 0.559435038696
H 1.899895915507 0.491227406736 -2.224351227612
H -0.626981161795 0.919061927482 -1.338765018630
H -0.651879275825 0.474005450214 1.332208996608
H 1.842074769968 -0.224450207491 2.074321897601
H 3.944450275072 3.330019689237 0.531100545351

H 2.554860410285 3.557984631138 -1.784633981956
H -0.065005288893 3.776957092790 -1.151292061838
H -0.279333456382 3.655821507379 1.550656797664
C 2.770372616701 5.686143378570 5.097393752227
C 4.575769102806 5.629716307739 2.583676928234
C 1.622485586930 6.522341399116 2.347765683410
C 4.281144741182 -2.452147709078 2.015097581457
C 2.318672001662 -3.060352922918 -0.314318566585
C 5.329885216443 -2.907008309527 -0.881390674675
H 4.952452226051 6.625814135495 2.850816428548
H 5.265349322035 4.886264758280 3.001742649901
H 4.608205349258 5.544039264736 1.491834959383
H 2.944598221358 6.755469698985 5.278939003936
H 1.793865794349 5.431307941063 5.525578503193
H 3.537653496464 5.129385734626 5.646000793407
H 1.890421594884 7.568769967806 2.544044663665
H 1.644474261801 6.364642423307 1.264286768277
H 0.592917307857 6.366650733177 2.690884606170
H 5.431321303878 -3.981514248715 -0.676299378890
H 5.112163062013 -2.781768684451 -1.947174408508
H 6.292839523692 -2.431604977814 -0.676811798357
H 2.432624526243 -4.149302111597 -0.231142304391
H 1.478419356646 -2.758936063167 0.319741730158
H 2.056462948874 -2.828559907754 -1.353402672439
H 4.394085158339 -3.515642489527 2.263581181922
H 5.201851835472 -1.932358541538 2.300519953722
H 3.467145216405 -2.046414111643 2.626435014566

**4b** *(transoid)*
E(B3LYP-D3/6-31+G*) = -5337.21757364
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5337.22326487
Sum of electronic and zero-point Energies= -5336.649415
Sum of electronic and thermal Energies= -5336.606908
Sum of electronic and thermal Enthalpies= -5336.605964
Sum of electronic and thermal Free Energies= -5336.724968
C -2.03576400 -0.46111400 0.16726200
C -1.25871500 -1.09136100 -0.86016500
C -0.31847300 -1.95677600 -0.23090500
C -0.47475400 -1.82900200 1.18453900
C -1.53021000 -0.90607300 1.43113400
Fe 0.00001500 -0.00009300 0.34632000
C 0.47465700 1.82900500 1.18425200
C 0.31841900 1.95651000 -0.23122000
C 1.25873400 1.09102700 -0.86029000
C 2.03582400 0.46106200 0.16729300
C 1.53016100 0.90619600 1.43105400
N 3.20684700 -0.35012200 -0.04120100
P 3.00164200 -1.93058900 0.51363300
Cl 3.36236200 -3.11958500 -1.25795300
N -3.20670300 0.35013500 -0.04143200
Si -4.61698800 -0.48705400 -0.84619000
C -6.05609700 0.70530200 -1.05619900
C -4.08671600 -1.05399700 -2.56660200
C -5.14828200 -1.97455400 0.24034900
C -5.27962100 -1.53014100 1.71202600
Si 4.61726400 0.48702200 -0.84593200
C 4.08733300 1.05313200 -2.56669500
C 5.14802400 1.97497400 0.24025100
C 5.27883800 1.53104100 1.71212200
C 6.05667800 -0.70515800 -1.05490700
C 6.53139600 2.45396300 -0.26372800
C 4.16259600 3.16069600 0.14755500
C -6.53151300 -2.45363100 -0.26398400
C -4.16292000 -3.16040300 0.14849700
Cl 4.80166800 -2.32509600 1.57867200
H -0.40339900 2.57813300 -0.74378100
P -3.00171700 1.93050600 0.51381800
H 1.37327800 0.92934000 -1.92203300
H 1.89548300 0.58279200 2.39694500
H -0.12296000 2.32661700 1.93580400
H -1.37321600 -0.92983800 -1.92193800
H 0.40320400 -2.57865900 -0.74334500
H 0.12273600 -2.32657200 1.93621900
H -1.89555800 -0.58249900 2.39695900
H -4.97813200 -1.37024600 -3.12368500
H -3.62577500 -0.22949800 -3.12369400
H -3.39069900 -1.89750100 -2.55265300
H -6.75445400 0.24948400 -1.76979600
H -6.59651200 0.88958200 -0.12423300
H -5.74599500 1.67121300 -1.46346900
H 6.75510500 -0.24956900 -1.76859400
H 6.59689800 -0.88873800 -0.12269000
H 5.74696700 -1.67138500 -1.46171100
H 4.97864100 1.37016000 -3.12350400
H 3.62741100 0.22801800 -3.12372300
H 3.39049500 1.89596700 -2.55320000
H -4.52907500 -3.99428900 0.76596600
H -4.06749700 -3.53507800 -0.87790400
H -3.16204400 -2.90324200 0.50660600
H -5.66482500 -2.35984100 2.32306300
H -4.31316800 -1.23099100 2.13156600
H -5.96764700 -0.68428000 1.83049700
H -6.85739000 -3.32667500 0.32019800
H -7.30320700 -1.68253900 -0.15616400
H -6.50490900 -2.76251500 -1.31752100
H 6.85693000 3.32734200 0.32014700
H 7.30314500 1.68302200 -0.15519900
H 6.50522300 2.76231400 -1.31743300
H 4.52822700 3.99472000 0.76514800
H 4.06788700 3.53517000 -0.87899100
H 3.16149500 2.90348700 0.50497600
H 5.66423700 2.36080600 2.32294800
H 4.31215600 1.23245800 2.13151100
H 5.96648800 0.68493900 1.83105400
Cl -3.36207200 3.11986900 -1.25754700
Cl -4.80203200 2.32470900 1.57846700

**4b** *(gauche)*
E(B3LYP-D3/6-31+G*) = -5337.21926463
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5337.22524178
Sum of electronic and zero-point Energies= -5336.650893
Sum of electronic and thermal Energies= -5336.608626
Sum of electronic and thermal Enthalpies= -5336.607682
Sum of electronic and thermal Free Energies= -5336.724533
C -1.66087100 1.28270000 0.06769500
C -1.58086900 2.55951800 -0.58240200
C -1.05150800 3.49338200 0.35265600
C -0.78121400 2.79658800 1.57182100
C -1.14872000 1.43436800 1.39600000
Fe 0.30899400 1.99004800 0.01897400

C 1.55295700 1.02609400 -1.33009400
C 1.56732400 2.43015200 -1.55340400
C 2.02267900 3.06153600 -0.35725700
C 2.29523500 2.04854700 0.60664400
C 2.01068900 0.77606700 0.00825600
N 2.38241700 -0.51103800 0.52535500
Si 3.65841400 -1.39867800 -0.44365600
C 3.02625700 -1.74531100 -2.18497800
N -2.31043200 0.11092600 -0.46762100
P -1.26524400 -0.70649100 -1.50631900
Cl -1.59216100 0.30429200 -3.44193500
Si -4.11392800 0.03127600 -0.20326500
C -4.65227800 1.79980800 0.17540100
C -4.98284500 -0.52537200 -1.77939500
C -4.53967600 -1.10398700 1.28170200
C -3.89418800 -0.58438500 2.58321900
P 1.89680300 -1.28533200 1.93737700
Cl 1.56290200 0.29258500 3.32187600
Cl -0.15772900 -1.86926900 1.59448800
C 5.26308200 -0.35186400 -0.44479200
C 5.57007100 0.12176100 0.99108400
C 3.97605200 -3.07001900 0.37713800
C 6.42037200 -1.25231600 -0.94005800
C 5.16592100 0.87256300 -1.38090800
Cl -2.30788300 -2.51299500 -1.89280700
C -6.07963000 -1.08850200 1.43971600
C -4.08288400 -2.55920000 1.05580400
H -1.86736600 2.74775100 -1.60828000
H -0.84080500 4.53716200 0.15698300
H -0.32919000 3.21677100 2.46103800
H -1.05085900 0.64912300 2.12612600
H 1.25387400 0.28094000 -2.04675600
H 1.24127500 2.92522500 -2.45866600
H 2.10353600 4.12797400 -0.18948800
H 2.64210600 2.20322100 1.61711300
H 3.63952500 -2.53946100 -2.63004900
H 1.98940900 -2.10144000 -2.16204100
H 3.07643100 -0.87721400 -2.84795800
H 4.65962900 -3.62546900 -0.27821600
H 4.44542000 -2.99747900 1.36349600
H 3.06533200 -3.67149700 0.47687200
H -5.73253400 1.81367200 0.36599300
H -4.14668600 2.23006700 1.04564400
H -4.45803500 2.45567400 -0.68069100
H -5.99270200 -0.09536500 -1.79473300
H -4.44938900 -0.17177600 -2.66828400
H -5.07205200 -1.61242600 -1.85442300
H -6.37439200 -1.74547300 2.27119300
H -6.46681000 -0.08734300 1.66660500
H -6.59056800 -1.45464000 0.54000800
H -4.39322600 -3.18122800 1.90885100
H -4.51968700 -2.99707000 0.15108100
H -2.99462600 -2.63702700 0.96967700
H -4.23859500 -1.18596500 3.43772400
H -2.80367200 -0.66700300 2.54905300
H -4.15295200 0.46076500 2.79295700
H 6.52266900 0.67103700 1.01288000
H 4.79196600 0.79224000 1.37180400
H 5.66347100 -0.71846100 1.69145400
H 7.35149500 -0.66899000 -0.98646100
H 6.60180800 -2.10164600 -0.27107500
H 6.23607800 -1.64586000 -1.94859400
H 6.12166900 1.41769300 -1.37533800
H 4.96598100 0.57888500 -2.41848600
H 4.38560200 1.57392000 -1.07413200

**4c** *(transoid)*

E(B3LYP-D3/6-31+G*) = -4677.06534621
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4677.07130204
Sum of electronic and zero-point Energies= -4676.590226
Sum of electronic and thermal Energies= -4676.556909
Sum of electronic and thermal Enthalpies= -4676.555964
Sum of electronic and thermal Free Energies= -4676.657293
C 1.20538000 -1.17993600 0.92315300
C 0.17297300 -1.97080000 0.34441000
C 0.28695800 -1.87963400 -1.07860900
C 1.40658000 -1.05493900 -1.38187600
C 1.98689400 -0.63186800 -0.14538100
Fe -0.00004100 -0.00011400 -0.26446000
C -0.28678900 1.87955000 -1.07840700
C -1.40649100 1.05502200 -1.38179900
C -1.98688400 0.63185000 -0.14536700
C -1.20535300 1.17973100 0.92325200
C -0.17283600 1.97053600 0.34462600
N -3.22611100 -0.06708300 0.00171200
P -3.18802600 -1.70742600 -0.36841900
Cl -5.16843300 -2.04224200 -1.04417200
N 3.22601400 0.06720000 0.00187800
C 4.27599100 -0.58541400 0.81766500
H 3.85242000 -0.82915900 1.80082900
C -4.27606000 0.58550000 0.81755700
C -4.93364700 1.84923600 0.20172200
C -3.99837000 3.07439600 0.25520300
C -5.36061300 1.58584200 -1.25148700
C -6.17945800 2.14393100 1.06322600
Cl -3.37143200 -2.64725200 1.58412300
H 0.58143900 2.51693800 0.89408900
H -1.76716200 0.77976700 -2.36414400
H 0.37992900 2.33560100 -1.79727300
H -1.38317500 1.02484600 1.97898100
H -0.37967200 -2.33570600 -1.79754300
H -0.58124200 -2.51739500 0.89376300
H 1.38315500 -1.02517600 1.97890800
H 1.76722100 -0.77956500 -2.36420000
C 4.93348800 -1.84917000 0.20177700
H 5.05074600 0.16599300 0.98613200
P 3.18803400 1.70747800 -0.36839400
H -5.05078900 -0.16592300 0.98607700
H -3.85244000 0.82927100 1.80069000
H -4.54071800 3.97110400 -0.06971700
H -3.63563000 3.25380700 1.27515100
H -3.12802400 2.96037900 -0.39608800
H -5.86588800 2.46838900 -1.66250300
H -4.49289700 1.36701100 -1.88348600
H -6.04643900 0.73503300 -1.32018300
H -6.68504300 3.04925500 0.70689000
H -6.90029800 1.31783800 1.02049500
H -5.90946800 2.30538300 2.11518400
Cl 3.37169400 2.64743100 1.58408000
Cl 5.16845000 2.04217600 -1.04434600

C 6.17969400 -2.14354700 1.06282800
C 3.99838900 -3.07442500 0.25586800
C 5.35983300 -1.58597800 -1.25164700
H 6.68507500 -3.04904200 0.70664200
H 6.90053400 -1.31749100 1.01940800
H 5.91018100 -2.30453600 2.11498000
H 4.54067300 -3.97111200 -0.06922100
H 3.63620100 -3.25376000 1.27602800
H 3.12768900 -2.96059400 -0.39498500
H 5.86552200 -2.46834300 -1.66254400
H 4.49178900 -1.36789200 -1.88345400
H 6.04510400 -0.73476500 -1.32083100

**4c** *(gauche)*
E(B3LYP-D3/6-31+G*) = -4677.06316397
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4677.06929238
Sum of electronic and zero-point Energies= -4676.587916
Sum of electronic and thermal Energies= -4676.554817
Sum of electronic and thermal Enthalpies= -4676.553873
Sum of electronic and thermal Free Energies= -4676.653935
C 1.29799800 -3.07185900 -1.13653100
C 0.86523000 -2.98903100 0.22368400
C 1.13410800 -1.67480000 0.69651500
C 1.72997800 -0.93637800 -0.37371500
C 1.81655900 -1.79931300 -1.51611300
Fe -0.15046200 -1.62375300 -0.93943300
C -1.71618500 -2.39160400 -2.03338700
C -2.17046800 -2.05440900 -0.72590000
C -1.94668000 -0.65340900 -0.52523200
C -1.34990500 -0.13717000 -1.72564200
C -1.21723200 -1.20738200 -2.65278800
N -2.43845300 0.14740100 0.54899100
C -3.07115400 1.44409300 0.17433100
N 2.28776700 0.37886400 -0.27976200
P 1.16393400 1.62266300 -0.43160600
Cl 1.42619000 2.26524100 -2.51718800
C 3.73764500 0.50991000 -0.54732800
P -2.25136400 0.04509400 2.22639800
Cl -1.85897600 -1.99653100 2.54590000
Cl -0.27606600 0.86199100 2.69576100
Cl 2.17862800 3.22438700 0.50983300
H 2.19923000 -1.51878500 -2.48850700
H 1.20071900 -3.93474800 -1.78292800
H 0.37927900 -3.77486700 0.78704500
H 0.92568400 -1.28366300 1.67941900
H -1.07041500 0.88600200 -1.91970100
H -0.77415700 -1.13335000 -3.63725100
H -1.71652800 -3.38544700 -2.46256400
H -2.59396800 -2.73479500 -0.00318100
H -3.06654600 2.08162600 1.06862000
H -2.42641700 1.94930800 -0.55131300
C -4.52789600 1.36211000 -0.34678400
C 4.67887900 -0.00163200 0.57426900
H 3.96647700 -0.00664000 -1.48899500
H 3.93430300 1.57114700 -0.71274000
C 6.08866600 0.51802600 0.22441300
C 4.24341200 0.55789900 1.93856600
C 4.72341000 -1.54204500 0.62758600
H 4.93426100 0.22444900 2.72269300
H 4.23201000 1.65316400 1.93431200
H 3.23649100 0.21789000 2.20271400
H 5.47659600 -1.86988400 1.35517400
H 3.76475900 -1.97398500 0.92557000
H 4.99424700 -1.96486000 -0.34851400
H 6.82067700 0.16450600 0.96053100
H 6.41221600 0.16398000 -0.76356700
H 6.12101400 1.61474500 0.21899900
C -4.99408300 2.81746200 -0.55755900
C -4.62321600 0.60680300 -1.68570300
C -5.42519800 0.67757100 0.69835900
H -6.02353200 2.83717200 -0.93413300
H -4.96960400 3.38848200 0.37946000
H -4.36154500 3.33727200 -1.28852900
H -6.46815800 0.67183400 0.35985300
H -5.12162900 -0.36251500 0.86274800
H -5.38796400 1.19932200 1.66315000
H -5.65337700 0.64635400 -2.06125500
H -3.97056600 1.05388100 -2.44466600
H -4.34465800 -0.44575600 -1.58312700

**4d** *(transoid)*
E(B3LYP-D3/6-31+G*) = -4362.51175316
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4362.51761429
Sum of electronic and zero-point Energies= -4362.264057
Sum of electronic and thermal Energies= -4362.241015
Sum of electronic and thermal Enthalpies= -4362.240071
Sum of electronic and thermal Free Energies= -4362.319555
C -1.66628400 1.22847600 0.22321500
C -0.92993200 1.33507100 -1.00354700
C 0.39582300 1.73799200 -0.67475000
C 0.48485800 1.87646900 0.74476200
C -0.78744900 1.56126800 1.30380500
Fe -0.05113300 -0.05938900 0.25019600
C -0.38861900 -1.99998300 -0.37055700
C 0.91904000 -1.58784000 -0.76312300
C 1.65278600 -1.25699000 0.42129800
C 0.78126000 -1.44166700 1.54197000
C -0.47193800 -1.91553000 1.05098500
N 3.01991400 -0.87072800 0.50271300
C 3.60796300 -0.81618900 1.84626100
N -3.07953900 1.01718000 0.34665400
P -3.56152100 -0.58330400 0.11232500
Cl -3.93511500 -0.68374900 -2.03302100
C -3.87685600 2.20214700 -0.02265100
Cl -5.56474000 -0.48880100 0.79562400
H -1.33710700 -2.14652900 1.65639400
H -1.32331500 1.11935300 -1.98825600
H 1.20749400 1.88553500 -1.37462000
H 1.37983200 2.13627600 1.29388200
H -1.05854700 1.55289600 2.35142500
H -1.17897200 -2.30130000 -1.04493400
H 1.28344500 -1.52868600 -1.77976100
H 1.02053200 -1.24203300 2.57679500
H -3.45695100 3.07003900 0.49311900
H -3.84469000 2.37292100 -1.10621200
H -4.91262900 2.06735500 0.29197500
P 3.66268500 -0.04564500 -0.83005200
H 4.68313700 -0.65294100 1.76824900
H 3.16790700 0.00038300 2.43212900
H 3.43508700 -1.76961400 2.35387700

Cl 4.01897000 1.92242700 -0.03530100
Cl 5.64795700 -0.75868900 -0.80935000

**4d** (gauche)
E(B3LYP-D3/6-31+G*) = -4362.50772420
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4362.51398507
Sum of electronic and zero-point Energies= -4362.259896
Sum of electronic and thermal Energies= -4362.236944
Sum of electronic and thermal Enthalpies= -4362.236000
Sum of electronic and thermal Free energies=-4362.314171
C 0.316459615423 0.117324561202 -0.014406177046
C 0.027350058362 0.064247731306 1.388012866683
C 1.276375885902 -0.089574748291 2.081421350671
C 2.319186083137 -0.129910767315 1.114390562582
C 1.726630441936 -0.006668367768 -0.177170281038
Fe 0.998673893972 -1.676818653330 0.774995359720
C 0.366344826692 -3.152151998233 -0.521931619451
C -0.242364766319 -3.354430758877 0.747127017772
C 0.801874714987 -3.521089350155 1.709990422875
C 2.061808177379 -3.422600422729 1.028497834899
C 1.785864843850 -3.206494516177 -0.352731863632
N 0.615198711499 -3.913568211580 3.075323737408
C 1.092097502695 -5.273770378683 3.376251508692
N -1.215120301822 0.358465479105 2.023311576118
P -2.776599310253 -0.272835003793 1.841582571789
Cl -2.778109454190 -2.161319853139 2.933010660003
C -1.088771826403 1.081977968601 3.308766495302
P 0.550439829354 -2.633411568904 4.164830544097
Cl -0.206874998053 -3.608786654018 5.881217985679
Cl 2.645109972645 -2.414231615056 4.783806639926
Cl -2.766901606638 -1.003843712663 -0.126495197292
H 3.035156561822 -3.484071078690 1.497432315715
H 2.523970817321 -3.055074170722 -1.130174099004
H -0.156748846926 -2.951033671489 -1.447849075030
H -1.297990407240 -3.367384595477 0.968937462513
H 1.415799847426 -0.146342290866 3.149664997009
H 3.369990950317 -0.270602632408 1.330824410177
H 2.248090733463 -0.042287949301 -1.125191191081
H -0.408926969451 0.216329040901 -0.807205514946
H -2.071896650781 1.450230137022 3.621065916905
H -0.696208957273 0.430600238030 4.097883033759
H -0.422757420509 1.938521772984 3.170900386342
H 0.735222539370 -5.942772977764 2.588370970745
H 2.188462416388 -5.307005324604 3.413866462894
H 0.689699958431 -5.607458651271 4.333752264777

**10a** *(transoid)*
E(B3LYP-D3/6-31+G*) = -3840.10959691
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3840.11569325
Sum of electronic and zero-point Energies= -3839.709293
Sum of electronic and thermal Energies= -3839.677870
Sum of electronic and thermal Enthalpies= -3839.676926
Sum of electronic and thermal Free Energies= -3839.772353
C -1.04189200 1.88252200 0.91128400
C -0.78762700 2.21355100 -0.45324600
C -1.83107700 1.63778700 -1.24211700
C -2.75729500 0.98281200 -0.37028200
C -2.23995800 1.10274800 0.95958500
Fe -0.80470800 0.16932300 -0.20382500
C 0.11228600 -1.40842500 0.77823700
C 1.03855500 -0.80059400 -0.12927700
C 0.47961600 -0.86647600 -1.44777700
C -0.77431400 -1.53971100 -1.35348300
C -1.00173000 -1.87138600 0.01625700
H -1.89038200 -2.34345600 0.41259400
N -3.92896700 0.33833500 -0.75733800
Si -5.21620400 -0.31771000 0.25183700
C -5.86412800 1.01911500 1.41307900
C -6.54235800 -0.87240700 -0.96738400
C -4.61094400 -1.79101700 1.26874300
H -4.04085500 0.27838200 -1.76264300
H 0.25074100 -1.48926500 1.84855500
N 2.36242200 -0.34742800 0.20773500
H 0.94139500 -0.46168900 -2.33885300
H -1.46205200 -1.72161400 -2.16990500
H -2.67111300 0.66827200 1.85148000
H -0.42848400 2.15057500 1.76052600
H 0.04834900 2.78344900 -0.83554200
H -1.91286700 1.68227800 -2.32152500
H -5.40239600 -2.15353600 1.93785600
H -4.31657000 -2.62292400 0.61703800
H -3.74589000 -1.53145900 1.89026400
H -6.64552100 0.62167300 2.07367200
H -5.06756800 1.42559500 2.04742000
H -6.29134000 1.85439000 0.84495500
H -7.39518800 -1.31114200 -0.43449200
H -6.92138100 -0.03204400 -1.56233200
H -6.16029900 -1.63504100 -1.65810800
P 2.39224700 1.31482900 0.46849400
Cl 4.23694400 1.53632800 1.53156300
Cl 3.01225500 2.12750400 -1.46648600
Si 3.70715100 -1.55901400 0.02426200
C 5.09906500 -0.82088500 -1.00019600
C 4.27642000 -2.08109100 1.74056500
C 2.97218400 -3.04240700 -0.87366800
H 5.84724700 -1.59757100 -1.20878800
H 4.72017400 -0.44466100 -1.95690200
H 5.60089300 0.00727500 -0.49202600
H 5.03609400 -2.87070600 1.66727200
H 4.70780300 -1.24158000 2.29439300
H 3.43604300 -2.47834900 2.32345700
H 3.73822900 -3.82571200 -0.94853200
H 2.10902100 -3.46194800 -0.34537800
H 2.64997100 -2.78618400 -1.88879000

**10a** *(gauche)*
E(B3LYP-D3/6-31+G*) = -3840.11025720
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3840.11516055
Sum of electronic and zero-point Energies= -3839.710302
Sum of electronic and thermal Energies= -3839.678862
Sum of electronic and thermal Enthalpies= -3839.677918
Sum of electronic and thermal Free Energies= -3839.773591
C 1.15567300 3.42884500 0.07642700
C 0.79367100 3.08222900 -1.26252600
C 0.92719500 1.66971600 -1.40784600
C 1.38222900 1.14295800 -0.15799900
C 1.50802300 2.23142400 0.76614800
Fe -0.44345500 2.12965000 0.07784000
C -2.11676400 3.26871200 0.37051400
C -2.37220800 2.30143200 -0.65025800

C -2.22263200 0.99480800 -0.08580000
C -1.83875300 1.16746800 1.28557300
C -1.79489600 2.56651100 1.57028900
N -2.42780300 -0.23064000 -0.72880700
Si -3.49331400 -1.52550400 -0.17128300
N 1.81500300 -0.20754900 0.07839400
P 0.53968300 -1.23852700 0.44750500
Cl 1.51570200 -2.69525200 1.68877400
Si 3.58722000 -0.51909400 -0.18323100
H -2.21579600 -0.21002600 -1.72013300
Cl 0.32869700 -2.45832800 -1.35203000
H 1.81640900 2.13872700 1.79931200
H 1.11964300 4.42207400 0.50560800
H 0.43839400 3.76882800 -2.02051900
H 0.72856500 1.07911600 -2.29289300
H -1.61648800 0.36853600 1.97861700
H -1.52629600 3.01271000 2.51921000
H -2.13303200 4.34415200 0.24445500
H -2.62556300 2.50842800 -1.68278200
C -3.78342100 -2.59528200 -1.69450200
C -2.71736000 -2.56512300 1.19937500
C -5.08892700 -0.76118100 0.48864000
C 4.20460100 0.83738900 -1.33446100
C 4.43434200 -0.38895500 1.49269700
C 3.85060400 -2.19930600 -0.97949800
H -3.45622900 -3.28101900 1.58423700
H -1.85889100 -3.13912200 0.83285900
H -2.38013400 -1.95690500 2.04703700
H -5.76351800 -1.52735100 0.89217100
H -4.87310500 -0.05000500 1.29630500
H -5.62411800 -0.21530100 -0.29811500
H -4.40120100 -3.46704700 -1.44499000
H -4.29555200 -2.04193400 -2.49182400
H -2.82987000 -2.96696900 -2.08997400
H 4.92565200 -2.33988500 -1.15630500
H 3.49882900 -3.02394300 -0.35355500
H 3.33400800 -2.26525300 -1.94284900
H 5.51787000 -0.53866400 1.39744800
H 4.27071200 0.60158200 1.93497400
H 4.04346700 -1.14053800 2.18677600
H 5.28220900 0.70626000 -1.50004200
H 3.70634000 0.79429100 -2.30972000
H 4.04416800 1.83894500 -0.92093000

**10b** *(transoid)*
E(RB3LYP) = -4076.00561313
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4076.01131359
Sum of electronic and zero-point Energies= -4075.432638
Sum of electronic and thermal Energies= -4075.394028
Sum of electronic and thermal Enthalpies= -4075.393084
Sum of electronic and thermal Free Energies= -4075.506883
C 2.62732900 -0.62221100 -0.98200600
C 2.00750800 -1.18213100 0.18069500
C 0.99020900 -2.09399300 -0.24194000
C 0.93926000 -2.06730800 -1.66686300
C 1.93797200 -1.14926800 -2.12126600
Fe 0.55923500 -0.19463300 -0.91371700
C 0.04275100 1.53709000 -1.90475400
C 0.48319300 1.82827400 -0.57835300
C -0.36899000 1.13668500 0.33583300
C -1.36693300 0.44761400 -0.43161200
C -1.09646700 0.68484300 -1.81881200
N -2.51076800 -0.25481200 0.09105000
P -2.42503100 -1.90576500 -0.24834800
Cl -2.51523600 -2.81982700 1.71955100
N 3.67933400 0.29005900 -1.02100400
Si 4.69882900 0.93123900 0.26731400
C 5.47500100 2.47572200 -0.49277000
C 3.66854200 1.38991400 1.78669200
C 6.04944300 -0.33220200 0.76187400
C 6.97537700 -0.59944400 -0.44319500
Si -3.71078400 0.74284500 1.02636500
C -2.86282400 1.39698100 2.58059100
C -4.32413000 2.17353000 -0.09378700
C -4.75439600 1.61255100 -1.46535400
C -5.17326200 -0.31315800 1.56100900
C -5.55408200 2.81336500 0.59525200
C -3.26004500 3.27358400 -0.29965900
C 6.88440300 0.22938800 1.93314300
C 5.39936500 -1.66385800 1.19564900
Cl -4.39870200 -2.36420600 -0.93403900
H 1.35193500 2.41878600 -0.31809100
H 3.87002400 0.62749000 -1.95764500
H -0.28306400 1.12155900 1.41279900
H -1.66683700 0.27729100 -2.64304200
H 0.50949000 1.88115100 -2.81903000
H 2.26280800 -0.95900800 1.20623000
H 0.36914000 -2.68598200 0.41651400
H 0.25232900 -2.62206800 -2.29205200
H 2.14044400 -0.88154700 -3.15156000
H 4.18834400 2.16070500 2.36975900
H 2.68821400 1.78639700 1.50150500
H 3.50275800 0.53730200 2.45490700
H 6.23737800 2.90270000 0.17010800
H 5.96179600 2.25710800 -1.45164300
H 4.71642000 3.24878400 -0.66740700
H -5.71271200 0.23617400 2.34342300
H -5.86910400 -0.50599500 0.74002600
H -4.86794600 -1.27629700 1.97817300
H -3.61687000 1.83519200 3.24712800
H -2.37773200 0.57595900 3.12229700
H -2.11397600 2.16774300 2.37577600
H 6.17681000 -2.39235700 1.47133900
H 4.74891500 -1.54110000 2.07101600
H 4.80053100 -2.10789500 0.39222300
H 7.73564600 -1.35050400 -0.18156500
H 6.41678200 -0.98518700 -1.30557700
H 7.50787500 0.30625100 -0.76069900
H 7.67068500 -0.48563000 2.21802900
H 7.38325900 1.17163500 1.67107000
H 6.27029300 0.40957900 2.82463700
H -5.92693900 3.65056300 -0.01309300
H -6.38096500 2.10342800 0.71437100
H -5.30881600 3.21838700 1.58620500
H -3.68223600 4.08775600 -0.90806000
H -2.93790300 3.71292100 0.65254800
H -2.37071500 2.90379300 -0.81724900
H -5.18702900 2.41453600 -2.08214700
H -3.90464500 1.19336300 -2.01416200
H -5.51006400 0.82279300 -1.37295100

**10b** *(gauche)*

E(B3LYP-D3/6-31+G*) = -4076.00667424
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4076.01177768
Sum of electronic and zero-point Energies= -4075.433717
Sum of electronic and thermal Energies= -4075.395202
Sum of electronic and thermal Enthalpies= -4075.394258
Sum of electronic and thermal Free Energies= -4075.504231

C -1.42917900 -3.35469200 0.07562000
C -1.03508500 -2.97551300 -1.24478700
C -1.11136000 -1.55408100 -1.34024100
C -1.56600500 -1.05273200 -0.07850600
C -1.73176900 -2.16836800 0.80773500
Fe 0.22036500 -2.12659800 0.14304100
C 1.76815700 -3.34797500 0.68276400
C 2.13721500 -2.59505300 -0.47570000
C 2.10755800 -1.20248500 -0.14399400
C 1.67896500 -1.10417300 1.22082600
C 1.49186600 -2.42462200 1.73393000
N 2.44230300 -0.14038500 -0.99072100
Si 3.56631500 1.18609200 -0.65497200
N -1.91225000 0.31605700 0.20655600
P -0.52498400 1.25825900 0.37658200
Cl -0.69166300 2.02628900 2.40860400
Si -3.67707800 0.67636800 0.45699300
H 2.38539200 -0.40237600 -1.96989800
Cl -1.00730500 3.04517600 -0.70593300
H -2.03112800 -2.10399500 1.84406200
H -1.44597800 -4.36348600 0.46772000
H -0.70533100 -3.64824500 -2.02618200
H -0.87501800 -0.94415900 -2.20233000
H 1.53991300 -0.18964300 1.77765800
H 1.16669200 -2.67200100 2.73619500
H 1.68507000 -4.42608800 0.73912900
H 2.39168300 -2.99894700 -1.44818700
C 3.71209400 2.06766700 -2.31758400
C 2.88943000 2.37173800 0.64322700
C 5.26868000 0.50258500 -0.08505900
C -4.63914300 0.17798500 -1.12571200
C -4.27450700 -0.29897400 1.95762400
C -3.92825000 2.50754500 0.80580900
H 3.65743300 3.10882100 0.91132500
H 2.02461200 2.92317800 0.25759800
H 2.58265000 1.87196200 1.56763100
C 6.31862000 1.63501600 -0.10664700
C 5.17417100 -0.06575600 1.34850800
C 5.72095600 -0.62370500 -1.03837800
H 4.33165000 2.96802800 -2.23110600
H 4.16276800 1.42961200 -3.08812500
H 2.72200200 2.38147200 -2.67097400
H -4.94044600 2.63112800 1.21203100
H -3.22212600 2.89544400 1.54453500
H -3.84526100 3.12226900 -0.09461600
H -5.29212400 0.01967000 2.21827600
H -4.29681500 -1.37938800 1.78734600
H -3.63037400 -0.09645400 2.82187200
C -6.06083600 0.77927400 -1.01969600
C -3.93806200 0.76557400 -2.36811100
C -4.76928500 -1.35277200 -1.28268000
H -6.65266700 0.49483800 -1.90230900
H -6.60072800 0.41145100 -0.13690800
H -6.04528900 1.87450600 -0.97611300
H -4.52762900 0.55042700 -3.27191600
H -3.82085800 1.85414800 -2.30100400
H -2.94142300 0.33518200 -2.51079300
H -5.35179900 -1.58530500 -2.18710900
H -3.79851900 -1.84717000 -1.38076200
H -5.29388000 -1.80671300 -0.43287300
H 6.70139200 -1.01596100 -0.72812700
H 5.01430000 -1.46254700 -1.03518100
H 5.82596600 -0.27121200 -2.07317400
H 7.29561000 1.25442300 0.22798200
H 6.45808500 2.04833800 -1.11365000
H 6.04836100 2.46236700 0.56230100
H 6.15696300 -0.44226500 1.67150000
H 4.86349600 0.69782500 2.07275700
H 4.46599700 -0.89941100 1.41538600

**10c** *(transoid)*

E(B3LYP-D3/6-31+G*) = -3415.85357024
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3415.85962940
Sum of electronic and zero-point Energies= -3415.372718
Sum of electronic and thermal Energies= -3415.343635
Sum of electronic and thermal Enthalpies= -3415.342691
Sum of electronic and thermal Free Energies= -3415.434188

C -0.37320800 1.17322100 -1.00928900
C -1.15647400 0.66180700 0.07353600
C -0.47422100 0.95900200 1.29892800
C 0.71113400 1.68300700 0.96922700
C 0.77818400 1.80267800 -0.45272000
Fe 0.74336600 -0.18567000 0.10192700
C 0.75261000 -2.22690100 0.39932800
C 1.11696400 -1.91277800 -0.94356500
C 2.30202900 -1.11122600 -0.90471500
C 2.68862600 -0.94651800 0.46237500
C 1.70270700 -1.60362600 1.26540600
N 3.81611900 -0.29739200 0.95327800
C 4.43021900 0.81779600 0.23082400
C 5.85363300 0.52096100 -0.30160600
C 5.80974600 -0.65293000 -1.29492100
N -2.46580700 0.09486900 -0.04253900
C -3.56244900 0.76300000 0.69148100
C -4.02539100 2.13018100 0.12279200
C -4.27275100 2.03000100 -1.39118400
C 6.36904400 1.78601100 -1.01089000
C 6.78129800 0.16943400 0.87464500
P -2.47860700 -1.51192800 -0.53955900
Cl -2.93731600 -2.59039800 1.30295900
Cl -4.39692200 -1.64621400 -1.44918600
C -5.34758900 2.46973600 0.84212300
C -3.00606900 3.25003100 0.41428000
H 1.45323800 2.04023500 1.67215600
H -0.62832400 1.08792900 -2.05726200
H 1.57865200 2.26805200 -1.01291100
H -0.81141700 0.68485200 2.28977600
H 0.58246900 -2.20917700 -1.83612400
H -0.09434100 -2.81703900 0.72038300
H 1.68765900 -1.62434400 2.34844200
H 2.81319300 -0.69892700 -1.76305500
H 3.77834500 1.10532800 -0.60297800

H 4.47908900 1.68890100 0.90014400
H 3.78648000 -0.17152900 1.95654900
H 7.80201800 -0.02173400 0.52125800
H 6.82791900 0.99177400 1.60174000
H 6.42871300 -0.72916400 1.39341800
H 7.37578500 1.62193000 -1.41406400
H 5.71705000 2.06858300 -1.84820500
H 6.42125500 2.63909400 -0.32138100
H 6.81907400 -0.90133700 -1.64561900
H 5.38087400 -1.54555200 -0.82683900
H 5.20424100 -0.40480900 -2.17639700
H -4.41057900 0.07485700 0.68407300
H -3.25904900 0.88343800 1.73992800
H -3.41521500 4.21864500 0.09999500
H -2.78186100 3.31236800 1.48673600
H -2.06239300 3.09881300 -0.11598400
H -4.64726200 2.98575000 -1.77823700
H -3.34843600 1.78523000 -1.92539900
H -5.00805900 1.25243700 -1.62474100
H -5.72174100 3.44739100 0.51499300
H -6.12325500 1.72428900 0.62643900
H -5.21090200 2.51280200 1.93081600

**10c** *(gauche)*
E(RB3LYP) = -3415.85289750
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3415.85833929
Sum of electronic and zero-point Energies= -3415.371700
Sum of electronic and thermal Energies= -3415.342720
Sum of electronic and thermal Enthalpies= -3415.341776
Sum of electronic and thermal Free Energies= -3415.432016
C -1.21724100 -1.20745000 -2.65275800
C -1.71621400 -2.39164900 -2.03333000
C -2.17049500 -2.05441900 -0.72585100
C -1.94669100 -0.65341600 -0.52522000
C -1.34990700 -0.13721600 -1.72564200
Fe -0.15048600 -1.62377800 -0.93939900
C 1.81653300 -1.79936300 -1.51607900
C 1.29796200 -3.07189300 -1.13645800
C 0.86519500 -2.98902000 0.22375400
C 1.13408700 -1.67478200 0.69655700
C 1.72996700 -0.93639200 -0.37369000
N 2.28777100 0.37884500 -0.27975800
C 3.73764900 0.50988200 -0.54732800
C 4.67889200 -0.00165100 0.57426600
C 4.72342400 -1.54206400 0.62760500
N -2.43846500 0.14742700 0.54897900
P -2.25137100 0.04516500 2.22638800
Cl -0.27607600 0.86209300 2.69571200
C -3.07116900 1.44410900 0.17429000
C -4.52791400 1.36211000 -0.34681500
C -5.42520100 0.67759100 0.69835400
P 1.16396500 1.62266400 -0.43163800
Cl 2.17867600 3.22438100 0.50979400
Cl 1.42627300 2.26519600 -2.51722700
Cl -1.85898500 -1.99645300 2.54593700
C -4.99411000 2.81745300 -0.55763600
C -4.62324200 0.60676200 -1.68570900
C 6.08867700 0.51799600 0.22438800
C 4.24343400 0.55789300 1.93856100
H 2.19920900 -1.51887200 -2.48848100
H 1.20067400 -3.93479700 -1.78283400
H 0.37923400 -3.77483000 0.78714300
H 0.92566800 -1.28361200 1.67944800
H -1.07041900 0.88595300 -1.91972300
H -0.77415300 -1.13344300 -3.63721800
H -1.71655800 -3.38550100 -2.46248500
H -2.59399100 -2.73477900 -0.00310600
H -3.06655200 2.08166300 1.06856500
H -2.42643800 1.94930800 -0.55137100
H 3.96648700 -0.00668300 -1.48898600
H 3.93431300 1.57111600 -0.71274700
H 4.93429400 0.22445200 2.72268200
H 4.23202400 1.65315800 1.93429800
H 3.23651300 0.21789400 2.20272100
H 5.47662000 -1.86988800 1.35519000
H 3.76477600 -1.97399600 0.92561300
H 4.99424300 -1.96490200 -0.34849000
H 6.82068900 0.16448100 0.96050800
H 6.41221800 0.16394300 -0.76359200
H 6.12103200 1.61471500 0.21895000
H -6.02356000 2.83715200 -0.93420600
H -4.96963000 3.38850300 0.37936600
H -4.36157900 3.33724600 -1.28862500
H -6.46816500 0.67183100 0.35986300
H -5.12162000 -0.36248800 0.86276900
H -5.38796200 1.19937200 1.66312800
H -5.65340200 0.64630700 -2.06126500
H -3.97059000 1.05381200 -2.44468800
H -4.34468700 -0.44579300 -1.58309400

**10d** *(transoid)*
E(B3LYP-D3/6-31+G*) = -3101.29898007
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3101.30496785
Sum of electronic and zero-point Energies= -3101.045471
Sum of electronic and thermal Energies= -3101.026515
Sum of electronic and thermal Enthalpies= -3101.025571
Sum of electronic and thermal Free Energies= -3101.095333
C 2.10821100 -1.40697600 -1.07773500
C 2.97950900 -0.93322400 -0.04504900
C 2.28752600 -1.07699000 1.19908400
C 1.01658800 -1.67652200 0.93795700
C 0.90866800 -1.89142600 -0.46907900
Fe 1.14899600 0.11499300 -0.07010300
C 0.01371700 1.29886900 -1.32364200
C 1.34722800 1.79668400 -1.24498300
C 1.63035500 2.11038200 0.11947900
C 0.47188900 1.81247800 0.89780100
C -0.53061500 1.31207900 0.00569000
N -1.89385900 1.04105000 0.36230300
C -2.82823200 2.11104500 -0.03086500
H 0.26828000 -1.91490000 1.68097800
P -2.26079000 -0.60478400 0.40044300
Cl -4.16984400 -0.55335500 1.33270900
Cl -2.89753900 -1.02230700 -1.64977300
H -0.50286400 0.94487500 -2.20601400
H 2.05091100 1.86566500 -2.06481300
H 2.57951500 2.46685700 0.49896600
H 0.35561600 1.92194000 1.96809400
H 0.06091100 -2.31334700 -0.99269800
H 2.32275500 -1.38098600 -2.13904400

N 4.24323300 -0.37192800 -0.25726600
H 2.65241200 -0.76575000 2.16847200
H -2.40968200 3.06607300 0.29851500
H -2.96433100 2.13087400 -1.11979500
H -3.79492900 1.95921200 0.45165900
H 4.77166500 -0.85957900 -0.97072600
C 5.03236900 -0.00287200 0.90812100
H 5.99284100 0.40008600 0.57447700
H 4.51153000 0.78506900 1.46440500
H 5.21993200 -0.84289700 1.59770800

**10d** *(gauche)*
E(B3LYP-D3/6-31+G*) = -3101.30144873
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3101.30740913
Sum of electronic and zero-point Energies= -3101.047182
Sum of electronic and thermal Energies= -3101.028725
Sum of electronic and thermal Enthalpies= -3101.027780
Sum of electronic and thermal Free Energies= -3101.093902
C 1.99325600 -2.25372200 0.69325400
C 2.28844200 -2.15708900 -0.70195200
C 1.14044800 -1.62617400 -1.36192700
C 0.12236000 -1.40981300 -0.37410900
C 0.65378900 -1.80860200 0.89702600
Fe 1.79804100 -0.30093400 0.05374600
C 3.42073000 0.93432600 -0.16327200
C 2.33335300 1.41680400 -0.95822900
C 1.23533400 1.69998100 -0.08659500
C 1.64107100 1.37044800 1.24742200
C 2.99656700 0.91744100 1.19995900
N -0.04649700 2.15446500 -0.45271900
C -0.54208100 3.34991300 0.23658900
N -1.19157300 -0.93951600 -0.66808600
P -1.85736500 0.16726900 0.42992500
Cl -3.35024600 -1.09101600 1.40845500
C -1.99872700 -1.83536800 -1.51410700
H -0.14630400 2.22766000 -1.46026700
Cl -3.20967800 1.22068600 -0.85662400
H 0.13084200 -1.75511600 1.84329000
H 2.67340300 -2.58785300 1.46625100
H 3.23144900 -2.40395300 -1.17234600
H 1.04771400 -1.40305300 -2.41696200
H 1.01618400 1.43444700 2.12809800
H 3.58323000 0.58633000 2.04707000
H 4.38754200 0.62056700 -0.53545200
H 2.32513600 1.52802000 -2.03574600
H -1.52796200 3.59796200 -0.16469500
H -0.65958300 3.12997600 1.30203500
H 0.12800300 4.21650400 0.13024000
H -1.42817500 -2.08874900 -2.41206300
H -2.25337200 -2.75458600 -0.97238900
H -2.91875400 -1.33082400 -1.81318400

**deprotonated 10a**
E(B3LYP-D3/6-31+G*) = -3839.53472936
Sum of electronic and zero-point Energies= -3839.148272
Sum of electronic and thermal Energies= -3839.117754
Sum of electronic and thermal Enthalpies= -3839.116810
Sum of electronic and thermal Free energies= -3839.208097
C 0.056641129476 -0.022652450976 0.028987331948
C -0.015748848767 -0.114945987071 1.457856274915
C 1.326323753189 -0.135348914495 1.955286989882
C 2.203032419676 -0.052860275441 0.825498711581
C 1.440296099477 0.171961203659 -0.392061280039
Fe 0.981130178398 -1.732513886255 0.764157163434
C 2.196313393522 -3.376700212227 0.628684662462
C 1.432529416133 -3.443856594409 1.833097379243
C 0.050991917091 -3.437245860055 1.476381309259
C -0.044272846613 -3.366764869163 0.055294818504
C 1.286720052087 -3.346288701856 -0.486544661194
N 1.661967765219 -3.376203910190 -1.871598693633
P 0.654746618507 -3.645908889211 -3.170977647178
Cl -0.983998307695 -2.270182021239 -2.966724613474
N 1.961662675884 0.389878633471 -1.600744028316
Si 1.352175598721 1.140357092782 -2.982381139682
C 2.226491883106 2.820931536749 -3.260112628037
C 1.743830517321 0.123033434705 -4.547779751189
C -0.519999225086 1.539298872308 -3.030246251286
Si 3.436383746377 -3.352921178514 -2.298902672819
C 4.290688675800 -1.861624200185 -1.560806972483
C 4.156403308608 -5.005303841222 -1.720072936302
C 3.644097201502 -3.293932879135 -4.176998158862
Cl -0.433979064707 -5.455357435876 -2.608197941916
H -0.788425754847 -3.442345092077 2.160856719761
H 1.840137307539 -3.451426616214 2.836545104315
H 3.273751201112 -3.332151542137 0.587306060155
H -0.963178965844 -3.333092954856 -0.507138419105
H 1.623722611415 -0.216834530233 2.995526782799
H -0.920648499011 -0.182807799845 2.052526969681
H -0.789338140256 -0.034546673932 -0.646119036291
H 3.286160356994 -0.057463475201 0.859015379348
H 1.452729501008 0.659010412763 -5.462954838334
H 2.821391269333 -0.081675289416 -4.606890129441
H 1.212934745800 -0.836314498039 -4.535887280839
H 1.916971951233 3.302005982085 -4.200342651660
H 2.005291885549 3.511517045572 -2.434486799983
H 3.315813429287 2.681817703457 -3.288314738360
H -0.770553891459 2.134013300326 -3.921445591085
H -1.125328422696 0.625381293214 -3.052609648088
H -0.817740957418 2.117551369868 -2.145092019269
H 5.197776075291 -1.654086671889 -2.146607802080
H 3.623151301418 -0.983127033099 -1.621742959993
H 4.585690497869 -1.995520712967 -0.515439505163
H 5.236425723573 -5.036964253726 -1.920270226128
H 4.001704753347 -5.181333786727 -0.650828065543
H 3.685451468691 -5.833988634178 -2.264232817812
H 4.726434511894 -3.235734767685 -4.364509882543
H 3.264788910202 -4.184635134584 -4.689399697441
H 3.181660284479 -2.410771072466 -4.627964301348

E(M06-2X/6-31+G*) = -3838.83597341
Sum of electronic and zero-point Energies= -3838.446489
Sum of electronic and thermal Energies= -3838.416051
Sum of electronic and thermal Enthalpies= -3838.415107
Sum of electronic and thermal Free energies=-3838.506827
C -0.056682000174 -0.059721444941 -0.025455404719
C -0.050495566629 -0.016126978738 1.393082669004
C 1.297908296329 0.011261345091 1.831601494616
C 2.140264591404 -0.014661665323 0.682263929982
C 1.292191030176 -0.061226194135 -0.466200534967
Fe 0.945555079258 -1.781976531085 0.720035806881

C 0.130958906209 -3.535169898293 1.495176676327
C 0.050801372536 -3.543959249637 0.076986619837
C 1.384041896497 -3.497766073315 -0.431100877913
C 2.332328619805 -3.518448872707 0.658497185279
C 1.512425702680 -3.477992347587 1.850957290199
N 3.679765809930 -3.463313354160 0.537307832266
Si 4.819600736636 -4.374989884397 1.362927446804
C 6.473296929723 -3.441307415858 1.440296152217
N 3.567936313099 -0.016382310491 0.646447581149
Si 4.391177885065 -0.023428650795 -0.967912757452
C 3.984207796220 1.630057252606 -1.779597799859
P 4.592910844965 0.081658567261 1.950685433211
Cl 3.917891478889 1.879881569102 2.920612766140
Cl 3.868967153042 -1.257848416757 3.394916818941
C 4.399125780812 -4.925547623764 3.144300808599
C 5.247160177676 -6.017503858248 0.479372485765
C 6.251561779104 -0.063454233392 -0.694904289269
C 3.922436372886 -1.495972562110 -2.010783795062
H -0.917785744902 -0.035177113897 2.039794058227
H -0.927397319699 -0.122300353212 -0.664679127171
H 1.605651556660 -0.139045670082 -1.496576324532
H 1.621632225534 0.018446472429 2.860850286718
H -0.859341919795 -3.551640159569 -0.511113317696
H -0.708090944940 -3.529557253677 2.180717493719
H 1.905019835498 -3.408740941960 2.858146300237
H 1.668666492738 -3.470236291001 -1.476223846621
H 7.250693586796 -4.034141445413 1.940308893307
H 6.823285703025 -3.220119825086 0.423542579383
H 6.372631579689 -2.490760306631 1.979569916803
H 6.043748079348 -6.573119705281 0.993863146206
H 4.361741877060 -6.663952305367 0.425061772336
H 5.574226239102 -5.821372610631 -0.549459416984
H 5.193828611940 -5.569873066817 3.545221969860
H 4.280562632488 -4.071366343368 3.820854800479
H 3.463286848790 -5.499011738086 3.159511932809
H 4.714993321640 -1.657480004470 -2.753724885677
H 3.878529637353 -2.372711081697 -1.341255690158
H 2.973054280734 -1.396247857950 -2.544553918526
H 4.479088982835 1.698911508588 -2.756596302155
H 2.910997727633 1.779763371809 -1.929465697344
H 4.350847517292 2.452504709643 -1.154042058803
H 6.718256870889 -0.075856558567 -1.689010735062
H 6.632122372235 0.809810571651 -0.155521101456
H 6.570796289524 -0.964582946743 -0.161948507293

**deprotonated 10b**

E(B3LYP-D3/6-31+G*) = -4075.43486027
Sum of electronic and zero-point Energies= -4074.875945
Sum of electronic and thermal Energies= -4074.838207
Sum of electronic and thermal Enthalpies= -4074.837263
Sum of electronic and thermal Free energies=-4074.943721
C -0.119564668132 0.038395779489 -0.125572926904
C -0.340794725305 0.014460127055 1.289517628340
C 0.933901043416 0.149140616048 1.925827458780
C 1.920379831180 0.258858286378 0.893451706171
C 1.282049561617 0.318175050941 -0.410898569660
Fe 0.874114496734 -1.529574992599 0.791670352811
C 2.237996690051 -3.050361453617 0.912409228422
C 1.305593897540 -3.158967868733 1.987658483989
C 0.001977704213 -3.295064409847 1.424179787629
C 0.124981064041 -3.270741595135 0.003644795923
C 1.517017696907 -3.136538335538 -0.329566539408
N 2.094910528923 -3.158265839177 -1.643861372318
P 1.289795190049 -3.509637833485 -3.064671321143
Cl -0.434977756974 -2.227041325942 -3.131865172329
N 1.907778439001 0.486951506206 -1.586304426858
Si 1.382380394518 1.366041869922 -2.926253209043
C 2.154810697185 3.157375613688 -2.841933827345
C 1.984414681217 0.603420178599 -4.565286667748
C -0.504911289207 1.617386628833 -3.136177044086
Si 3.881820344210 -2.868098295739 -1.908761320687
C 4.505861923815 -1.413490109903 -0.910220108935
C 4.831830374024 -4.517258783520 -1.575434258212
C 4.168488126531 -2.416822277621 -3.723104378822
Cl 0.245722553224 -5.366277645026 -2.610453653871
H -0.930602779792 -3.363385830421 1.970597093286
H 1.551702197562 -3.102716504896 3.040954735682
H 3.298909254660 -2.909338391599 1.032604131236
H -0.695562226245 -3.333685881694 -0.692229831059
H 1.120020546951 0.151506911765 2.994593384174
H -1.295471020268 -0.112253072790 1.788755405149
H -0.877484891180 -0.096627649218 -0.885603286574
H 2.988240769092 0.358514921260 1.045184725766
H 1.671734000673 1.212138854918 -5.424963182937
H 3.077732070853 0.518563144598 -4.597723782291
H 1.556580463267 -0.398297976913 -4.695651001606
C 1.752203090280 4.041233126957 -4.037546595922
C 1.676364123969 3.824687208415 -1.537236312278
C 3.690771835774 3.040292541895 -2.799122226752
H -0.730984974045 2.250173719101 -4.006003076329
H -1.000905751333 0.651197286593 -3.289308891311
H -0.953798153411 2.085769619952 -2.250944477651
H 5.489048415085 -1.126920870224 -1.308843199624
H 3.802379193948 -0.582551005939 -1.083420124471
H 4.607339094930 -1.580532399806 0.164575481502
C 6.292523462485 -4.321987077832 -2.045342078855
C 4.851853112100 -4.920664767664 -0.088012101577
C 4.193375932154 -5.666930045386 -2.382169664736
H 5.200621067122 -2.049659150416 -3.803120572532
H 4.050451097007 -3.246923337621 -4.426417977454
H 3.510272113186 -1.602360310395 -4.034374638136
H 2.212672660726 5.042249078513 -3.958411474655
H 2.077524028367 3.609024656775 -4.993629825072
H 0.665378680907 4.188132255650 -4.091455265074
H 2.128846789632 4.825113922365 -1.417013104924
H 0.585739302021 3.955504713484 -1.525301378357
H 1.947250291000 3.222165374790 -0.661912936891
H 4.157459040159 4.032200157810 -2.662948255452
H 4.009532374289 2.393752387631 -1.973160178718
H 4.091588530032 2.616598112243 -3.730416644011
H 4.782012952440 -6.589986551119 -2.257223990318
H 3.171716860275 -5.879590960687 -2.048676060763
H 4.154431112638 -5.449562776789 -3.457167407677
H 6.873548662688 -5.239158404767 -1.859343099987
H 6.357305353868 -4.107434339901 -3.118957264449
H 6.790808937800 -3.504773205868 -1.506712724575
H 5.454261746599 -5.834015899622 0.044823321948
H 5.298304716385 -4.140833639554 0.542350626838
H 3.846727279440 -5.127385096695 0.292398664903

E(M06-2X/6-31+G*) = -4074.59780988
Sum of electronic and zero-point Energies= -4074.035255
Sum of electronic and thermal Energies= -4073.998559
Sum of electronic and thermal Enthalpies= -4073.997615
Sum of electronic and thermal Free energies=-4074.100565
C -0.300695747368 -0.182716203917 -0.376880838747
C -0.447411425080 -0.192471572691 1.033533237840
C 0.841094529243 -0.083256851967 1.615161009664
C 1.799189295794 0.000493046803 0.561056094276
C 1.083034339460 -0.057136555255 -0.670631161028
Fe 0.754598938938 -1.846508385326 0.445553234934
C 0.124203580710 -3.615989911808 1.345265967571
C -0.043226718420 -3.710614502882 -0.061979126689
C 1.247715261783 -3.586828424811 -0.657281615692
C 2.254892743869 -3.457488029657 0.370962723649
C 1.514685576004 -3.431436405986 1.607031436036
N 3.604755648931 -3.299564533953 0.201148630693
Si 4.570068819279 -4.616707778127 -0.196572894912
C 6.169480823509 -4.115182187366 -1.105876007509
N 3.217624103622 0.105020897259 0.698433439764
Si 4.362402211536 -0.099197352595 -0.708612718066
C 4.699913386615 1.669783466376 -1.367167390310
C 3.392285639631 2.340031507186 -1.810227912085
P 4.033142426065 0.447879007762 2.107840231097
Cl 2.945345826136 2.108341677343 2.882795903954
Cl 3.403765990918 -0.980187100971 3.534024637513
C 5.171172190304 -5.611886564235 1.352185572304
C 5.688469693820 -4.617830411910 2.398542811303
C 3.721805112976 -5.892746507367 -1.339673858200
C 3.976110477696 -6.370068191827 1.943055730218
C 6.282505904041 -6.609862897089 1.013097918697
C 5.954091194186 -0.839154643812 -0.046969576208
C 3.692791663584 -1.123515297318 -2.128830867500
C 5.359344675640 2.562577421324 -0.308499276648
C 5.646264858900 1.552949766998 -2.572284579748
H -1.372732856420 -0.310398450188 1.582000900657
H -1.091335785110 -0.283315985309 -1.108477983759
H 1.508627228064 -0.045772468714 -1.661820938455
H 1.053735924996 -0.106126908519 2.672763261575
H -0.984862774730 -3.820209685968 -0.586612147013
H -0.669791029748 -3.632536663245 2.082500008687
H 1.968793273761 -3.272605006802 2.577399915518
H 1.462606661048 -3.604482417437 -1.720077720841
H 6.641178646603 -5.002589269731 -1.548193783120
H 5.946954223777 -3.414300833615 -1.919330553064
H 6.906466068380 -3.640655900956 -0.446736400559
H 4.314080197911 -6.809536033409 -1.462104547506
H 2.734354565901 -6.172101987833 -0.951704864864
H 3.568326157521 -5.457301662844 -2.336189087733
H 4.556181286522 -1.603768060745 -2.605246436645
H 3.050809411883 -1.922444584454 -1.754014071436
H 3.176896377576 -0.527478577500 -2.889863961320
H 6.570365419035 -1.173241439396 -0.890496235838
H 6.547252687131 -0.150632800941 0.561992283117
H 5.690671242654 -1.724797058890 0.544360812867
H 5.613642787550 3.539485757772 -0.748333831206
H 4.687991400418 2.756746601818 0.536609467142
H 6.285332532061 2.126968269104 0.085721492129
H 3.595847880635 3.354975467521 -2.186043646215
H 2.897653726001 1.786470250185 -2.617947936634
H 2.681347630399 2.425885083093 -0.979025987211
H 5.856976780294 2.549313327419 -2.990415951254
H 6.607855067228 1.104794524095 -2.290075936896
H 5.214393783245 0.943612865678 -3.376042265422
H 6.570554187199 -7.193718507949 1.904072404246
H 5.967727097279 -7.325297779250 0.241457373860
H 7.184435442062 -6.101470970998 0.648978494585
H 6.006072797201 -5.143319111796 3.315080310722
H 6.554905247770 -4.053032647870 2.026336175187
H 4.912889375451 -3.889791686639 2.662642312469
H 4.256770647865 -6.870048093619 2.885768676227
H 3.139842286069 -5.692556582326 2.156771404041
H 3.609870607411 -7.142999839392 1.254657325503

**deprotonated 10c**

E(B3LYP-D3/6-31+G*) = -3415.27382446
Sum of electronic and zero-point Energies= -3414.808204
Sum of electronic and thermal Energies= -3414.779611
Sum of electronic and thermal Enthalpies= -3414.778667
Sum of electronic and thermal Free energies=-3414.866828
C 0.095313386989 -0.059166846564 -0.081408533830
C 0.368710275049 0.004949307577 1.327048250036
C 1.795759516863 -0.074300488381 1.490627893158
C 2.391123411590 -0.169240475872 0.195954197100
C 1.341167505006 -0.158329028310 -0.771266227708
N -0.586910874316 0.123624078878 2.383868079755
C -0.185168229664 -0.435183174853 3.705837848523
C 0.178926841818 0.602119302378 4.804586686344
C 1.137276140731 1.689237881538 4.287253856315
Fe 1.084099510870 -1.747613398450 0.535335057379
C 1.687745355106 -3.446694416351 1.606945212360
C 0.238347337181 -3.513708904228 1.813427566293
C -0.296116033148 -3.297294314436 0.475572976140
C 0.742469501740 -3.442821889134 -0.501359304819
C 1.986292603076 -3.521202442208 0.202308948803
N -0.483726836066 -3.626117668073 2.917641349542
C 0.241610640654 -3.879601477353 4.133288927374
C -0.678900459266 -4.443859052321 5.251011729787
C -1.256928837763 -5.795904723278 4.796960219048
C 0.147612171605 -4.640122512243 6.534238921769
C -1.835693798634 -3.467908848612 5.530614285514
P -2.212420195625 0.482439290834 2.266878777540
Cl -2.169169314105 2.254050851256 1.049704460462
Cl -3.121460570875 -0.841886839587 0.779803914542
C -1.085257277553 1.286538596638 5.361643647635
C 0.857422897212 -0.182891154594 5.945901490916
H 1.456883188656 -0.250739508660 -1.844405464698
H 3.450816163161 -0.272107719581 -0.003572851125
H 2.336257770001 -0.089552690369 2.424716205414
H -0.880322044379 -0.056048449194 -0.541555349638
H 2.972102514755 -3.621032941417 -0.240547606342
H 0.611940829474 -3.457663904971 -1.578321161239
H -1.351408572341 -3.171833565278 0.267822381324
H 2.430742171967 -3.458992729326 2.395912518683
H 1.067985207726 -4.610838457655 3.993147937652
H 0.736072121124 -2.970540274998 4.546252925699
H 0.656726119658 -1.095585119101 3.496659734360
H -0.973415673731 -1.100216138764 4.068138289248
H -0.827506051346 1.915128991617 6.225014148095
H -1.558826335999 1.933620673812 4.614542612830

H -1.829145884412 0.548412160014 5.686538739137
H 1.283437193520 2.459571810552 5.056574963800
H 2.121193902831 1.278401082095 4.039310831597
H 0.737992715122 2.170633122399 3.388119535598
H 0.192952108728 -0.954027646902 6.352879965267
H 1.767484092763 -0.684951341517 5.595097907341
H 1.134956487315 0.493393359830 6.765497540493
H -2.525863016564 -3.878584386215 6.282287007864
H -1.458520961224 -2.510807412229 5.915408696686
H -2.387666369633 -3.269831779751 4.606481752086
H -1.932631860928 -6.215168561202 5.557408267949
H -1.806641444025 -5.667214467161 3.859033332801
H -0.452010676751 -6.522932266225 4.618731697370
H -0.473506579363 -5.042074789353 7.347668921304
H 0.978381147971 -5.339874985762 6.367404325821
H 0.576545494387 -3.688440841989 6.878127736941

E(M06-2X/6-31+G*) = -3414.65316164
Sum of electronic and zero-point Energies= -3414.180431
Sum of electronic and thermal Energies= -3414.153347
Sum of electronic and thermal Enthalpies= -3414.152403
Sum of electronic and thermal Free energies=-3414.236370
C -0.552851782177 -0.222281527573 0.353952203410
C -0.390758776740 -0.419754304071 1.759577485340
C 0.997662215952 -0.347206562183 2.047186677993
C 1.695879705173 -0.106939115950 0.828060759231
C 0.738857015160 -0.014905451764 -0.218141017684
Fe 0.594008961632 -1.911118693716 0.678689817580
C -0.594347784709 -3.342313659670 -0.222565571503
C 0.694311125985 -3.364742852967 -0.837104684933
C 1.648389401706 -3.677225568017 0.168386050310
C 0.950778983876 -3.870508753843 1.396185749652
C -0.433934199015 -3.664310569900 1.160058424780
N -1.833218921360 -3.025411295501 -0.837296316499
C -2.919565921583 -4.002477108129 -0.643314457340
C -2.979032327095 -5.103433062927 -1.716883338328
C -3.253016122937 -4.486816390639 -3.091086081461
N -1.796513962657 -0.266505147555 -0.327601458769
C -2.858338429256 0.604237459778 0.207948288356
C -2.884257545133 2.017424027639 -0.400653585836
C -4.011456626573 2.787149645660 0.297026829470
P -2.358437120564 -1.496738823450 -1.351107292815
Cl -0.910178833715 -1.213900014618 -2.986596397496
C -1.669083483055 -5.896395258561 -1.765555202594
C -4.128604637790 -6.042768076375 -1.334891427756
C -1.554315053008 2.741560041577 -0.168259655925
C -3.166900663565 1.940259141937 -1.903272244918
H 2.769767831125 -0.036179586755 0.711223577767
H 1.451033974804 -0.500501481905 3.018020428017
H -1.204134098361 -0.692993487003 2.425746544421
H 0.936465380224 0.119500361079 -1.273268760125
H 1.403353921913 -4.085922797595 2.355527838221
H 2.720648012976 -3.729135112148 0.028890865574
H 0.893490039355 -3.118385690523 -1.871532561755
H -1.243195714227 -3.626338358437 1.883713022969
H -2.811470418436 -4.438338500619 0.355720746946
H -3.872903256982 -3.462382504094 -0.613288389363
H -2.744021129441 0.651099027645 1.296277461586
H -3.825361438741 0.113845225935 0.047212920981
H -3.212270408825 2.946721011235 -2.339948964574
H -2.380661701013 1.379560827163 -2.421514332741
H -4.124410580165 1.440582813804 -2.098044952254
H -1.627835206633 3.786637236438 -0.498069516221
H -1.278325438349 2.733747258794 0.893840784405
H -0.741861177601 2.265253243996 -0.725753635171
H -4.976928113084 2.286290900893 0.155675400671
H -3.828145177529 2.861855226033 1.375745600322
H -4.093009739572 3.804590808089 -0.106227871596
H -3.322115494271 -5.269031105272 -3.858600425824
H -4.196613356791 -3.926405034148 -3.089451676722
H -2.450463006821 -3.798004249992 -3.378452542783
H -1.767879217270 -6.752197203138 -2.446878339738
H -0.842283964368 -5.273063906387 -2.119973556834
H -1.397621755539 -6.275921443974 -0.772297757066
H -4.234426351768 -6.846296167267 -2.074891381011
H -3.951987614715 -6.502945000116 -0.355163126447
H -5.080317047273 -5.500075846736 -1.282879033470
Cl -3.502721908696 -2.119830717294 2.102951355879

**deprotonated 10d**
E(B3LYP-D3/6-31+G*) = -3100.72701358
Sum of electronic and zero-point Energies= -3100.488947
Sum of electronic and thermal Energies= -3100.470342
Sum of electronic and thermal Enthalpies= -3100.469398
Sum of electronic and thermal Free energies=-3100.537124
C 0.002125202521 -0.097938607438 0.007026757947
C 0.002333552163 -0.105773287250 1.438119907835
C 1.372034500363 -0.099152510545 1.870254976189
C 2.255825832692 0.108145559462 0.720036663300
C 1.369307119251 -0.100127411889 -0.420511541475
Fe 0.880835701525 -1.770750826454 0.722410243120
C -0.228148242333 -3.413738111789 0.121321715494
C -0.083360579743 -3.419894502053 1.545782429354
C 1.310220290142 -3.430848543546 1.848319462801
C 2.035546858183 -3.464043331727 0.607140948854
C 1.074173162524 -3.442161951586 -0.462802560748
N 3.459358667675 -3.620801528159 0.486122149430
C 4.159635748240 -2.746724876467 -0.468537940725
N 3.563887670175 0.275313156395 0.643276066646
C 4.258045867748 0.250728889578 1.912433340241
P 3.923777082515 -5.156635090739 0.935577634471
Cl 5.990120838065 -4.851953443174 1.438744533941
Cl 4.251457911147 -6.251602784690 -0.987976184371
H 1.307523561411 -3.435366788184 -1.519545650318
H -1.164042199138 -3.360224790458 -0.422133431625
H -0.888106002448 -3.367375988351 2.268827135685
H 1.763823779595 -3.408455224437 2.831276459253
H 1.712250397574 -0.115274926350 -1.448888880564
H -0.873223387773 -0.115646926627 -0.633667025533
H -0.873146026218 -0.122556081244 2.079293926620
H 1.692975163358 -0.132891627623 2.904169840240
H 5.322568754143 0.472182158735 1.753674015188
H 3.877175392977 0.993079143638 2.646501143190
H 4.204785649855 -0.737734866960 2.416925696914
H 5.236505297892 -2.904164631391 -0.377447080366
H 3.851695054476 -2.990490899499 -1.493986635303
H 3.923992805510 -1.701216085957 -0.235339464237

E(M06-2X/6-31+G*) = -3100.21074131
Sum of electronic and zero-point Energies= -3099.970300

Sum of electronic and thermal Energies= -3099.952748
Sum of electronic and thermal Enthalpies= -3099.951804
Sum of electronic and thermal Free Energies= 3100.016587
C 0.035318241161 -0.170378077116 -0.077896529908
C -0.016743577479 -0.179720433628 1.338293172178
C 1.321642978391 -0.179918164653 1.824158207860
C 2.202725711393 -0.160888187858 0.703808744033
C 1.406183277710 -0.147438813948 -0.468095665410
Fe 0.971367276024 1.592756161306 0.691333637759
C 0.082258298128 3.290956628059 -0.066587598501
C -0.111362537050 3.293125198804 1.354744939056
C 1.171157798429 3.466544955676 2.022766882511
C 2.143422381375 3.340090833827 0.950718677451
C 1.478437544238 3.330023253121 -0.313704103283
N 1.468379224381 3.570013793486 3.312026500732
C 0.322136695014 3.452628550678 4.173805911894
N 1.694945732380 -0.276760087967 3.204484558328
P 1.395609788565 -1.790126687002 3.813354913297
Cl 3.345002700717 -2.737454136273 3.861333781712
C 2.749188460780 0.632374106264 3.673453550003
Cl 1.291302968494 -1.374424623346 5.873628616631
H 3.283140339700 -0.122754255499 0.752018364014
H 1.777253507448 -0.086825812484 -1.483053105427
H -0.816930749754 -0.130750989889 -0.743228011975
H -0.901183481525 -0.152216128156 1.962111330919
H 3.215581162233 3.351713630923 1.109389477234
H 1.953340858062 3.305045366017 -1.287704820504
H -0.697309963649 3.240034542882 -0.818023733253
H -1.073151731895 3.242001632000 1.849769731383
H 0.627704640157 3.583271501930 5.219994156103
H -0.470089104153 4.204340335217 3.970589981085
H -0.177716763956 2.459616091189 4.104357782038
H 2.880995488469 0.497598392156 4.748940414647
H 3.696109280644 0.398321756887 3.169814002093
H 2.444000720743 1.671254287751 3.477741753038

**van der Waals complex of 10a and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4014.61853836
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4014.61365562
Sum of electronic and zero-point Energies= -4014.094016
Sum of electronic and thermal Energies= -4014.056374
Sum of electronic and thermal Enthalpies= -4014.055430
Sum of electronic and thermal Free Energies=-4014.163248
C -0.506482673129 -0.261351087100 0.376707900504
C -0.243784792801 -0.225931696586 1.779392710699
C 1.158589173276 0.003612471222 1.961431415911
C 1.760398219916 0.088746850607 0.661065442218
C 0.732898483323 -0.076982493400 -0.311467825722
Fe 0.821998583959 -1.747132699882 0.894759342875
C 0.150774089755 -3.458809549150 -0.000066829055
C -0.038503684862 -3.562546666559 1.412975924023
C 1.238896305715 -3.483751635093 2.054384704660
C 2.213484920601 -3.277505794704 1.021066127785
C 1.546422529214 -3.291913725930 -0.244006227601
N 1.500127779410 -3.598295324383 3.423398789530
Si 2.672435772849 -4.758636520849 4.066056265347
N 1.810007687803 0.242255669425 3.225574004102
P 3.093704411395 -0.829923870745 3.471029684842
Cl 3.139013381531 -1.006839691237 5.608219173073
Si 1.518122984234 1.922322531463 3.861556663497
Cl 4.840537162862 0.465290375988 3.246546847719
N -0.974348286749 -2.919476400239 5.178260080921
C -0.479177048081 -1.606989502666 5.592665374533
C -2.151974889869 -2.789953973995 4.324266834820
C -1.257415422062 -3.769068874971 6.333038291711
H 0.872243088018 -0.094824866890 -1.384885994992
H -1.470249457237 -0.437345214354 -0.083696422025
H 2.814161212597 0.248652485391 0.471837627913
H -0.965269954598 -0.338819585594 2.575098838221
H 3.271848316348 -3.125926204261 1.179502924251
H 2.016376107039 -3.158603430566 -1.210026778973
H -0.631710294297 -3.477217722957 -0.748461534610
H -0.982561999625 -3.693737449679 1.923132160423
C -0.329012888994 2.104640824789 4.195760441896
C 2.053108845501 3.111628259977 2.504833155734
C 2.472766730098 2.247303388434 5.444912489495
C 2.482572718858 -6.411794838915 3.168883505196
C 2.264613233006 -4.923413670535 5.898245168483
C 4.456887785374 -4.180393797800 3.856564311013
H 0.662939445559 -3.455859332659 4.002952544869
H -1.245203078932 -1.023598718442 6.140252889526
H -0.160047256440 -1.039973314978 4.714669771453
H 0.395425701988 -1.727468584785 6.236240322037
H -1.904681263441 -2.189883234909 3.444029321531
H -2.475577223697 -3.780457544292 3.985071364663
H -3.001027225558 -2.309144150768 4.848353981307
H -2.066594335661 -3.358713984048 6.968092439162
H -1.558286559705 -4.766712046260 5.994219200685
H -0.356986802562 -3.871090403616 6.945472645504
H -0.511317864963 3.082359699908 4.661512110146
H -0.921517372418 2.058647496305 3.276142322867
H -0.698176195011 1.335761766781 4.884160791602
H 2.345163300640 3.309981276714 5.693777943169
H 2.100036008931 1.654163113583 6.285298368271
H 3.543436947260 2.051508056453 5.338881838602
H 1.874919441409 4.150734794786 2.811057683795
H 3.122622510207 2.995391553916 2.294808343939
H 1.502286776708 2.933250199800 1.574242818117
H 3.018745104909 -5.536417203732 6.407578524374
H 2.251948380301 -3.939503872482 6.382039893213
H 1.288647645093 -5.398283647832 6.051062660322
H 3.215196080429 -7.148264954427 3.524168638304
H 1.479507739985 -6.831770969676 3.315871119939
H 2.632713503050 -6.286287758664 2.089017367968
H 5.136078739413 -4.983191717537 4.174429811056
H 4.702262671883 -3.941632686557 2.815403097569
H 4.677962082998 -3.299022042551 4.467995870763

**van der Waals complex of 10a and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -4132.57530424
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4132.5797132
Sum of electronic and zero-point Energies= -4131.964999
Sum of electronic and thermal Energies= -4131.923183
Sum of electronic and thermal Enthalpies= -4131.922239
Sum of electronic and thermal Free Energies=-4132.040100
C 0.039409316082 -0.006743345471 -0.036921395100
C 0.026018650351 -0.000373863662 1.395212542899

C 1.378135627864 -0.009587369731 1.865403682016
C 2.215616120392 -0.151235182739 0.709546510689
C 1.397374027399 -0.094831775769 -0.462701363997
Fe 0.874669437937 -1.738131674891 0.627636490762
C 0.590483805325 -3.258276397783 -0.731957870585
C 1.784360562588 -3.494580780032 0.007652619079
C 1.429096234790 -3.590881090036 1.393351564977
C 0.014567601032 -3.400258416965 1.503317720131
C -0.503097306942 -3.207184197192 0.188288647983
N 2.298613078236 -3.999120125884 2.463599910135
P 3.363199766166 -2.789670760986 2.927771909404
Cl 3.578737587208 -3.258007877379 5.027110657089
N 1.822546315292 0.117485536978 3.171321603528
Si 0.867011576251 0.042459776622 4.648331729076
C -0.082411280439 -1.587052446416 4.718918051800
Si 2.137456489046 -5.737488191011 2.972950620662
C 0.914875770230 -5.791808456461 4.403037352820
C 1.464112719086 -6.663409392488 1.478196475284
C 3.808896306340 -6.449264549471 3.451788771832
C 2.079946902545 0.185395693270 6.080052148433
C -0.364569751414 1.476230505510 4.736431660572
Cl 5.313379771899 -3.496120233367 2.257688414932
N 4.739887246479 1.396242378210 3.090354463706
C 5.882438696685 0.482565581379 3.277427689024
C 5.843833014880 -0.297905224377 4.591775644928
C 4.748087584399 1.997755378732 1.742392514834
C 5.815268442212 3.069545909102 1.459191063184
C 4.631655393000 2.388978492206 4.171291786743
C 3.428688317214 3.324078050763 4.025122310394
H 2.821169847998 0.343075029111 3.232039605608
H 0.526313356461 -3.102174791860 -1.801496742645
H -1.537131464779 -3.009626755761 -0.064184892122
H -0.544056696709 -3.404887301888 2.428692741218
H 2.789548860743 -3.583376824036 -0.383850963230
H -0.833667301847 0.020315346348 -0.676989605214
H 1.747187006042 -0.149942440588 -1.485783539763
H 3.290400998140 -0.251211013529 0.736713840759
H -0.860084882470 0.041999264687 2.013590427388
H 5.559277054592 2.985902351562 4.264593572835
H 4.528309601094 1.836396878568 5.108839998435
H 4.880570371635 1.175989582320 1.030859770682
H 3.751978409030 2.409547305678 1.547166303847
H 6.846202374141 1.021474840939 3.209364160708
H 5.856223559871 -0.230773251661 2.444844074080
H 3.548838178137 4.034624622177 3.200517952551
H 2.511169607608 2.753829338698 3.847251154094
H 3.301747313234 3.906508843164 4.945115268003
H 6.549831658359 -1.133693565416 4.543838815774
H 6.116367014806 0.319082196214 5.454794912636
H 4.849306808909 -0.714431922470 4.771355511551
H 5.735705532805 3.396384646371 0.415285571917
H 5.689223489623 3.954793501108 2.092293044759
H 6.830807771582 2.687947068467 1.611320835578
H 0.733608651197 -6.825946802707 4.724138119358
H 1.296062879193 -5.227793109520 5.261101870357
H -0.049246505861 -5.357045205307 4.112770342107
H 3.675441220131 -7.506530779181 3.719061324939
H 4.514087986589 -6.395536014005 2.615868049816
H 4.261447771167 -5.937951852913 4.305683475814
H 1.368273826424 -7.729534400816 1.723063037471
H 0.480850118385 -6.295692583760 1.166291806296
H 2.141441338891 -6.573933374184 0.620908423690
H -0.975180426225 1.407190240623 5.646742493299
H 0.159655675429 2.439824764912 4.757969904779
H -1.048430939949 1.493037456132 3.879826666759
H -0.605785927989 -1.688558993042 5.678560370018
H -0.833004655098 -1.645709491016 3.922453664508
H 0.593876073174 -2.441952997125 4.610250823536
H 1.537356994921 0.127602001964 7.032468339446
H 2.822009576456 -0.619398308535 6.070883563499
H 2.607502632268 1.145666844327 6.061147632628

**van der Waals complex of 10b and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4250.44055100
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4250.50686725
N 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 0.000000000000 1.185730000000
N 0.232601993895 0.000000000000 2.643246460983
P -1.410087847711 -1.227154940173 3.155718535825
Cl -2.990299405656 -3.206262265420 2.879529406072
N -1.764333611780 -0.660583701730 4.747059228174
Si -2.388020889133 -1.760865479087 6.095492194545
Cl -2.828519811738 -0.103761466544 1.905826828551
C 0.238083430122 1.409096544681 2.918668504095
C -0.684238038484 2.345724964752 2.321638042980
C -0.429509781605 3.651334404260 2.837607955531
C 0.665631454685 3.552770740032 3.746464213815
C 1.076331548302 2.184968307841 3.806459839848
Fe -0.878274483351 2.327005630799 4.345581282635
C -1.876803593856 0.731445731165 5.120799265916
C -1.068496569963 1.373955106840 6.127482982997
C -1.503960023562 2.721090494831 6.275375406573
C -2.579063327422 2.932151945734 5.361180478621
C -2.817672435370 1.715379772324 4.657716346973
Si 1.710441089796 -0.872571941341 3.321038578664
C 1.406034398338 0.340919118787 -0.403762189057
C -0.399597137393 -1.407595665765 -0.285991253140
C -0.962772676255 0.958020830953 -0.605797248745
H 1.925713178452 0.723717507465 0.467787782311
H 0.298268038137 -2.087683241311 0.199972475814
H -0.993391008197 0.792693161455 -1.688543847718
H -3.108303239818 3.863294509408 5.203374268659
H -1.069091834773 3.456962526322 6.939605542281
H -0.257195795867 0.902692694765 6.659329383207
H -3.554005006478 1.561686003286 3.886296678183
H 1.093689036281 4.362169475510 4.324002713138
H -0.991298322577 4.546419559622 2.603789016177
H -1.520708244138 2.076221122225 1.698411932974
H 1.867668145750 1.815332066192 4.441025331983
C 1.596773093926 -0.827279213926 5.210799529052
C 2.010044911418 -2.736916739177 2.837671109384
C 3.287203257484 0.051514859806 2.770860466577
C -1.760392228549 -3.530057945991 5.943732420096
C -1.552415300940 -1.218566137328 7.718351322873
C -4.288766956842 -1.558041603428 6.335224547691
H 1.403839796159 1.118438588649 -1.169686187412
H 1.927363562226 -0.534896002871 -0.791026892332
H -1.951693817436 0.793414943557 -0.176852463595
H -0.636796835104 1.976577351006 -0.397070129860
H -0.409813468117 -1.586924923962 -1.366497086074

H -1.393199370451 -1.575606876671 0.133904582197
H 4.071648733872 -0.083119935397 3.525273763076
H 3.681817466832 -0.338436633364 1.829451751924
H 3.135245805898 1.129075105758 2.653038861253
C 3.124932648420 -3.242389338123 3.793167736691
C 0.781001074256 -3.643881781203 3.010881241996
C 2.553062003837 -2.913378715854 1.397586517909
H 2.593508555730 -0.850176045885 5.666156473001
H 1.093086950940 0.079666767325 5.546446263522
H 1.020459314176 -1.676289659354 5.595567896077
H -1.869834513728 -1.932905773238 8.489801163128
H -0.459837623490 -1.290507389803 7.641816541722
H -1.808914762993 -0.217716677619 8.070249488490
H -1.775797492857 -3.971982229265 6.947773711908
H -2.322535284623 -4.157988648256 5.253068700919
H -0.715539110647 -3.518532195458 5.611803540088
C -4.779530020577 -2.768338744106 7.168286932165
C -4.585350259767 -0.266171746199 7.135956304288
C -5.087263728289 -1.516942528422 5.015783700184
H 1.000576480522 -4.670633850842 2.685175760167
H 0.457989209362 -3.702611892175 4.054448018878
H -0.087291777544 -3.279198323164 2.462454623820
H 3.402849406127 -4.267845817890 3.510713869699
H 4.035786100504 -2.632554722666 3.741793681819
H 2.802828695133 -3.281148111811 4.838390371236
H 2.750091510656 -3.977474075833 1.205310356131
H 1.852926483687 -2.582565790036 0.624978467949
H 3.499418998742 -2.384464602620 1.238147073515
H -6.123279085075 -1.214918036968 5.233018396958
H -4.675031197487 -0.800304861314 4.297513608966
H -5.108802477685 -2.492074461919 4.523512734586
H -5.860693809491 -2.677554254389 7.351647029266
H -4.616093561443 -3.719515530038 6.648264423945
H -4.289260002358 -2.827755535616 8.149323808766
H -5.669497140510 -0.186671087855 7.306241481116
H -4.104147739762 -0.261937279949 8.120161853529
H -4.268851392235 0.636594471894 6.602955842392

**van der Waals complex of 10b and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -4368.46780527
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4368.4718779
Sum of electronic and zero-point Energies= -4367.684949
Sum of electronic and thermal Energies= -4367.635709
Sum of electronic and thermal Enthalpies= -4367.634765
Sum of electronic and thermal Free Energies=-4367.767104
C 0.485832128995 -0.192289470538 -0.053718751693
C 0.169779954760 0.003210225160 1.329736122646
C 1.388631722252 -0.010582734929 2.080065521166
C 2.443770559192 -0.295440683710 1.154743187871
C 1.894846416053 -0.377439872979 -0.160341635634
Fe 1.054535151856 -1.845632696030 0.995720824138
C 0.496097240758 -3.460213055607 -0.151764874303
C 1.778024509621 -3.701109602795 0.421187856292
C 1.628105205181 -3.669129253406 1.847789825375
C 0.260648631722 -3.376903669935 2.146243429340
C -0.439873840245 -3.257055642894 0.910495052941
N 2.626821701857 -4.043008721977 2.823309742756
P 3.529573321791 -2.686143416790 3.231280455272
Cl 4.620602448648 -3.390018530559 4.929019648163
N 1.552984076939 0.208687513227 3.440753466033
Si 0.296370292197 0.460295951086 4.647997267765
C -0.995015256482 -0.919976968952 4.578342309275
Si 2.727668440154 -5.828077741691 3.198490685849
C 2.690286678947 -6.113288244986 5.062653939738
C 1.139525235498 -6.552831551408 2.482969624233
C 4.246574658408 -6.662038905876 2.380251239717
C 1.155795399173 0.449842344513 6.355922841840
C -0.559121915697 2.114244124131 4.323500892904
Cl 5.191463595179 -2.666351863120 1.773277923693
N 5.105211975346 1.304994636355 3.195801878727
C 6.130551303713 0.583717094929 3.968612838482
C 5.672635188754 0.166479176201 5.367439126297
C 5.436827335044 1.339179538992 1.758469145145
C 6.657576597715 2.177795155289 1.338661492312
C 4.819885545952 2.635141033986 3.754186016848
C 3.633318158608 3.334698099883 3.087083473169
H 2.532234822294 0.245412161038 3.709189858936
H 0.278273267389 -3.390826211902 -1.210141238561
H -1.489197739669 -3.016741072653 0.794797472848
H -0.150212162332 -3.281137529198 3.141266231769
H 2.706548770394 -3.871377520088 -0.105005156950
H -0.230318443022 -0.223132065677 -0.865355852793
H 2.451643916754 -0.578427020504 -1.066586937870
H 3.483685444120 -0.394241993230 1.416442144372
H -0.824906396934 0.152190469289 1.726319567662
H 5.711805724585 3.290410391165 3.715569793494
H 4.590011051400 2.505506988050 4.814534785883
H 5.594082859267 0.301073542877 1.444784989421
H 4.554574477361 1.694148107015 1.216214669781
H 7.062440583239 1.174880055757 4.056647049748
H 6.379532378191 -0.320357466148 3.401804045879
H 3.858089912562 3.650517302565 2.062502475754
H 2.761149164693 2.672312711959 3.056221817165
H 3.366603780807 4.233441676386 3.655930310307
H 6.423421867473 -0.490799525059 5.820435521644
H 5.533076860297 1.019797386567 6.039660812451
H 4.732186662074 -0.389775314211 5.318529491587
H 6.814110356275 2.076615332673 0.257714070421
H 6.519495753163 3.243713264229 1.553397549756
H 7.574303053593 1.846738220318 1.839541538002
H 2.295793556015 -7.118670877744 5.259574053190
H 3.673362579594 -6.032217997600 5.532485864085
H 2.026924505989 -5.390990070013 5.552220536778
C 4.069900229673 -8.192213271857 2.543754472006
C 4.304352072371 -6.322121995349 0.875889955474
C 5.579610735469 -6.253072071569 3.040806019801
H 1.102589458742 -7.623999184046 2.715120840589
H 0.256062007948 -6.084818644604 2.930292043658
H 1.061539341042 -6.433173661258 1.397677455693
H -1.393901142523 2.285160845627 5.014862893754
H 0.146542818611 2.947136106817 4.427640325525
H -0.958762680431 2.153479574402 3.302568996929
H -1.879113927461 -0.645008652281 5.167107579052
H -1.325113301168 -1.126903497038 3.555531187742
H -0.595932534837 -1.853949179853 4.990324326111
C 0.093012174920 0.686055295960 7.452241676353
C 1.839861532285 -0.911515578092 6.607236116047
C 2.213282173899 1.569639776259 6.436108902483
H 2.692488134826 1.571272307270 7.426641123579
H 3.007201928167 1.434562439965 5.696275296012

H 1.774728325528 2.563066707936 6.280642477479
H 2.349988630256 -0.907132976577 7.581919037864
H 1.118452241549 -1.737857512471 6.622761984664
H 2.594557886459 -1.146760149364 5.849517318943
H 0.567604312662 0.679830859277 8.444693460812
H -0.409466697816 1.654931952884 7.337719946507
H -0.676800132132 -0.096117074123 7.455114531389
H 5.117754954486 -6.886193494463 0.395348924287
H 3.373674273586 -6.581677769737 0.355461356766
H 4.503705883487 -5.258167236533 0.714151967526
H 6.407248337700 -6.806462893727 2.571859232622
H 5.790116516464 -5.187396144614 2.922899394425
H 5.597521994654 -6.483295371616 4.112639138211
H 4.943067822705 -8.711656476616 2.122416715028
H 3.993622364362 -8.491486828309 3.597533271503
H 3.184361430744 -8.568552073518 2.017834389246

**van der Waals complex of 10c and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -3590.36032438
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3590.36685383
Sum of electronic and zero-point Energies= -3589.755634
Sum of electronic and thermal Energies= -3589.720065
Sum of electronic and thermal Enthalpies= -3589.719121
Sum of electronic and thermal Free Energies= 3589.823125
C 0.103721926059 -0.001231138243 0.052030637228
C 0.070895069037 -0.038401694481 1.485927000042
C 1.423094785791 -0.093132482326 1.957984835888
C 2.283646416460 -0.060973288213 0.819806328607
C 1.468507469460 -0.022188830753 -0.353137747464
Fe 1.055009895574 -1.715114631506 0.754998805244
C 1.831389756849 -3.374459693771 1.719370126332
C 0.408112709541 -3.521005863767 1.730117261978
C -0.029344852756 -3.447493095328 0.364310937625
C 1.120814784235 -3.351762586470 -0.480828450323
C 2.272033117570 -3.299675025096 0.358782335709
N -0.409914726886 -3.713564033270 2.828276433372
C -0.117583739467 -3.092371180927 4.116864817078
C 0.278766078868 -4.074455473393 5.248428576294
C -0.867389159872 -5.071808065333 5.486568657843
N -1.090406991898 0.040975634213 2.324346815837
C -1.126421217402 1.143808205208 3.314763723729
C -1.715758445408 2.511856832656 2.875324146632
C -1.240066022114 2.895731687095 1.464619240666
P -2.229305867763 -1.125908282513 1.915297676180
Cl -3.536636655888 -1.015333833620 3.594359187138
Cl -3.545195219208 -0.191409435567 0.406466061620
C 1.557198869685 -4.842367967980 4.874868041143
C 0.520772849614 -3.249499654739 6.525128993734
C -3.254569671070 2.500021834895 2.924357058669
C -1.197849441508 3.546994406466 3.896165633968
N -3.229759824770 -4.680937966545 2.040185204658
C -2.643252015986 -5.948127934040 1.602948835408
C -4.038840582151 -4.861082034808 3.246069958269
C -4.023155729065 -4.076266743365 0.970318972907
H 1.824513109541 -0.032935381256 -1.375367352170
H 3.364786337529 -0.106064920028 0.844134801956
H 1.729732362588 -0.149096515524 2.994051404048
H -0.763904881461 0.032960415036 -0.592646029302
H 3.299287243406 -3.196373780576 0.032530164086
H 1.111183489961 -3.293046326763 -1.561647197500
H -1.060137247449 -3.473050244382 0.039495922552
H 2.468703402860 -3.341023940847 2.590990286510
H 0.681009430346 -2.352331971167 3.976461309503
H -1.005455199795 -2.534919351836 4.446529105587
H -1.658591270049 0.787348683700 4.200651500036
H -0.082559369462 1.291598337387 3.607097644270
H -1.399072793768 -3.834227399629 2.600208350092
H -3.413579267983 -6.697749893390 1.338148606018
H -2.007461596889 -5.778529878462 0.727654938440
H -2.015129481745 -6.358917513998 2.399726926857
H -4.850832892160 -4.734846756856 0.642805728305
H -4.454771086638 -3.130976202185 1.311168854528
H -3.388288195225 -3.866619162142 0.103391562530
H -4.902975796834 -5.531594553719 3.073113325697
H -3.423909412793 -5.290894421996 4.041987371803
H -4.411792462110 -3.889844764081 3.585085320213
H -0.622920467984 -5.760105136888 6.305250344413
H -1.796360444840 -4.549720948784 5.750720688733
H -1.052481562374 -5.667747629141 4.586095461498
H 0.809589427323 -3.899449916087 7.360398257951
H 1.325889623162 -2.517048988800 6.378560091115
H -0.382554847868 -2.701691790332 6.823927989979
H 1.806594052510 -5.579520579773 5.648533025702
H 1.431033196307 -5.372407744754 3.924421180967
H 2.413720932031 -4.162562786023 4.777908648641
H -1.583788929980 3.907059866066 1.214388922269
H -0.146097610190 2.879403007426 1.388796467990
H -1.641155154627 2.208214302398 0.713979875494
H -3.645755635556 3.491270097688 2.662344763839
H -3.681724552918 1.780254236815 2.223410030276
H -3.615996398235 2.248960979135 3.929212349628
H -1.630785688953 4.534025601232 3.694021043101
H -1.471491685164 3.268200656745 4.922602694319
H -0.105347030033 3.644212494526 3.849920226943

**van der Waals complex of 10c and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -3708.31537763
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3708.31956833
Sum of electronic and zero-point Energies= -3707.624092
Sum of electronic and thermal Energies= -3707.584663
Sum of electronic and thermal Enthalpies= -3707.583718
Sum of electronic and thermal Free Energies=-3707.696273
C 0.996673932277 -0.213831814533 -0.565782528130
C 0.707893049606 -0.019966078226 0.813793578767
C 1.910856604589 -0.290956496287 1.550956548912
C 2.929290914044 -0.672151610163 0.618957617889
C 2.364756582851 -0.610733387337 -0.688682326545
Fe 1.322426462317 -1.966054888239 0.468928309772
C 0.894428242778 -3.536807204910 -0.753962769386
C 1.979091865044 -3.902467201257 0.105416215045
C 1.514516937859 -3.882707866891 1.458026558407
C 0.159865671328 -3.405593398584 1.427530902208
C -0.233676393580 -3.236045486167 0.064259245510
N 2.208341029877 -4.278266753553 2.587182832165
C 3.627662833893 -3.970350091491 2.738349393496
N 2.122278774521 -0.073202273915 2.950390556284
C 2.967346430602 1.080194447225 3.336243248083
P 1.310359984089 -1.214213500948 3.882811785741
Cl -0.801296744661 -0.546783951018 4.019770891527
Cl 1.930133634781 -0.643075837741 5.844316561690

N 0.323710962472 -4.819750488598 5.098178779622
C -1.055669894734 -4.465430209829 4.709858819507
C -2.187192359808 -4.962044075126 5.625356104285
C 0.563839931187 -6.272612078481 5.147370053665
C 0.248799105600 -6.998834424769 3.837889410015
C 0.718376548721 -4.163958998244 6.357254137941
C 2.230929870292 -4.111337328923 6.579138750358
H 0.288547547084 -0.123052151117 -1.379826205609
H 2.871019258126 -0.868519178149 -1.610115598535
H 3.943444718938 -0.948224982339 0.875779537769
H -0.238550933981 0.265602136591 1.251514237295
H 0.938947177443 -3.472674186099 -1.834068586164
H -1.202721395602 -2.895610252881 -0.277564687756
H -0.458040921233 -3.217056937056 2.292637123142
H 2.975565822607 -4.168675882664 -0.215711694780
H 3.924359572260 -3.283153153020 1.935156713432
H 3.768675413613 -3.423635148467 3.681940320687
C 4.578390390040 -5.194873778414 2.740421949629
H 3.289500118415 0.907512853682 4.363918833752
H 3.862212888368 1.023566016882 2.703640329048
C 2.368010335690 2.507627243820 3.236705191626
H 1.654594796837 -4.253683445942 3.446397317332
H 0.001559305285 -6.740457391440 5.978101227560
H 1.623033718784 -6.417157142252 5.375724856202
H -1.100667490315 -3.373003589976 4.645381055623
H -1.225173282483 -4.840353521157 3.695564500332
H 0.244124308171 -4.653129425693 7.228815807004
H 0.334307532949 -3.138693680143 6.326369340035
H 2.451824076731 -3.502349822673 7.462682714534
H 2.665301125906 -5.103074558834 6.741583941689
H 2.733437360823 -3.649837180610 5.723417744145
H -3.151442368285 -4.615628684836 5.234453047457
H -2.223540467930 -6.056356960824 5.677061759512
H -2.085252623575 -4.576452132941 6.645901437102
H 0.614482819596 -8.030858838959 3.895363122228
H -0.826745469237 -7.044535140686 3.634850781169
H 0.740319589678 -6.506695787043 2.991975282338
C 3.361661047325 3.432405735863 3.971843817065
C 2.248480116299 2.978299710837 1.774520430270
C 0.996734505595 2.575682489419 3.925024811814
H 1.919799904565 4.024848920409 1.742079719921
H 3.214428347070 2.913856042740 1.256821137270
H 1.526327603133 2.384517977936 1.209041224270
H 0.638589553693 3.612231035894 3.956053386594
H 0.253171325794 1.978175683911 3.391178232782
H 1.044665581277 2.200181966358 4.953753583714
H 3.031790331912 4.476180495230 3.906009291563
H 3.439241187141 3.171849872438 5.035083452644
H 4.366699394901 3.372964746415 3.532900901789
C 6.009046637784 -4.677223429409 2.973496147482
C 4.184002451059 -6.159888471508 3.870461385020
C 4.505150026377 -5.932696371455 1.393712966092
H 4.875983303711 -7.010346127290 3.914829839250
H 4.202387019652 -5.658177506234 4.845702454356
H 3.175121657247 -6.550668291113 3.705691150891
H 5.139228468893 -6.828134440310 1.407396548827
H 3.477789227763 -6.244610251590 1.176106338699
H 4.853138729948 -5.293837082431 0.571338156020
H 6.728664047742 -5.505160026295 2.969863700122
H 6.310144772079 -3.970198977158 2.188772746559
H 6.094879796971 -4.163896484139 3.940253873922

**van der Waals complex of 10d and $NMe_3$**

E(B3LYP-D3/6-31+G*) = -3275.80892842
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3275.81480746
Sum of electronic and zero-point Energies= -3275.431798
Sum of electronic and thermal Energies= -3275.406282
Sum of electronic and thermal Enthalpies= -3275.405338
Sum of electronic and thermal Free Energies=-3275.487804
C 0.057684239334 0.055834971357 -0.023158596717
C 0.035523109822 0.058218352087 1.408245614391
C 1.396401770875 0.040054770503 1.859403221438
C 2.248446668899 -0.011017742339 0.711826002472
C 1.421607465082 0.008467062726 -0.452222851837
Fe 1.101908890197 1.695470236824 0.665118296236
C 0.072996236251 3.338237861564 0.012492550309
C 0.201145658768 3.364110230299 1.441585708019
C 1.601611320597 3.385293011548 1.755111089858
C 2.327133351465 3.354341845307 0.528548072319
C 1.385572710111 3.342486534619 -0.546749114592
N -0.898050640301 3.413006405422 2.350098284427
C -1.683785560313 4.656476265640 2.300936371086
N -1.100806289668 0.144878525039 2.228985395513
C -1.212952149324 -0.855655789688 3.291095398972
P -0.727492594693 2.453767609683 3.739771014003
Cl -0.247415165403 4.007437324457 5.221142964729
Cl -2.785574844378 2.211257058298 4.297447004104
N -3.698857214888 0.489581630490 0.714938619986
C -3.868567061268 -0.224798460652 -0.547429865872
C -4.691148856312 0.064137432441 1.702867387239
C -3.732432517195 1.938810309779 0.519837717360
H 3.404775901819 3.325466994428 0.431201402263
H 1.624223495064 3.301910298254 -1.601719088569
H 2.023353005618 3.399422942249 2.751931060706
H -0.859817782068 3.302680093546 -0.533957294125
H 1.716390349628 0.079154814528 2.892128055903
H 3.330582630460 -0.025454879581 0.726517228161
H 1.764098117286 0.008281206513 -1.479250608293
H -0.815620850036 0.101300615525 -0.660143727227
H -1.999964047944 4.835455876351 1.268965108217
H -1.088623369880 5.508291061231 2.652394479278
H -2.570606340461 4.559466946401 2.929308870842
H -1.183919455974 -1.889124333912 2.911516344382
H -2.154616795821 -0.692461807359 3.822020552935
H -0.397903228987 -0.730000831106 4.011940093800
H -1.962933912966 0.218742119060 1.673364416364
H -4.706276081933 2.286941062166 0.125159266273
H -2.947811822471 2.228394244932 -0.186631592858
H -3.534192085060 2.439130007147 1.470844883482
H -3.098597153857 0.090644275006 -1.259940864604
H -3.762438591099 -1.302268554983 -0.380885155152
H -4.858215774358 -0.038543882467 -1.007797793804
H -5.726262468592 0.285488732298 1.379175799877
H -4.605379912038 -1.015557369878 1.867897351474
H -4.505158381620 0.576082591106 2.651164488522

**van der Waals complex of 10d and $NEt_3$**

E(B3LYP-D3/6-31+G*) = -3393.72983541
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3393.76192089
Sum of electronic and zero-point Energies= -3393.267373

Sum of electronic and thermal Energies= -3393.239746
Sum of electronic and thermal Enthalpies= -3393.238802
Sum of electronic and thermal Free Energies=-3393.323174
C 0.000000000000 0.000000000000 0.000000000000
N 0.000000000000 0.000000000000 1.430182820712
P 1.500748200111 0.000000000000 2.486769108842
Cl 2.659667083888 0.871551757004 5.196549120686
C -0.510118730632 -1.055456798922 -0.840054760238
C -0.270708702024 -0.699934981777 -2.202178502478
C 0.369314899757 0.574630959810 -2.218033627782
C 0.523159132784 1.017543471084 -0.869877064194
Fe 1.491965024068 -0.778811840616 -1.119926552316
C 3.424447686615 -1.013417607215 -1.836678338427
C 3.432088537361 -0.417864240902 -0.541624188834
C 2.761514318024 -1.313977841188 0.359977093619
C 2.371518822921 -2.476012978321 -0.388932481957
C 2.772095338602 -2.283073568237 -1.744377113930
N 2.529463256131 -1.132728760130 1.752849027436
C 3.617961038860 -1.637429226920 2.627977735044
Cl 2.288269739139 1.918667518415 1.750920275883
C -0.913232037441 -1.017177809176 1.992886207032
N -0.959507352981 2.487763944939 2.862824681141
C -0.576412858171 3.720971240880 2.069382654616
C -1.363737044806 4.976259631085 2.428412558579
C -2.434100121254 2.184318735950 2.835841751470
C -2.982715765683 2.063146024559 1.415787755142
C -0.357724915279 2.538753456722 4.269448794098
C -0.785177497695 1.409309841881 5.192455060575
H 3.821533981068 -0.567685757068 -2.739678816696
H 2.588671989594 -2.966004982092 -2.563886508313
H 1.828154585626 -3.321145177303 0.013940152878
H 3.816213675878 0.557471668563 -0.278114152830
H -0.514527947813 -1.306337962390 -3.064902144021
H 0.707113890558 1.109256683767 -3.096567746532
H 1.018648692221 1.921598687197 -0.552636741141
H -0.952918764911 -1.982730556603 -0.505028044564
H -0.603998146094 -2.045108435244 1.758474736651
H -0.938440837148 -0.921325968343 3.081519641902
H -1.924286490003 -0.861401642672 1.600029111944
H 3.431228631541 -1.330829612793 3.662082536949
H 3.658930229146 -2.730141315272 2.557530291221
H 4.579922228862 -1.215709933611 2.314216772674
H -0.517737981685 1.677130269695 2.367048998487
H -2.944663403096 2.959808676447 3.413072757085
H -2.556504977133 1.238590162534 3.364748551663
H 0.489925462012 3.858478676202 2.247817561261
H -0.697217481113 3.462924209809 1.014942781648
H -0.632897818144 3.511281150903 4.684237190135
H 0.728877328676 2.495159202127 4.141165012913
H -3.015263527191 3.023646887376 0.893982748866
H -2.385469172058 1.368652246729 0.816161448701
H -4.006353346222 1.677782904697 1.465047730008
H -0.125134636206 1.453235031803 6.063851682401
H -1.828922697351 1.484762398295 5.517287714207
H -0.596379457326 0.429361199875 4.746293794733
H -0.943016616553 5.812707257273 1.860600645175
H -2.424325841405 4.903886469261 2.168306580470
H -1.282218512679 5.230426306536 3.489401723387

**TS(1a/10a) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4475.38997447
E(PCM-B3LYP-D3/6-31+G* (ether)) = 4475.40765588
Sum of electronic and zero-point Energies= -4474.854708
Sum of electronic and thermal Energies= -4474.815710
Sum of electronic and thermal Enthalpies= -4474.814766
Sum of electronic and thermal Free Energies=-4474.923496
N 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 0.000000000000 1.425340000000
N 0.130065001418 0.000000000000 2.695879982766
P -1.646609419993 -0.151234878647 3.468141553922
Cl -2.911752515223 -1.227051122752 1.455341007814
C 0.660464432418 -1.289070322369 3.152537154766
C 0.117579134662 -2.556228211878 2.751745469726
C 0.577117783005 -3.552910445085 3.659326975218
C 1.417557220372 -2.955838294404 4.645272910857
C 1.514812947654 -1.564650843562 4.384622719157
Fe 2.200098502244 -2.676611714665 2.744914745523
C 3.610403803214 -2.155579546886 1.286365374805
C 3.008936140835 -3.380321764120 0.858083833504
C 3.164678943401 -4.320196753436 1.923974203629
C 3.944334183615 -3.714244684766 2.960202877608
C 4.224454549230 -2.372721775125 2.576389016124
N 2.424256888338 -3.614412660930 -0.381718169226
Si 1.447259726075 -4.988812059806 -0.916471941829
C 0.892594022404 -4.521022520131 -2.655835337019
Si 1.204195445184 1.512492408884 3.058786250969
C 1.255475149675 2.134099187921 4.826881589659
Cl -2.311622508842 1.813116824991 3.019680997928
Cl -1.100723555833 0.185237156528 5.662211630204
C -1.108579070920 0.813165346646 -0.563252741672
C -0.134103793666 -1.409298688188 -0.442722012288
C 1.294839294459 0.520023531869 -0.483411311906
C 2.976474442757 1.072719853850 2.595644246642
C 0.607645876956 2.954117880051 1.995967531822
C -0.025482811758 -5.226043318270 0.233230351208
C 2.489452445135 / -6.561493137005 -0.951528514437
H 2.548375467788 -2.850874217172 -1.035417004464
H -2.054490056781 0.449587261469 -0.162662952591
H -0.975623743429 1.860975403372 -0.289968329567
H -1.108587860437 0.733641445875 -1.660566966822
H 0.629698328715 -2.009212095061 0.052905805583
H -0.001369328665 -1.474722486328 -1.534666628020
H -1.122915825346 -1.772687867109 -0.171572783965
H 2.095026619192 -0.103686772290 -0.085927916231
H 1.438626460301 1.549496350593 -0.151979343476
H 1.334253406414 0.497131187157 -1.580799304111
H 4.791399134260 -1.646715022559 3.146140171138
H 4.233936320985 -4.184150243272 3.890328632215
H 3.666675472975 -1.249357569032 0.701547564701
H 2.776727912162 -5.329281208806 1.943530141095
H 2.057642275757 -0.834166465663 4.964643068824
H 1.937390758638 -3.471960493610 5.441726890767
H 0.351328334873 -4.608166870495 3.599611444823
H -0.580545959374 -2.701420094177 1.943313488574
H 0.298072587141 2.545529440377 5.150960044476
H 1.568138584535 1.396000978550 5.568572464317
H 1.995148501771 2.948855480665 4.815906675054
H 3.596098905259 1.928526904768 2.896859957040
H 3.333471458084 0.188563409390 3.126184939222
H 3.135996406497 0.913882828663 1.528266852659

H 1.473499248741 3.461115661238 1.549124977672
H -0.080391067673 2.679285757733 1.198909815732
H 0.082944323904 3.676285095041 2.630047958052
H 2.852376241728 -6.840047938273 0.045199642861
H 1.902143526936 -7.406070590354 -1.333786146403
H 3.365810454069 -6.434556600437 -1.599345593619
H -0.556255351148 -6.158177496468 0.001004829078
H 0.295801954084 -5.277074604694 1.279205899255
H -0.744215887104 -4.402540857456 0.150420809867
H 0.303737301266 -5.333128459007 -3.099985665055
H 0.259463899709 -3.625327717071 -2.648433448997
H 1.746813741648 -4.334237460972 -3.319234261506

**TS(1a/10a) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -4593.32949664
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4593.34796001
Sum of electronic and zero-point Energies= -4592.706405
Sum of electronic and thermal Energies= -4592.664237
Sum of electronic and thermal Enthalpies= -4592.663293
Sum of electronic and thermal Free Energies=-4592.778014
C -0.003431624754 -0.003710402619 0.001483852225
C -0.001517964661 -0.002082005366 1.423141836820
C 1.372070825758 -0.003484418641 1.861639789416
C 2.196427140870 0.017264875898 0.687428741677
C 1.346990171256 0.008347895647 -0.452259590421
Fe 0.957996504076 1.684830292895 0.676960365573
C 1.053822143704 3.588789386281 1.553753040250
C 2.040195689265 3.429655013744 0.529043079025
C 1.352155552171 3.148648992356 -0.685653272900
C -0.051840480609 3.127933824818 -0.405417570911
C -0.246658479442 3.448960680916 0.974421131459
N -1.452177317441 3.634827365081 1.642076002005
Si -3.099452998879 3.131813275929 1.223910807029
C -3.492814555099 3.625028285495 -0.555994373792
N 1.774206845122 -0.432162575606 3.211060631574
P 0.814153622783 -2.130797483430 3.175168097190
Cl 1.571323600591 -2.962397968235 4.978052401408
Si 3.627218924165 -0.386644343206 3.533348008980
C 4.214341650029 1.323913014799 2.961377187360
C 3.912127178236 -0.669073006344 5.375259857388
C 4.675063733982 -1.665880966753 2.647774255893
C -3.365570605702 1.279659778297 1.432350976109
C -4.189817319801 4.107215461144 2.414886042194
Cl 2.081542579320 -3.263003152440 1.713462638486
N 0.783877880967 1.309819959350 5.046813259578
C 1.649483014150 2.526670196922 4.871267998246
C 2.814070059991 2.720004838770 5.842450101829
C 0.664705143970 0.944517924757 6.494776496000
C -0.262969750329 -0.219111375518 6.817014863681
C -0.555498532944 1.578378127877 4.416573506168
C -1.466841473653 2.575647942850 5.133580189807
Cl -1.729548845175 -1.621941318792 4.116330940597
H 1.284390132614 0.317418102909 4.155008335180
H -1.324265185001 3.955863211430 2.594998656742
H -1.302780552148 -0.031628793072 6.543144204428
H 0.034017699813 -1.134984063228 6.307525046609
H -0.218009022351 -0.394202723718 7.898917271836
H -1.050336114462 3.587791302741 5.205843347582
H -1.732640848060 2.245850749291 6.142012006370
H -2.400370993533 2.640126944165 4.565906256336
H -5.244583386622 3.846069019138 2.262602725874
H -4.085191956635 5.186962172026 2.251663320292
H -3.955908449290 3.900513485705 3.466267499206
H -3.111081962657 4.625463954946 -0.791745332534
H -3.083195368375 2.920864709794 -1.289567489256
H -4.581468738954 3.638219263583 -0.698557521185
H -4.422052622540 1.027261981895 1.269465743159
H -2.782181168477 0.707337475210 0.702522711912
H 1.669635412972 0.704642907612 6.845948520807
H 0.347278710892 1.841079418428 7.045858939597
H -0.344375763013 1.916534633348 3.399510594323
H -1.064852742729 0.616351033401 4.337714216219
H 2.021204128631 2.478952391811 3.848701611898
H 1.014277722897 3.417240794927 4.939589737976
H 3.111673821670 3.515454304179 0.654081230015
H 1.805278378013 2.949987203691 -1.648459380105
H 1.240690276512 3.855943295679 2.582245536658
H -0.831488194425 2.912595128912 -1.121486033464
H 3.275524323805 0.021074533796 0.658865335228
H 1.675000259594 0.051052926888 -1.482681585891
H -0.884888434612 0.024086070375 -0.625483155185
H -0.870450792098 -0.043422055202 2.062973672330
H 3.399808832838 3.579862793873 5.497096839156
H 2.475575577117 2.942943275531 6.858236609420
H 3.483435770455 1.860468047487 5.886119478366
H 4.770609430664 -0.070524111319 5.706889073264
H 3.058928285089 -0.433864297560 6.012335078561
H 4.152496091748 -1.723087385685 5.542854355101
H 4.451450508121 1.984696818284 3.799910840256
H 5.133036751262 1.194589189262 2.375298946749
H 3.486528046256 1.825294911946 2.318055284397
H 4.486039198211 -2.677219911013 3.013652576415
H 4.569995866467 -1.678394220188 1.560924328103
H 5.714758941649 -1.399931990249 2.892227658189
H -3.091666728469 0.912014040635 2.428412733418

**TS(1b/10b) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4711.27303761
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4711.28972154
Sum of electronic and zero-point Energies= -4710.563832
Sum of electronic and thermal Energies= -4710.518060
Sum of electronic and thermal Enthalpies= -4710.517116
Sum of electronic and thermal Free Energies=-4710.638605
C -0.062662846314 -0.158329193516 -0.142612554820
C 0.057401715214 -0.200632291377 1.280152120735
C 1.443335878227 -0.316375140698 1.618755454048
C 2.197615137482 -0.283152603742 0.411900551044
C 1.269761013540 -0.151486402811 -0.670182525109
Fe 1.138470137822 1.459493337100 0.666514663134
C 0.297936835667 3.349230623016 0.367020442941
C 1.686644995339 3.402054182463 -0.007764352897
C 2.447911437878 2.981284857658 1.137866545072
C 1.544135126310 2.742070504224 2.211716192668
C 0.222384078493 2.964733043203 1.733019085069
N 2.172633892295 4.107062633375 -1.222665473385
Si 4.082412400985 3.951066078265 -1.413045551861
C 4.983240644195 4.853641210056 -2.867633293809
C 4.378331131762 4.624895831682 -4.264182223946
N -1.228937933783 -0.153580389678 -0.898242022998
Si -2.908079953693 0.247834600418 -0.495151316992

C -3.821172178862 -1.320968478707 0.119421187264
C -3.807724766068 -2.390922742305 -0.992573810580
P 1.333107379991 5.822073854095 -0.971838952495
Cl 2.976889005793 6.925130994281 0.064631355313
Cl 1.692073177890 6.634833952201 -2.881494556909
C -3.641272989727 0.840390912483 -2.129100660006
C -2.984881680012 1.615425884054 0.796512544475
C 5.014222947121 4.450978113559 0.164537752063
C 4.290280815930 2.082258218746 -1.643037579648
C -3.121195425057 -1.893517916064 1.370112530320
C -5.283414480274 -0.974678988014 0.474444168194
C 5.191776344060 6.368302060622 -2.646439319589
C 6.393907452271 4.189968400847 -2.858626190625
Cl -1.299230732225 5.412977002858 -1.830306118012
N 0.937258600957 2.985274168604 -3.355177287632
C 0.552912730897 3.929258933260 -4.436326452695
C -0.284045673775 2.338285119029 -2.815855561685
C 1.826861842883 1.944481047971 -3.907451977752
H 1.592884356490 3.611151593648 -2.262030568808
H -1.047915790429 -0.279882255398 -1.886757111132
H -0.110344766665 4.689824524921 -4.025103156878
H 1.446300959534 4.400626045289 -4.846714910999
H 0.037157574376 3.378083454207 -5.235888295133
H -0.014970352208 1.759504590843 -1.937646741687
H -0.731304443802 1.686664635767 -3.581022167024
H -0.996205574059 3.111413334885 -2.527951102263
H 2.113634258181 1.252643747711 -3.117155671992
H 2.721920846376 2.405879420182 -4.322676896068
H 1.314196625443 1.388121508407 -4.704856718005
H 3.274312651348 -0.348369377067 0.325559493644
H 1.842507117976 -0.383346542344 2.622798263333
H 1.518997953808 -0.130958139353 -1.722248774040
H -0.762458521788 -0.173741001180 1.982948216317
H 3.512744614994 2.836547246540 1.198456524281
H 1.820552251033 2.396154979162 3.199446673070
H -0.691791724933 2.829456161878 2.293847292275
H -0.530656589394 3.634196790275 -0.264526221194
H 5.698566610185 5.273210259412 -0.058774839845
H 4.381093315240 4.788490627971 0.982545324372
H 5.613849693572 3.599024278748 0.510435932161
H 5.225050324262 1.773101147097 -1.160467133595
H 3.473098898693 1.533043535302 -1.169298352785
H 4.353635120874 1.783769617467 -2.692899490844
H -4.030546401793 1.897060871584 0.971246909004
H -2.558261671324 1.318268236068 1.759986192644
H -2.458503484180 2.509066792657 0.446935303187
H -4.732578819397 0.926444204182 -2.064543573399
H -3.248190960671 1.828328390427 -2.396470710640
H -3.417443157314 0.148847662579 -2.951426629715
H 7.015906562223 4.677835273046 -3.621873424911
H 6.913506394395 4.308359227747 -1.900498593268
H 6.364173543415 3.121671278412 -3.101092757143
H 5.005827842006 5.113269467077 -5.023330553816
H 4.339743197465 3.561180403887 -4.525299275971
H 3.375833135899 5.047798994177 -4.349926387992
H 5.847990900261 6.756766449630 -3.438912593050
H 4.260128241071 6.930862603164 -2.680046448847
H 5.672121430413 6.588856664037 -1.688603528716
H -3.647680057310 -2.793135194610 1.723083007497
H -2.083716500906 -2.180537084412 1.161502709086
H -3.116364383309 -1.176644687997 2.201887451625
H -5.818155654006 -1.876865220335 0.807272501184
H -5.346141639361 -0.241197983296 1.288065725735
H -5.833714434453 -0.571163216122 -0.385210557450
H -4.308482597500 -3.308010924100 -0.647174778673
H -4.334832234322 -2.052972113234 -1.894034906440
H -2.783814143222 -2.663523783628 -1.278527320681

**TS(1b/10b) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -4829.21671871
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4829.23348406
Sum of electronic and zero-point Energies= -4828.420008
Sum of electronic and thermal Energies= -4828.370665
Sum of electronic and thermal Enthalpies= -4828.369721
Sum of electronic and thermal Free Energies=-4828.497568
C -0.205278131736 -0.175469604629 0.100245804286
C 0.034449222692 -0.162176850477 1.510306788385
C 1.433508254767 0.046333791507 1.692862417959
C 2.049924905948 0.222471386075 0.412789462496
C 1.031367225723 0.092757372102 -0.573102987006
Fe 1.184091455032 -1.650941711708 0.483032712742
C 2.343045350220 -3.161863481525 -0.377522912404
C 2.152024435550 -3.440546499366 1.023935001009
C 0.730395284633 -3.518577427352 1.239358855970
C 0.076529801437 -3.317587618387 -0.001148912572
C 1.069140965532 -3.090203071331 -0.996553206672
N 3.166556708648 -3.997980186825 1.950580775083
Si 4.779954506751 -2.925805630340 2.089531590289
C 6.427224554557 -3.671027568604 2.825167074361
C 6.268764359714 -4.359839001791 4.194375163956
N -0.895991217079 -0.315306233818 2.534643495986
Si -2.643080390097 -0.531335461502 2.452579987961
C -3.072651506758 -2.120172004824 1.528159707473
P 3.207746287781 -5.725565309090 1.073581313106
Cl 4.990444550178 -5.278326459120 -0.515507902028
Cl 1.185831776993 -6.637093981432 2.058912197679
Cl 4.446566718053 -6.828616865957 2.397986446097
C -3.215279065589 -0.623893529404 4.279012516851
C -2.881367949307 0.686029330386 5.025511828686
C -3.435592837165 0.929794093784 1.559408423823
C -2.534317369794 -1.803660663602 5.005461155337
C -4.745948334699 -0.836930127589 4.311521381107
C 5.183474471908 -2.036090069463 0.477654804567
C 4.327028126059 -1.484719135879 3.232583335846
C 7.189365540947 -4.607019268724 1.864825108789
C 7.347322243583 -2.434777664501 3.059843242345
N 1.876896942439 -3.953257258378 4.377485421679
C 0.738582944496 -4.891564021869 4.651526575650
C 0.001279423935 -4.670045494005 5.974451129108
C 1.363087770052 -2.534209448092 4.283703181441
C 1.477336375557 -1.632246223326 5.513936546098
C 2.960293275548 -4.117301941898 5.399456284281
C 3.354041279945 -5.567063854723 5.673028693630
H 2.519236728222 -4.116663238423 3.145237452240
H -0.473897153268 -0.270887294485 3.453218409147
H 2.606456007952 -6.088113607912 6.278787999705
H 3.505167812903 -6.134062876842 4.753267384228
H 4.294633302919 -5.571627978900 6.233669299820
H -0.532024823005 -3.715380475609 6.004712998346
H 0.666487404468 -4.721615887302 6.842974443651

H -0.745740497117 -5.464114571735 6.085553171826
H -2.992664308685 1.069557938647 0.566020951294
H -4.513361722509 0.776626133455 1.421814900912
H -3.291639350916 1.863840332021 2.114916125181
H -4.148372145539 -2.328606262317 1.581087206715
H -2.811956619206 -2.038545626048 0.466805499779
H 3.819600228992 -3.560793936665 5.031131420053
H 2.654957620344 -3.647885649497 6.339099260916
H 0.041914041289 -4.805188975811 3.817820900321
H 1.128160259204 -5.903805840213 4.590806972988
H 1.867863568285 -2.066416615090 3.443870715299
H 0.315553818596 -2.603618581814 3.987828755398
H 3.095721635408 0.432137808469 0.233997458516
H 1.166148131744 0.147222432080 -1.645648601327
H 1.914634535191 0.139429424706 2.656247419883
H -1.154515050531 -0.367663920877 -0.381804994961
H 3.288269488427 -3.080261490737 -0.885057527720
H 0.890850719798 -2.863577388248 -2.039669923479
H -0.993609847984 -3.301915201390 -0.150276895740
H 0.236507293803 -3.753102348955 2.163991818918
H 1.007067023121 -0.670101678389 5.275441913647
H 0.966561756490 -2.035998879555 6.392419954658
H 2.514899873072 -1.417130602122 5.783044645742
H 5.120640001157 -0.738780797602 3.114776182597
H 3.406245317974 -1.011334930734 2.902634358967
H 4.249657811572 -1.711679416537 4.297624672618
H 5.976431584851 -1.314587676963 0.708199000583
H 5.532201223468 -2.695723005974 -0.317157969947
H 4.320298829983 -1.467201360455 0.125791888759
H -2.537536452789 -2.985798134662 1.935067505489
H -2.928641746449 -1.901159003962 6.028033085782
H -2.703770580429 -2.760294378645 4.495961349728
H -1.451341881285 -1.659190533731 5.095576275602
H -5.101533525676 -0.865756388244 5.351903660343
H -5.285055754322 -0.025829056349 3.806145040731
H -5.040841999368 -1.783065942834 3.841343710731
H -3.217670059091 0.622863388272 6.071132286217
H -1.803956500499 0.895377909443 5.043955869220
H -3.377899023783 1.553281866120 4.574417360840
H 7.253051467548 -4.701445022225 4.546210137575
H 5.882892121668 -3.672478374592 4.957338843591
H 5.619151049152 -5.232807261036 4.147605411423
H 8.321272488181 -2.796476130198 3.417825833382
H 7.539633574180 -1.862982122179 2.145799829203
H 6.962953050167 -1.751168792588 3.823973368979
H 8.177065919953 -4.830333002872 2.295595021591
H 6.674620675874 -5.551203181710 1.698369485803
H 7.346089440732 -4.148140223716 0.884012877226

**TS(1c/10c) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4051.13164090
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4051.14725858
Sum of electronic and zero-point Energies= -4050.514573
Sum of electronic and thermal Energies= -4050.478150
Sum of electronic and thermal Enthalpies= -4050.477206
Sum of electronic and thermal Free Energies=-4050.580036
N 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 0.000000000000 1.377180000000
N 0.137751749809 0.000000000000 2.694879309336
P -1.448732128093 0.553838328595 3.634332893361
Cl -2.953619048165 -0.250084431898 1.750829500782
C 0.108618446634 -1.407141908638 3.140428321437
C -0.580575026179 -2.470353463101 2.473354241934
C -0.551839867256 -3.609646671145 3.317678335149
C 0.146716216089 -3.267673334369 4.512069658465
C 0.566412731169 -1.914485313555 4.410903616555
Fe 1.386945069868 -3.013751602527 2.883519937041
C 3.416134177257 -2.635659043284 2.839145863569
C 2.899810589169 -2.687114860119 1.509774053837
C 2.328244061548 -3.979826050401 1.291050017944
C 2.477397013704 -4.724274010988 2.507880325517
C 3.149602289129 -3.892263689769 3.456887438234
N 1.716455205995 -4.367138060910 0.072295750952
C 0.823325078417 -5.525849577847 0.148119131014
C 0.133184734168 -5.863763574690 -1.191865295784
C -0.652582846086 -4.649755177605 -1.719314762034
C 1.541696328207 0.546568352265 2.998796176749
C 2.061701121142 2.023901015537 2.891481711450
C 1.613979118799 2.854261925155 1.678324709439
Cl -0.395148092036 0.974217362435 5.663457605179
Cl -1.617179361329 2.563767245920 2.996280346910
C 1.382237580728 0.037880069546 -0.531498899027
C -0.746279875248 1.215280706058 -0.427666028848
C -0.656727917890 -1.203415762745 -0.579717012567
C 1.784887723872 2.853567150658 4.162159225508
C 3.599188986456 1.834158300505 2.798979608730
C 1.172053535264 -6.309313880605 -2.240222441404
C -0.841341495753 -7.027423755526 -0.925068862233
H 2.427004487726 -4.498903441433 -0.644304736272
H -1.747648797301 1.180023915260 0.000967328198
H -0.230448888145 2.105240547912 -0.073613143380
H -0.804522930126 1.245418277618 -1.524047514313
H -0.089173145827 -2.091919059214 -0.296999672746
H -0.662231542470 -1.122600880791 -1.675336408255
H -1.681135025104 -1.262390248938 -0.213084295772
H 1.844349992762 -0.934765398318 -0.378087163436
H 1.968219416913 0.800683845101 -0.025446315062
H 1.368677479163 0.251863729355 -1.608679411236
H 2.147948882870 -0.077337506378 2.336568896166
H 1.776100952266 0.238244435666 4.016588869716
H 3.891259579706 -1.782966045451 3.306529288540
H 3.371919628888 -4.157133394260 4.482982393687
H 2.951735764466 -1.896851917969 0.778700856686
H 2.107139217268 -5.723294606538 2.693655066677
H 1.111266925946 -1.369205623567 5.164887604372
H 0.368142143740 -3.933411592372 5.336156061972
H -0.972452830909 -4.578073201659 3.081072099588
H -1.085223548033 -2.405338872745 1.528962545798
H 0.057750222415 -5.278907375869 0.893686172769
H 1.347320626655 -6.428524272383 0.511528875089
H 2.356584459590 3.789023885163 4.110072476315
H 0.731619763420 3.108583065352 4.269806789812
H 2.088179875554 2.318030677244 5.066530227433
H 2.000456415046 3.874815039362 1.785348061826
H 2.007409164533 2.473394768918 0.732709322211
H 0.529488910266 2.925600231332 1.614640896188
H 4.095492442909 2.810926957756 2.780785431975
H 3.988550664902 1.280741399856 3.663033157345
H 3.891212203044 1.293165466441 1.889027880163
H 0.673794476001 -6.616906093494 -3.167676629694

H 1.865155859458 -5.500445501169 -2.505178253582
H 1.762283165731 -7.161072824594 -1.878106745048
H -1.223627576108 -4.921210068097 -2.615852199880
H -1.362011392317 -4.283250513953 -0.966886869095
H 0.018314840413 -3.824682131320 -1.977678096991
H -1.339544019690 -7.335690753001 -1.852090691750
H -0.318614289120 -7.903039623093 -0.518917725347
H -1.619813562667 -6.735518407837 -0.208829904769

**TS(1c/10c) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -4169.07347160
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4169.08978541
Sum of electronic and zero-point Energies= -4168.370530
Sum of electronic and thermal Energies= -4168.330006
Sum of electronic and thermal Enthalpies= -4168.329061
Sum of electronic and thermal Free Energies=-4168.440495
N 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 0.000000000000 1.452590000000
N 0.342232728300 0.000000000000 2.733933961347
P -1.058090406629 0.811222721084 3.760945015125
Cl -2.846099740511 0.129625501730 2.188277436734
Cl -0.775485439933 2.770230774073 3.003919778196
Cl 0.031975005480 1.106364423904 5.846761748317
C 0.296089611102 -1.374796383944 3.226005852908
C -0.490340650216 -2.397807100608 2.604605507522
C -0.504059169317 -3.529164076295 3.462003002921
C 0.262316969255 -3.211580947593 4.621800979027
C 0.760356873504 -1.887879682976 4.481626078586
Fe 1.450550461253 -3.095199485292 2.943213019023
C 3.511655813202 -3.167372352442 3.136253790569
C 3.160964722471 -2.848383924862 1.791675463256
C 2.377839678100 -3.930367966886 1.258763131063
C 2.236520902848 -4.903179170711 2.301699122505
C 2.930425922342 -4.429541681686 3.452733887928
N 1.952075671733 -4.027325291431 -0.085437996222
C 0.581549179612 -4.321848862544 -0.480903875504
C 0.289316473944 -5.684502749931 -1.157366271065
C 1.034509101393 -5.771342572040 -2.501322044440
C 1.734877278721 0.606805338199 2.521481225386
C 2.795632720255 1.223882359066 3.496634376289
C 3.194563320940 0.361001364462 4.701997756333
C -1.197504229478 -0.751086680664 -0.515706830509
C -1.376360588176 -0.800789894509 -2.037534174502
C 0.016547738243 1.406921464340 -0.528872694419
C -1.302865793457 2.165902881840 -0.397741850179
C 1.231096383575 -0.789369003279 -0.390812300465
C 2.514487891592 -0.022414803723 -0.711830890561
C 2.460440504101 2.657287907396 3.947141592547
C 4.049512915173 1.326542128581 2.580803375184
C -1.233112226420 -5.734610485744 -1.412818610372
C 0.705267997908 -6.860461964984 -0.263375476967
H 2.686990355199 -3.858659817467 -0.767855980219
H 0.468658227986 -3.874154288422 5.452268544236
H -0.997439424988 -4.470754505479 3.259268327691
H -1.039365377965 -2.286513483319 1.686310427673
H 3.465518532555 -1.965832096250 1.246264889115
H -0.004220933242 -4.231155350311 0.436991044327
H -1.797691670556 -5.693263852293 -0.472706631078
H -1.109407387466 -1.770025403510 -0.134533850268
H -2.075552067234 -0.318048889446 -0.044341030039
H -0.551564388703 -1.295885837803 -2.561082205420
H -2.285243269997 -1.375789344157 -2.248438785756
H -1.509451052378 0.191001747448 -2.479236283453
H 0.317364224125 1.384050273436 -1.583736505093
H 0.797692789260 1.944253619538 0.012704460212
H 1.391258902569 -1.507748605430 0.413794700603
H 0.993199662407 -1.382879394471 -1.274858921672
H 2.231703137893 -0.221514110220 2.018624687968
H 1.546256703860 1.392686690559 1.791038730003
H 4.092669399332 -2.550460221913 3.807451106124
H 2.974931910737 -4.925387960446 4.414312633560
H 1.683397927459 -5.827165120507 2.230604053055
H 1.359300361456 -1.361321196768 5.202086548317
H 0.234746809175 -3.536781916379 -1.168590364309
H 3.308023749349 -0.760359892338 -0.878860004455
H 2.425331536854 0.564198895632 -1.630911040995
H 2.847707027591 0.641966217010 0.084287406543
H -1.113651755149 3.223152534584 -0.615408904192
H -2.058128090159 1.812686517816 -1.105363043469
H -1.723436418311 2.092772227748 0.603577348582
H 4.110216844862 0.766602871354 5.149764255882
H 2.425005273209 0.366408884382 5.472966645385
H 3.397766849717 -0.670403492809 4.401832586383
H 4.867274804738 1.801960492441 3.133107687974
H 4.399469274610 0.339514001307 2.251474723919
H 3.860509083778 1.939701332001 1.690422895256
H 3.322384558366 3.079486151872 4.479262972073
H 2.249259806463 3.301218728254 3.084934283938
H 1.604737695755 2.693251057773 4.617559729155
H 0.526528537414 -7.814171769237 -0.775321794508
H 1.769275405845 -6.803500328485 -0.009181090954
H 0.125972795159 -6.872776556591 0.667899104668
H 0.773804675981 -6.696823891905 -3.029341334812
H 0.774252881608 -4.927722972833 -3.154036512894
H 2.121824366481 -5.766698909817 -2.357663429199
H -1.510810190409 -6.661632279982 -1.928979077464
H -1.560967334143 -4.894683561895 -2.039631895436

**TS(1d/10d) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -3736.60922955
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3736.6253048
Sum of electronic and zero-point Energies= -3736.219751
Sum of electronic and thermal Energies= -3736.193672
Sum of electronic and thermal Enthalpies= -3736.192728
Sum of electronic and thermal Free Energies=-3736.273734
N 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 0.000000000000 1.377560000000
N 0.227854327556 0.000000000000 2.649908738952
P -0.894872197851 1.254015136843 3.565220482686
Cl -0.253852292359 2.987728859106 2.535214089066
Cl -2.713300279482 0.744912112233 1.948030666560
C -0.136744481676 -1.269618584901 3.258920538772
C 0.310337502856 -1.750194241902 4.534986463402
C -0.429935869950 -2.929247990159 4.829103254185
C -1.320375162738 -3.182562940286 3.743243314674
C -1.145230537885 -2.157851941571 2.771751292080
Fe 0.636151071393 -3.182693752012 3.083503192133
C 1.763482077491 -4.845723154568 3.478629598130
C 2.618586501922 -3.742050672701 3.185072688233
C 2.310889646712 -3.290045727315 1.865690317653

C 1.279492376868 -4.126411274405 1.329885476390
C 0.934816456350 -5.084024110188 2.337962899999
N 0.740128510337 -3.984759685597 0.028964325691
C -0.492855123483 -4.719366869163 -0.242931454415
C 1.695936755617 0.262983365650 2.716775717507
Cl 0.582092831277 1.556485062313 5.372825643892
C 1.333035412928 -0.428506939010 -0.481907091327
C -0.286636910088 1.378654488349 -0.468151204300
C -1.024913017546 -0.940459151970 -0.518250985316
H -1.258913800619 1.688541089453 -0.085564607160
H 0.477490285294 2.056902590298 -0.083604935083
H -0.281488587261 1.408284463692 -1.566712066674
H -0.755598135677 -1.952612909299 -0.213536777706
H -1.048992555816 -0.894348121349 -1.616390779757
H -1.997906940231 -0.659679936789 -0.115121335775
H 1.522782421692 -1.444911553740 -0.135377155184
H 2.099561515431 0.252333493058 -0.105364828693
H 1.361124089533 -0.418518233023 -1.580740733321
H 2.189686854300 -0.531834679887 2.158689336147
H 1.898117075016 1.235875374971 2.266044140531
H 2.059856609111 0.268769365667 3.742490498885
H 3.343886765575 -3.299733413877 3.855523163674
H 1.718072068396 -5.384535849200 4.416486953749
H 2.792261599025 -2.475202332798 1.343225976229
H 0.159718947918 -5.834775271360 2.265258936165
H 1.053570603394 -1.283891477960 5.163716330675
H -0.304646710862 -3.548231576652 5.707895481897
H -1.993046378501 -4.025773096810 3.655410432704
H -1.699602618040 -2.037820869785 1.856038239647
H -1.264513932858 -4.382486193454 0.457817822050
H -0.392959446671 -5.812468544098 -0.145253855384
H -0.827613533602 -4.490255586106 -1.259386610280
H 1.447676623711 -4.174193033686 -0.676427791600

**TS(1d/10d) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -3854.55070430
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3854.57117182
Sum of electronic and zero-point Energies= -3854.075874
Sum of electronic and thermal Energies= -3854.045420
Sum of electronic and thermal Enthalpies= -3854.044476
Sum of electronic and thermal Free Energies=-3854.136030
N 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 0.000000000000 1.400000000000
N 0.187887574722 0.000000000000 2.686350752814
P 1.385029117882 1.391126439527 2.918986422672
Cl 1.824930590096 1.077700921849 4.960910597068
C 0.021905691174 -1.447107878986 -0.412363301701
C 1.377979571473 -2.147925325910 -0.342312555287
C -1.307851682255 0.578583024035 -0.455931170196
C -1.459670966628 2.081565605519 -0.228210523322
C 1.177142989448 0.781826201457 -0.495860355024
C 1.303491236086 0.890645894624 -2.019185685785
C -1.092542725987 0.128640850415 3.383256920673
C -1.326171144092 -0.233111977163 4.747890496106
C -2.647710644955 0.170078839550 5.084249997050
C -3.235921804804 0.765510000327 3.934306702357
C -2.292688759060 0.729311304425 2.876925479963
C 0.777259943634 -1.347402773754 3.020346361640
Fe -2.702582631691 -1.173199941057 3.512880189216
C -4.496025602517 -2.057722187603 3.030902623209
C -3.589634887308 -2.193541804156 1.932362251481
C -2.441658682104 -2.897590889892 2.410139609416
C -2.641658288881 -3.210225819336 3.789887857895
C -3.907225275302 -2.685062181043 4.177570162749
N -3.720848965422 -1.691746355635 0.616397550891
C -4.810533635289 -0.768239154225 0.355703836137
Cl 3.481409318957 0.045103974826 2.077311343717
Cl -0.169606207931 3.042825318125 3.233850138380
H -3.747903167721 -2.441460291655 -0.066295650628
H -4.767521987662 -0.464248534989 -0.696344151262
H -1.582348536219 -3.161877278825 1.809041143512
H -5.808785865894 -1.189272482595 0.552801679921
H -4.660694961039 0.113524950268 0.982007984414
H -2.462784243859 1.110184940609 1.888022881715
H -0.618592727191 -0.712177305287 5.408822236428
H -3.126680173111 0.007928301575 6.042780085099
H -4.247400163400 1.149308264334 3.866358627882
H -4.339540595539 -2.722458624581 5.169253914897
H -5.441527011177 -1.538535529571 3.016360211992
H -1.937811714461 -3.730781486810 4.426577467206
H 0.990942282560 -1.407506903776 4.085174162364
H 0.023072177332 -2.083871313889 2.751651321136
H 1.705420944393 -1.485919232191 2.473148199733
H -0.371356038182 -1.527353678788 -1.435544564844
H -0.711338342643 -1.942218341026 0.229551249800
H -1.428894577868 0.361625222979 -1.525976099924
H -2.089625090587 0.016829937931 0.059797335249
H 2.075974916731 0.344039214856 -0.070984071396
H 1.104391409944 1.780137735204 -0.056502107154
H 1.217825964244 -3.227150917889 -0.447839930692
H 2.042214284455 -1.833057977518 -1.150939003005
H 1.901142684299 -1.967894937852 0.597330603648
H -2.512064538848 2.356451214582 -0.366217833089
H -1.159653046526 2.392618734041 0.774482679767
H -0.876083173764 2.663505733952 -0.947260144311
H 2.225595337454 1.434894652664 -2.250137324883
H 1.371209540983 -0.089328640671 -2.502138293390
H 0.472859193001 1.437912775658 -2.476927758012

**TS(10a/2a) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4014.58037701
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4014.5953484
Sum of electronic and zero-point Energies= -4014.052384
Sum of electronic and thermal Energies= -4014.016542
Sum of electronic and thermal Enthalpies= -4014.015598
Sum of electronic and thermal Free Energies=-4014.116884
C 0.000000000000 0.000000000000 0.000000000000
C 0.000000000000 0.000000000000 1.425394000000
C 1.357501862126 0.000000000000 1.865216112906
C 2.219879610186 -0.010886347973 0.706794693527
C 1.354611802366 0.012792609759 -0.445914934801
Fe 1.037748794605 -1.649091159939 0.726735361800
C 0.348624316259 -3.413987698289 1.542501268579
C 0.284978504218 -3.485166111961 0.116388199544
C 1.598731553278 -3.288957162919 -0.400090274744
C 2.490873001477 -3.078176883907 0.706839717024
C 1.704118483279 -3.162449667796 1.908344965459
N 3.900319136421 -2.846261776982 0.669719802806
P 4.650797926951 -1.469818276037 0.009637726874
Cl 3.807582340600 -1.405718494929 -2.016395131041

N 3.656188325110 -0.064912876049 0.700109987278
Si 4.469615522097 0.421794734598 2.249592246586
C 6.339410478405 0.545331594571 2.008612389749
C 3.805070845380 2.124160057681 2.754489427221
C 4.200229596899 -0.827598242350 3.642971227330
Si 4.963409402535 -4.257106769204 1.152891315228
C 4.071017851780 -5.149551729874 2.564572392716
C 5.126759502388 -5.435765096287 -0.292701424266
C 6.581082423659 -3.627796083674 1.875833353169
Cl 6.977365801674 -2.573668676474 -1.413135565252
N 4.704607523104 1.774565492178 -1.349186854112
C 6.000294182466 1.214638108264 -1.876895344078
C 3.717221407989 2.010422947579 -2.448326619535
C 4.930696516636 3.030075414031 -0.572307172299
H -0.608256820201 -3.639889887165 -0.475140777228
H -0.487155028581 -3.504757381313 2.224458731715
H 2.082403135048 -3.019519883017 2.910381586657
H 1.881994860140 -3.257668597324 -1.441126105813
H -0.870805098275 -0.026349771410 2.067683250645
H -0.872520654357 -0.031979562531 -0.639742483899
H 1.674282373658 -0.051335680254 -1.473166367641
H 1.670462425794 -0.042037124404 2.896866725655
H 4.283530439136 1.075861508943 -0.666441583708
H 5.296144441220 3.806064230100 -1.249030656636
H 3.988122032280 3.338098269134 -0.116690070232
H 5.669312827530 2.839552632929 0.205300425688
H 4.128438306933 2.757611438068 -3.131960445234
H 3.546468073841 1.068986505750 -2.966899686281
H 2.783265499282 2.366665151970 -2.009421550726
H 6.481004981457 1.986282529462 -2.483831491516
H 6.636891721691 0.932377660595 -1.039027901389
H 5.800270021490 0.318708250857 -2.463492943150
H 4.720714153873 -5.974411058035 2.888791730278
H 3.906885507339 -4.503935631264 3.435395788545
H 3.108791678884 -5.579986583868 2.268151984058
H 7.228567500081 -4.497781724567 2.054162153572
H 7.125679500550 -2.958603808195 1.203339533615
H 6.411221498138 -3.142432988193 2.846317465009
H 5.723887892960 -6.312336685092 -0.006887350152
H 4.136899331061 -5.792446744760 -0.606848858352
H 5.623044572106 -4.940424546901 -1.134557738674
H 6.752288198088 1.079301921582 2.876355497450
H 6.819648728154 -0.436722153953 1.956220120743
H 6.645940276115 1.093822852801 1.112676981482
H 4.960319721967 -0.667252178526 4.419058891600
H 3.218726891494 -0.756838627589 4.122566282353
H 4.317614578387 -1.848306769176 3.266609022286
H 3.848469200414 2.221955611422 3.846974780621
H 4.409546401203 2.937521013086 2.336325378630
H 2.764093495883 2.278084062048 2.451400637691

**TS(10a/2a) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -4132.52697105
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4132.53837761
Sum of electronic and zero-point Energies= -4131.916422
Sum of electronic and thermal Energies= -4131.876904
Sum of electronic and thermal Enthalpies= -4131.875960
Sum of electronic and thermal Free Energies=-4131.984044
N 0.000000000000 0.000000000000 0.000000000000
H 0.000000000000 0.000000000000 1.185730000000
N 0.141871429481 0.000000000000 2.654855732910
P -1.780147495621 -0.766404942115 3.085475642634
Cl -3.923709575927 -2.085537465610 2.691463204461
N -1.966478744724 -0.290858873142 4.715474804418
Si -2.854119284915 -1.379655246184 5.896586365918
C -4.676530835180 -0.930953616350 5.902453492159
Cl -2.740883575111 0.851394461296 1.978992349058
C 0.561870484495 1.329875243161 3.015669615828
C -0.005997867956 2.571950919473 2.538862311376
C 0.673618271364 3.679233736609 3.134322382984
C 1.681778377300 3.165215877951 3.997982353063
C 1.622809301661 1.741926120115 3.934878078583
Fe -0.170493371257 2.492675650415 4.596164438282
C -1.560164652057 1.234498247169 5.382437516417
C -0.533554745703 1.543669807821 6.342919682038
C -0.540606252491 2.952478827663 6.560836612639
C -1.558229037281 3.520672943175 5.733288474464
C -2.197012540644 2.468111941467 5.014189522355
Si 1.211209056234 -1.318092386566 3.315267438099
C 3.021704793520 -1.105402205568 2.781536341186
C 1.359013353474 -0.513408834602 -0.380592962806
C 2.491268517289 0.476759049278 -0.110864220854
C -1.092634532630 -0.881592825655 -0.569093004310
C -1.099114666405 -2.333628390717 -0.118396608215
C -0.223301103986 1.416377309480 -0.473591005446
C -0.144570752866 1.639025095167 -1.985048925588
C 1.215223549703 -1.450639525026 5.204217791758
C 0.714596297526 -3.038556154351 2.713426386265
C -2.525927338551 -3.190486697106 5.497488114477
C -2.123013017577 -1.109016106185 7.621987041916
H -1.791192774051 4.574213417166 5.644578980282
H 0.133244670438 3.491238843497 7.214693342689
H 0.130490795690 0.827229677097 6.800541983916
H -2.983380994897 2.576349805365 4.283125635460
H 2.355064114924 3.743025432973 4.618134584100
H 0.430006305523 4.722887168515 2.981821488529
H -0.868023869434 2.652969898611 1.900760066828
H 2.250400124028 1.090531150878 4.521597917009
H 1.335557300236 -0.800105644624 -1.437921435092
H 1.513585045737 -1.425708911454 0.197969875859
H -1.209122850107 1.697200283015 -0.103081771433
H 0.503342802197 2.040561917129 0.043864352556
H -0.989524459629 -0.840176055208 -1.657919135355
H -2.037250613666 -0.410312781389 -0.295461608186
H 2.494961297299 1.302214798414 -0.828356701805
H 2.429096049190 0.896452219440 0.896392780280
H 3.450194823348 -0.042750276494 -0.200500016427
H -1.943005691392 -2.828378370293 -0.610294338810
H -0.187534338201 -2.866888727945 -0.408092654447
H -1.261061524060 -2.434637200021 0.954618291108
H -0.215496014254 2.716116612875 -2.173100449451
H 0.798795330048 1.292406742776 -2.418968962991
H -0.967660295812 1.161673378006 -2.524295624733
H -2.882944548082 -3.795048786512 6.342590001354
H -3.036748648730 -3.521929398414 4.591680940174
H -1.451344106264 -3.385371986582 5.389573378425
H -5.191368628947 -1.443697549373 6.726179053171
H -4.790098217539 0.149772314482 6.058472230150
H -5.155574217181 -1.200421914840 4.957932388730
H -2.672389158486 -1.780482192275 8.296841883169

H -1.062491385626 -1.376366393742 7.689876471058
H -2.248124657910 -0.087735116289 7.994628310003
H 3.635581392228 -1.697796664011 3.473490697583
H 3.206038234879 -1.497885295614 1.775912770074
H 3.386805514661 -0.075349051707 2.817359828010
H 1.737957695095 -2.379330552613 5.469978682874
H 1.731403670802 -0.627496547513 5.706012126321
H 0.204078108851 -1.505904599836 5.609670586534
H 1.399607976951 -3.736602490619 3.214787610108
H -0.305233960342 -3.329679257164 2.982376585001
H 0.839852770361 -3.190112530301 1.637935355590

**TS(10b/2b) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4250.46073527
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4250.48735718
Sum of electronic and zero-point Energies= -4249.762925
Sum of electronic and thermal Energies= -4249.720392
Sum of electronic and thermal Enthalpies= -4249.719448
Sum of electronic and thermal Free Energies=-4249.831791
C 0.000000000000 0.000000000000 0.000000000000
C 0.000000000000 0.000000000000 1.427417926481
C 1.361420569774 0.000000000000 1.867118770991
C 2.205388895981 -0.022836100470 0.717283816238
C 1.366152083565 -0.033956485673 -0.446735924573
Fe 0.955251866389 -1.664016640536 0.694634473519
C 2.148025187521 -3.321951097664 0.467443273633
C 1.339209273625 -3.472538601622 1.632815802359
C -0.031224455635 -3.387962726537 1.238234495432
C -0.070609359573 -3.172718208159 -0.173245270444
C 1.284507400629 -3.125704227394 -0.666275388982
N 1.663444874505 -2.883843835992 -2.023200753004
Si 0.824917179511 -3.871270802392 -3.284005927489
C -0.968781132883 -3.297971065636 -3.495723742692
N 1.780252464309 -0.127242305861 -1.807125129591
Si 1.690675614628 1.339695480494 -2.868175307418
C 1.419361909944 0.735944713238 -4.635630585669
P 2.504819493977 -1.478800541893 -2.574649122813
Cl 4.371819510737 -1.801462191845 -1.303631461252
C 1.605578220474 -3.686268320783 -4.975446015589
C 0.932473605293 -5.715465703784 -2.719841427117
C 0.190718690486 2.338899456529 -2.306279958121
C 3.273497098591 2.412296207144 -2.756746637530
Cl 4.340744965079 -1.754298975241 -4.857002399649
N 5.735717786141 -4.084765129653 -3.363745432119
C 5.598264542165 -4.717894287030 -4.719615632655
C 6.796412692384 -3.015013061941 -3.377143824126
C 5.964648530367 -5.069397722401 -2.264639767778
H 1.697871811401 -0.017856022260 2.896057470864
H -0.874984058945 -0.002327389684 2.064688717428
H -0.864939794320 -0.032800471932 -0.649212339101
H 3.284262707173 -0.082875339938 0.706371721471
H -0.891010973398 -3.439509469135 1.893849226622
H 1.705228907539 -3.603762646796 2.643215944198
H 3.225351230041 -3.300232301052 0.437560648972
H -0.961047308682 -3.022124448273 -0.765051895789
H 4.817308683925 -3.629354045535 -3.236474689869
H 6.542267265179 -5.201665668026 -4.979699644829
H 4.789671373975 -5.451776484456 -4.680253110046
H 5.342052883769 -3.914607312274 -5.416984823675
H 6.956466004047 -5.507821948811 -2.393984218702
H 5.900669727691 -4.532956526830 -1.316283101235
H 5.200619306410 -5.846617043639 -2.303196202252
H 7.719636334240 -3.478620275097 -3.734777126079
H 6.445448527331 -2.215574718002 -4.033626612648
H 6.915458383533 -2.635449035666 -2.363823497803
H 0.153001553900 3.275847610300 -2.877071367734
H -0.741485357980 1.794207701961 -2.498846345231
H 0.223295344058 2.592932470947 -1.242105720402
H 1.018260932133 1.555890513724 -5.245593566295
H 2.342804488103 0.370614670640 -5.100379591101
H 0.694233003090 -0.086417775573 -4.662907496592
C 3.352053067758 3.310791560677 -4.010483022987
C 3.224263115015 3.305307320610 -1.498726185424
C 4.535700729549 1.528783749248 -2.698057704450
H 1.046554340255 -4.329444889900 -5.667123735013
H 1.548319590888 -2.659918244718 -5.346583731952
H 2.663467934037 -3.948801747382 -5.026598259650
H -1.403674220242 -3.758435434667 -4.392838594121
H -1.624456859687 -3.541067060216 -2.653941249355
H -0.991850671641 -2.210187282571 -3.642274361151
C -0.162203636084 -6.156369044371 -1.732130377534
C 0.822360330153 -6.603655504334 -3.986868970022
C 2.326444616865 -5.955027232540 -2.106935537613
H 5.433356872554 2.162161107637 -2.771374752699
H 4.593705257202 0.980031129544 -1.754298780026
H 4.583471068144 0.794145866017 -3.511617544269
H 4.208286332259 3.996566046662 -3.925434354404
H 3.491494048598 2.719724741453 -4.922342354732
H 2.453211210826 3.930069453170 -4.139201601498
H 4.158662029437 3.879054397826 -1.407656820309
H 2.397159425793 4.025076606401 -1.536652577869
H 3.111336264677 2.711593654834 -0.581877989587
H 0.862906245603 -7.665847034986 -3.703624522561
H -0.122088226461 -6.445628653477 -4.523496354277
H 1.642315021143 -6.418815518448 -4.695184957341
H 2.518324346816 -7.031983404299 -1.986200007112
H 3.106835566107 -5.550242672856 -2.765254607475
H 2.435102281329 -5.472133153284 -1.130828116636
H -0.050297533830 -7.227154775230 -1.502622672670
H -0.109008412657 -5.608396655594 -0.788157704904
H -1.164548441284 -6.014866480154 -2.154514683363

**TS(10b/2b) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -4368.40435998
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4368.41817834
Sum of electronic and zero-point Energies= -4367.617625
Sum of electronic and thermal Energies= -4367.570665
Sum of electronic and thermal Enthalpies= -4367.569721
Sum of electronic and thermal Free Energies=-4367.693715
C -0.009880666385 0.004842745186 0.003075182565
C -0.007532617889 0.000210441595 1.431884125956
C 1.354188584224 -0.002600423164 1.918000780492
C 2.177133514273 0.050264570999 0.729314853885
C 1.347177598910 0.029882282205 -0.432867262261
Fe 0.946618717481 1.675868405109 0.717532066403
C 1.190257993958 3.291588313132 1.962077530072
C 2.200247477320 3.250956422652 0.940970331220
C 1.555173382633 3.331218422119 -0.330158939101
C 0.145962435680 3.402839026787 -0.103307027954
C -0.082667679299 3.380691563110 1.302867632462

N 1.454244277053 3.380062353405 3.380187417421
Si 1.867537823280 5.072514693530 4.010145868593
C 3.251960092500 4.812588310260 5.266713332626
N 1.743781242284 -0.004155036268 3.263142103823
Si 3.466248299745 -0.055100438886 3.672553486515
C 4.443329300311 1.423338652173 2.974617670483
C 3.690254765826 0.100440420217 5.551046347729
C 4.471293097630 -1.680602729455 3.205901056511
C 5.977539587097 -1.323077953558 3.173528245174
P 1.077412460697 2.124667746447 4.465250666181
Cl -1.069021644134 1.809417962613 4.051735045160
C 4.290632852955 -2.764218763681 4.293327971875
C 4.110867170981 -2.306575564792 1.842758429341
C 2.550349225133 6.323050999332 2.695478950430
C 2.691172405157 7.656146953418 3.485968367249
C 0.265388028373 5.820706326129 4.678057845878
C 3.952430774513 5.962380823916 2.161753442095
C 1.595079642804 6.590917045259 1.513463119210
Cl 0.533575140881 3.192710923207 6.646228647070
N -0.257682881105 -1.520892360031 4.798029136635
C -1.500440978177 -1.694571453208 3.950668051994
C -2.501849279967 -2.720022731271 4.475170928282
C 0.533677283320 -2.797228694569 4.934405980152
C 0.765405867594 -3.503525879399 3.603339522387
C -0.628995512402 -0.944203990476 6.151716686316
C 0.544795919491 -0.564167566216 7.039764968289
H 0.406927953028 -0.847067382113 4.275209307732
H -0.621237008815 3.436076920456 -0.866440666117
H 2.047916947045 3.299688644615 -1.293552033566
H 3.259629901707 3.146379267844 1.113031202550
H -1.041476651207 3.404367165181 1.798029768986
H 1.691581914265 0.067302631442 -1.458918825187
H -0.887420858845 0.021191550507 -0.631261475299
H -0.887687342275 0.078524816707 2.046699885663
H 3.252702323293 0.130355979871 0.712771807023
H 0.008611491069 -3.438053360252 5.649292765213
H 1.486063229932 -2.506688823453 5.378280052074
H -1.955328340269 -0.705998326051 3.889304652922
H -1.158154168215 -1.959108295880 2.951253048289
H -1.254914887653 -1.694454386314 6.641911412257
H -1.234639857540 -0.060969349446 5.945418481648
H -0.147459664940 -3.952599050304 3.202218887256
H 1.173581644633 -2.809034904125 2.864389425286
H 1.490280112958 -4.309573692383 3.750361261254
H 0.139254049353 -0.122762903979 7.955613059279
H 1.161514329570 -1.422544761641 7.323931708131
H 1.169886455393 0.198598023187 6.578067078918
H -3.316974825835 -2.795367072190 3.747445592481
H -2.068145351409 -3.719055147737 4.584815523027
H -2.945935591474 -2.426457118674 5.430668248698
H 3.607350875306 5.774854823277 5.653442094131
H 2.925851126595 4.213645463823 6.119106326479
H 4.102279463215 4.308641996385 4.791137896357
H 0.437894151214 6.295606143995 5.650769334857
H -0.134652945523 6.575191524045 3.991059627895
H -0.494572216079 5.051551352866 4.830822681006
H 5.411715120784 1.496131561176 3.484452085901
H 4.642393069605 1.361499021433 1.899502675487
H 3.899898644495 2.353862798133 3.160828976650
H 4.765817799261 0.043194887975 5.763816071545
H 3.336241209390 1.058153556138 5.946824497380
H 3.209891664806 -0.698108933833 6.123768935849
H 4.881656974715 -3.657288393488 4.037833165117
H 4.628811235047 -2.426159722908 5.278810256341
H 3.251496278151 -3.087884175506 4.386834972622
H 4.649740235983 -3.258261909702 1.712814397175
H 3.040827231553 -2.511903521957 1.738989694580
H 4.398957676805 -1.662426633661 1.006133555384
H 6.574549015114 -2.231394129548 2.997630098561
H 6.216967773752 -0.614976898396 2.372588397507
H 6.323947449057 -0.887191089819 4.119336062839
H 4.330750866988 6.778784937758 1.527729006775
H 4.676913359893 5.819158854938 2.972399721605
H 3.946054348812 5.058347397296 1.550088306509
H 1.973649852621 7.436825382087 0.919300533172
H 1.505724633612 5.734004440647 0.845228382100
H 0.586955862999 6.858959651194 1.851371241106
H 3.078930542900 8.432363540855 2.810206130071
H 1.733921009396 8.018476337368 3.877035652391
H 3.394080295419 7.581179244062 4.323620671907

**TS(10c/2c) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -3590.30854017
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3590.3280207
Sum of electronic and zero-point Energies= -3589.704553
Sum of electronic and thermal Energies= -3589.670541
Sum of electronic and thermal Enthalpies= -3589.669596
Sum of electronic and thermal Free Energies=-3589.767112
C 4.078537008826 1.454985857570 -0.747222936439
C 2.724328522099 1.505916469463 -1.181218625687
C 1.873913204724 1.470047833798 -0.025619791815
C 2.729710942166 1.407875638044 1.128955265511
C 4.085582107435 1.397562346098 0.679900155909
Fe 3.046736013126 -0.217172792581 -0.067603438488
C 3.760863762431 -1.950407203326 0.803617589440
C 2.430199968671 -1.669384579167 1.228517668258
C 1.586058072548 -1.619895982397 0.062521085580
C 2.407553460703 -1.909025921677 -1.077040861868
C 3.744052833917 -2.097364247254 -0.619154287469
N 0.208508587736 -1.305545086760 0.071480558413
C -0.609065623040 -1.943970438760 1.118425014871
C -0.996624742290 -3.418134645480 0.856338979117
C 0.145340763179 -4.385876934001 1.222237775432
N 0.448132618824 1.491882953373 -0.042120534743
C -0.251031584611 2.252890820958 1.042685606577
C -0.590991393861 3.715983809925 0.646413175278
C -1.802353127817 3.692717622837 -0.317523512374
P -0.502684006099 0.158475880186 -0.580284334928
Cl 0.110861626071 0.018939575724 -2.679225873906
C -2.214240541500 -3.713976192440 1.756237613406
C -1.394921608131 -3.580574291642 -0.616510844346
C -1.011737889025 4.430747733462 1.946927006450
C 0.607013373926 4.428387323610 0.005769563287
Cl -3.484787028163 0.688649451876 1.597832798208
C -3.544439819230 -0.868992639856 -2.020703603283
N -4.192515464696 -0.268919938595 -0.813650241986
C -4.494143238525 1.179856408220 -1.041242998261
C -5.419753353474 -0.998487232030 -0.354413904322
H 4.943392408043 1.448798991214 -1.398104746511
H 4.970107278211 1.331005981585 1.300263051882

H 2.404818441943 1.336841879506 2.157995700078
H 2.381516886898 1.532065326897 -2.204728398079
H 4.638752833525 -2.017384329997 1.432957062924
H 4.602236917081 -2.305330078288 -1.245470150640
H 2.071211564066 -1.929686390021 -2.102941415824
H 2.110571788646 -1.473442447856 2.244274041475
H -0.112576723052 -1.841184732526 2.093567695658
H -1.530729966429 -1.362133774831 1.213037724785
H -1.198584312837 1.740241593765 1.269317874323
H 0.354481626985 2.209951453512 1.953004178294
H -3.547757728496 -0.270683918342 0.047655887853
H -4.075487444265 -0.505452105521 -2.907648603810
H -2.502676649064 -0.562124691130 -2.079316229657
H -3.646776802831 -1.957459694942 -2.021170556106
H -5.229280303025 1.266683504705 -1.844874817285
H -4.868154079509 1.598271299367 -0.106015680663
H -3.567398501088 1.686794028528 -1.316398047043
H -6.289796316746 -0.633829134640 -0.905866962533
H -5.285699853695 -2.066896994314 -0.526352108700
H -5.518844753301 -0.804513483042 0.717017981484
H -0.516522662194 -3.569289327669 -1.269829168591
H -2.019460520653 -4.452068483810 -0.854217711483
H -2.006974024866 -2.715855206409 -0.902022602114
H -2.453258475770 -4.784988319316 1.749349680437
H -2.020766184631 -3.415114140937 2.794143766052
H -3.097164024495 -3.155804003239 1.421761678926
H -0.138921137988 -5.421985641175 0.997514361882
H 1.059659407942 -4.157381973497 0.663535769604
H 0.383586846463 -4.322321589412 2.291724739160
H 0.372971334221 5.487591930643 -0.164915927915
H 1.494935795237 4.374197007440 0.648167084223
H 0.865455505015 3.979370874618 -0.957688491530
H -2.291384396390 4.672393778229 -0.370540395826
H -1.489940939045 3.400125980783 -1.328162289233
H -2.520586070324 2.945725638016 0.030950465536
H -1.309585511944 5.466270436503 1.739298440358
H -1.860512707952 3.921065524413 2.419757874170
H -0.184989745693 4.460661334455 2.669266684618

**TS(10c/2c) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -3708.26037966
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3708.27445758
Sum of electronic and zero-point Energies= -3707.570547
Sum of electronic and thermal Energies= -3707.532671
Sum of electronic and thermal Enthalpies= -3707.531727
Sum of electronic and thermal Free Energies=-3707.637164
Fe 0.000000000000 0.000000000000 0.000000000000
C 0.000000000000 0.000000000000 2.068816000000
H 0.880775070770 0.000000000000 2.698320055884
C -0.652833708959 -1.161482791076 1.554952739849
H -0.330938497476 -2.179876666999 1.703389815233
C -0.683266221744 1.149852915334 1.574815548635
H -0.422516919498 2.182997585191 1.765688471094
C 0.005797543933 0.591469532192 -1.946519446039
H -0.763720335139 1.205608199599 -2.396533324914
C 1.198996639657 1.053155993603 -1.316623698384
H 1.499836896695 2.087119762178 -1.206775598446
C 1.902312919744 -0.087569442794 -0.819197034495
H 2.833086824143 -0.070125276383 -0.266564953208
C 1.158406592715 -1.257340934209 -1.154311326811
H 1.408564794849 -2.275477955121 -0.896429512573
C -0.034248642823 -0.844086921478 -1.837182003080
N -1.076271650396 -1.644850414606 -2.377717348697
C -1.153479686560 -1.583535885852 -3.856465242247
H -2.080799363432 -2.035853147138 -4.207757682984
H -1.130620822458 -0.531561944608 -4.158756998553
H -0.317498524826 -2.123750427759 -4.311427910230
P -2.028109034785 -2.830526913346 -1.603007248220
Cl -0.710845766064 -3.918805122950 -0.256369357463
Cl -1.658644190457 -4.650846333010 -3.346606272349
C -1.752436241010 -0.741892516344 0.724084596612
C -1.765265956453 0.701215912441 0.755799912909
H -2.442063799605 1.346013272219 0.213089583595
C -3.722763119017 -0.823440101667 -0.633749988585
H -4.398142228180 -1.511620955780 -1.150494815658
C -4.488766609565 -0.090369186411 0.355363597245
H -3.347081077236 -0.107404822542 -1.377758516176
N -2.634839773741 -1.588033455087 -0.004531996452
H -2.753761307829 -2.599938292593 1.063346362802
N -2.908424478090 -3.351675261880 1.967186207947
C -1.606343834762 -3.356818557519 2.721347914648
H -1.348749651452 -2.312733704226 2.904845135540
H -0.862790848030 -3.746566232300 2.023140814981
C -1.601174559829 -4.151280852071 4.026202614603
H -2.339693521305 -3.780455079210 4.744855643971
H -1.777567421621 -5.219487770807 3.869056436164
H -0.613447744791 -4.048702332242 4.488681024398
C -3.211716722796 -4.719686464459 1.415041987801
C -4.474897008841 -4.806170292855 0.563639930605
H -4.516492939310 -5.806803656198 0.121530772348
H -5.390130712108 -4.661527272557 1.146503776905
H -4.453485753923 -4.095668242572 -0.265844431398
H -3.283386066849 -5.414739731774 2.258456462270
H -2.342337572875 -4.997461752966 0.813979316212
C -4.051867863646 -2.786831190744 2.755105108096
H -4.353048941224 -3.520900318958 3.511825865330
H -4.881429071521 -2.679624557000 2.053583253058
C -3.746442789181 -1.431211915074 3.390359682168
H -4.679446275497 -1.003970991723 3.773036425062
H -3.050892125412 -1.510286440656 4.231140769348
H -3.324349603143 -0.730758097218 2.663083488541
C -5.591809139061 0.590206025452 -0.294724519182
C -5.006931700024 -1.013168185007 1.346548215377
C -3.633562480158 0.884925515577 1.003380681372
H -5.582226735339 -0.462606649343 2.089406625700
H -5.649219491006 -1.745648137052 0.859865039781
H -4.178508724423 -1.524303637227 1.834786807645
H -6.167104174376 1.140767561117 0.448133891142
H -5.202649288365 1.283259894053 -1.039138346178
H -6.234096930043 -0.142273926593 -0.781407694777
H -4.208857515473 1.435487051242 1.746239091695
H -2.805139504557 0.373790063357 1.491619273640
H -3.244402629462 1.577979384178 0.258966854375

**TS(10d/2d) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -3275.76935136
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3275.80190463
Sum of electronic and zero-point Energies= -3275.390038
Sum of electronic and thermal Energies= -3275.366366
Sum of electronic and thermal Enthalpies= -3275.365422

Sum of electronic and thermal Free Energies=-3275.441539
C 0.001692973654 -0.031958928622 0.027001453272
C -0.005801962544 -0.059706071730 1.464581243603
C 1.347194862311 -0.102681294411 1.913732964496
C 2.195035241850 -0.088043259599 0.762204159557
C 1.372871736564 -0.027494260738 -0.401078363417
Fe 0.906819202199 -1.711495384281 0.686306117376
C -0.297590279651 -3.084396774295 -0.188711651104
C 1.051143481944 -3.258666925466 -0.657538314456
C 1.886815855461 -3.524420745315 0.469366126730
C 1.070338968444 -3.540778243296 1.638726339020
C -0.276162564253 -3.278736108715 1.240121854184
N -1.441533845612 -2.749954821099 -0.980012045430
C -2.704719370116 -2.969658303973 -0.244708487151
N -1.171992038949 0.028250003674 -0.776216394981
C -1.788132997067 1.377397815663 -0.812736184809
P -1.707266456357 -1.106885580939 -1.918016965315
Cl 0.052295784873 -1.441398459261 -3.206618876261
Cl -2.657686704581 0.578232946991 -3.984665015386
N -1.823892009692 -4.316095796401 -3.265933583633
C -2.622407895118 -3.501685570519 -4.243037713980
C -0.548243853547 -4.808381179409 -3.865718992388
C -2.626589955781 -5.441209600005 -2.705931119986
H 3.276429069485 -0.138547710861 0.768555127136
H 1.673036782755 -0.165892033767 2.943986903358
H -0.895056422966 -0.085976831563 2.081310586328
H 1.703623053009 -0.039137797342 -1.429208123744
H 1.407664426502 -3.700009300750 2.654786590299
H 2.960122821005 -3.660580780443 0.437408356877
H 1.384395762135 -3.122446817171 -1.674480151641
H -1.120494031636 -3.194857849936 1.909873330193
H -2.814713633989 -2.301171555669 0.620468272963
H -3.550688653192 -2.780490657000 -0.913750703008
H -2.754696316555 -4.005837692528 0.110128122800
H -2.676945237597 1.363864842581 -1.444082161112
H -2.049908703237 1.668409250608 0.210884138013
H -1.084738815269 2.103794498116 -1.233938030134
H -1.576204781419 -3.685787358024 -2.417306043087
H -2.881713294623 -6.140957837559 -3.506322344682
H -2.037228291074 -5.947728581895 -1.938530301581
H -3.537934187385 -5.038630759194 -2.261391214614
H -0.779909830099 -5.495098200595 -4.684912134858
H 0.014320947442 -3.950000322291 -4.230346658570
H 0.027036118097 -5.321225161841 -3.091945344320
H -2.916633343875 -4.146517562068 -5.076040082518
H -3.504264612338 -3.105332935273 -3.737782071079
H -2.023309360228 -2.660996373183 -4.594852473760

**TS(10d/2d) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -3393.72983541
E(PCM-B3LYP-D3/6-31+G* (ether)) = -3393.75090734
Sum of electronic and zero-point Energies= -3393.267373
Sum of electronic and thermal Energies= -3393.239746
Sum of electronic and thermal Enthalpies= -3393.238802
Sum of electronic and thermal Free Energies=-3393.323174
C 0.000000000000 0.000000000000 0.000000000000
N 0.000000000000 0.000000000000 1.430182820712
P 1.500748200111 0.000000000000 2.486769108842
Cl 2.659667083888 0.871551757004 5.196549120686
C -0.510118730632 -1.055456798922 -0.840054760238
C -0.270708702024 -0.699934981777 -2.202178502478
C 0.369314899757 0.574630959810 -2.218033627782
C 0.523159132784 1.017543471084 -0.869877064194
Fe 1.491965024068 -0.778811840616 -1.119926552316
C 3.424447686615 -1.013417607215 -1.836678338427
C 3.432088537361 -0.417864240902 -0.541624188834
C 2.761514318024 -1.313977841188 0.359977093619
C 2.371518822921 -2.476012978321 -0.388932481957
C 2.772095338602 -2.283073568237 -1.744377113930
N 2.529463256131 -1.132728760130 1.752849027436
C 3.617961038860 -1.637429226920 2.627977735044
Cl 2.288269739139 1.918667518415 1.750920275883
C -0.913232037441 -1.017177809176 1.992886207032
N -0.959507352981 2.487763944939 2.862824681141
C -0.576412858171 3.720971240880 2.069382654616
C -1.363737044806 4.976259631085 2.428412558579
C -2.434100121254 2.184318735950 2.835841751470
C -2.982715765683 2.063146024559 1.415787755142
C -0.357724915279 2.538753456722 4.269448794098
C -0.785177497695 1.409309841881 5.192455060575
H 3.821533981068 -0.567685757068 -2.739678816696
H 2.588671989594 -2.966004982092 -2.563886508313
H 1.828154585626 -3.321145177303 0.013940152878
H 3.816213675878 0.557471668563 -0.278114152830
H -0.514527947813 -1.306337962390 -3.064902144021
H 0.707113890558 1.109256683767 -3.096567746532
H 1.018648692221 1.921598687197 -0.552636741141
H -0.952918764911 -1.982730556603 -0.505028044564
H -0.603998146094 -2.045108435244 1.758474736651
H -0.938440837148 -0.921325968343 3.081519641902
H -1.924286490003 -0.861401642672 1.600029111944
H 3.431228631541 -1.330829612793 3.662082536949
H 3.658930229146 -2.730141315272 2.557530291221
H 4.579922228862 -1.215709933611 2.314216772674
H -0.517737981685 1.677130269695 2.367048998487
H -2.944663403096 2.959808676447 3.413072757085
H -2.556504977133 1.238590162534 3.364748551663
H 0.489925462012 3.858478676202 2.247817561261
H -0.697217481113 3.462924209809 1.014942781648
H -0.632897818144 3.511281150903 4.684237190135
H 0.728877328676 2.495159202127 4.141165012913
H -3.015263527191 3.023646887376 0.893982748866
H -2.385469172058 1.368652246729 0.816161448701
H -4.006353346222 1.677782904697 1.465047730008
H -0.125134636206 1.453235031803 6.063851682401
H -1.828922697351 1.484762398295 5.517287714207
H -0.596379457326 0.429361199875 4.746293794733
H -0.943016616553 5.812707257273 1.860600645175
H -2.424325841405 4.903886469261 2.168306580470
H -1.282218512679 5.230426306536 3.489401723387

**deprotonated TS(10a/2a)**

E(B3LYP-D3/6-31+G*) = -3839.53226372
Sum of electronic and zero-point Energies= -3839.145863
Sum of electronic and thermal Energies= -3839.116100
Sum of electronic and thermal Enthalpies= -3839.115155
Sum of electronic and thermal Free Energies=-3839.203995
C -0.020648980232 -0.083640259919 -0.084719793838
C -0.072835055562 -0.097035822447 1.341211813700
C 1.263339155185 -0.108098746352 1.838542496184

C 2.164260563462 -0.112542406051 0.720406145061
C 1.353330729719 -0.099923455969 -0.471791220584
Fe 0.950532837263 -1.762037974086 0.626500869236
C 0.124846903963 -3.529757209922 1.230314708513
C 0.136853482046 -3.434404426394 -0.197612008203
C 1.502099989632 -3.317083066191 -0.609204349396
C 2.388281555033 -3.421562153647 0.538456531882
C 1.482415793590 -3.474079190096 1.677887634465
N 3.737744907847 -3.349994752148 0.509416528617
Si 4.839169668957 -4.460164599616 1.138541112669
C 6.591047716789 -3.715796122286 1.065730454031
N 3.586799832839 -0.168591232280 0.737664270004
Si 4.484798414426 0.083712176322 -0.825640113836
C 4.007512775833 1.805981190532 -1.441342033279
P 4.633045315949 -0.464882467714 2.008119317784
Cl 4.593351684333 1.557925945384 3.056546473070
Cl 3.629870636920 -1.505920304048 3.551306473958
C 4.550348596196 -5.062624427876 2.933731199524
C 4.916966023535 -6.077022527131 0.107879284336
C 6.347994234435 0.101526789153 -0.506076328855
C 4.142986673652 -1.298741558481 -2.047834063842
H -0.967594199473 -0.115766906214 1.951220036462
H -0.865759783690 -0.096888853125 -0.762048745734
H 1.703584675276 -0.143945497237 -1.491487382730
H 1.542156090968 -0.125568196044 2.879042321364
H -0.731708236155 -3.432126940178 -0.847425429438
H -0.755091478445 -3.612678052813 1.858870299209
H 1.807284182365 -3.480949975844 2.709204213529
H 1.849416860514 -3.196180099343 -1.627855210760
H 7.351735334599 -4.455294972617 1.354411292719
H 6.818432878743 -3.380337074019 0.044563008970
H 6.691425001172 -2.849523070267 1.731700771641
H 5.647622518755 -6.794600688816 0.511427569422
H 3.933807834552 -6.568333316636 0.094236781026
H 5.189920659529 -5.860759868507 -0.934327916151
H 5.283549778981 -5.830965521297 3.222061213358
H 4.620492125924 -4.234089729040 3.648388944890
H 3.548461514696 -5.502895353625 3.033934418469
H 4.966830963893 -1.354340175639 -2.773322469273
H 4.108223959984 -2.233598602578 -1.466370318666
H 3.205858246292 -1.194033603735 -2.603840806219
H 4.527430070459 2.027715857840 -2.383751921172
H 2.931609784535 1.914339829140 -1.610039858679
H 4.306494351852 2.557203599160 -0.699600057858
H 6.821357646415 0.346904798787 -1.468621071595
H 6.663818737738 0.856750447003 0.222179273132
H 6.727080886164 -0.873977077642 -0.185633015334

E(M06-2X/6-31+G*) = -3838.83507341
Sum of electronic and zero-point Energies= -3838.445692
Sum of electronic and thermal Energies= -3838.416004
Sum of electronic and thermal Enthalpies= -3838.415060
Sum of electronic and thermal Free Energies=-3838.504290
C -0.000399801740 -0.001535219062 -0.002154813210
C -0.001991205708 -0.000610423192 1.423932059539
C 1.352538500624 0.000467306828 1.924301673510
C 2.175076194541 -0.064496674212 0.735136349956
C 1.353897380708 -0.040239332060 -0.430035326410
Fe 0.896447013523 -1.755732477105 0.682364256438
C 1.174449183692 -3.643608882578 -0.305594500729
C 2.004381840264 -3.594187246367 0.844237026204
C 1.174497171577 -3.401969887734 1.985617128600
C -0.178041336563 -3.352552668209 1.523092796210
C -0.174194414055 -3.502819447085 0.111840850598
N 1.571668221909 -3.197997927786 3.336006915450
P 3.102417260678 -2.911292735654 3.938514458074
N 1.731259933636 -0.045777872239 3.236840427273
Si 2.726879318434 1.116611504213 3.936373357493
C 4.233640453560 1.694041052927 2.913755192138
C 1.812143669227 2.742761484022 4.357571450181
C 3.402924857048 0.476104151088 5.589787454687
Si 0.291859987130 -3.166596476341 4.607565987952
C 1.117552773428 -3.057029608253 6.295098610743
C -0.869012074735 -1.710116797976 4.449158570417
C -0.575404547832 -4.837987923862 4.531189268240
Cl 4.291864656885 -2.044615496231 2.456695397258
Cl 3.968616205848 -4.919524262157 3.707084067492
H 1.523240076009 -3.753262307715 -1.324003366954
H -1.047237891498 -3.472428162430 -0.526494995732
H -1.056194842272 -3.162390000166 2.122327598833
H 3.080813576342 -3.662642031697 0.844080635409
H -0.873708651890 -0.003352074359 -0.643556963931
H 1.697915145285 -0.074974760304 -1.456892444588
H 3.254811894004 -0.134707587345 0.743421727705
H -0.881412749648 -0.004109291730 2.056141599411
H 3.935299076789 1.266773617603 6.134899893759
H 2.580954057039 0.123418497700 6.225723242555
H 4.096662797212 -0.360872275733 5.443745889889
H 2.475865797671 3.494586759376 4.806622754643
H 1.374189494724 3.174764475801 3.448383669505
H 0.989829947765 2.547864241865 5.057691371503
H 4.812160457989 2.449108608303 3.463961251126
H 4.900946351373 0.856310635962 2.677944063437
H 3.910856964461 2.143472051175 1.965831693617
H -1.352846165779 -1.536620594300 5.419361758443
H -0.247010339320 -0.838766083953 4.193656113482
H -1.652639786261 -1.826905519934 3.695018629878
H -1.317302526635 -4.908358376842 5.336707352669
H -1.083981517239 -5.020995995889 3.580606760353
H 0.162717615758 -5.635944825434 4.674290851415
H 0.321706672517 -3.146080503897 7.047023909284
H 1.840350662628 -3.860409456616 6.474682280828
H 1.621825538721 -2.098005976856 6.447655084277

**deprotonated TS(10b/2b)**
E(B3LYP-D3/6-31+G*) = -4075.43133562
Sum of electronic and zero-point Energies= -4074.871595
Sum of electronic and thermal Energies= -4074.834919
Sum of electronic and thermal Enthalpies= -4074.833975
Sum of electronic and thermal Free Energies=-4074.936646
C -0.125799484983 0.040366282989 -0.091456690777
C -0.150885599074 0.123215422772 1.334992906344
C 1.204811137759 0.143394295726 1.790882300447
C 2.047595137453 0.069332374376 0.637865871349
C 1.246780464606 0.072038461329 -0.575013332618
Fe 0.834721039500 -1.583979434677 0.777951192525
C 2.159562808797 -3.112158348717 0.821430524033
C 1.313572985740 -3.198860495446 1.967673306526
C -0.030490105084 -3.332915380906 1.508297013182
C -0.016149944660 -3.349943191228 0.083037535954

C 1.342103080702 -3.212050997519 -0.361794836703
N 1.816489442135 -3.119442865140 -1.701774872864
P 0.936539016118 -2.820229346146 -3.106732597099
Cl -0.958901584022 -1.974352517275 -2.678552881476
N 1.718303208796 0.012444759941 -1.848972213559
Si 1.379674614336 1.172353531663 -3.031355752967
C 2.407510791175 2.805918874508 -2.721068565167
C 1.892499179398 0.536050559677 -4.750861743252
C -0.448267254830 1.721686049652 -3.169165210622
Si 3.605139625037 -3.169525379508 -2.052723440728
C 4.543360771335 -1.799914926186 -1.168803849993
C 4.285966470518 -4.941390349638 -1.685913335002
C 3.884712865869 -2.829197178634 -3.894799245642
Cl 0.080101869328 -4.905401769872 -3.494350176065
H -0.917868815553 -3.395262448833 2.125878719086
H 1.641702548979 -3.134121947340 2.997863982219
H 3.225191871976 -2.960828845183 0.855672759233
H -0.884198120013 -3.438210878507 -0.548777374427
H 1.533733106234 0.185780707794 2.823537279643
H -1.036618549059 0.150481158371 1.960060712009
H -0.992874227017 -0.027064005935 -0.732345602663
H 3.129659333135 0.035650027920 0.648910373122
H 1.644670935911 1.265763325580 -5.533762154910
H 2.971682492190 0.343295786939 -4.804811763235
H 1.373445895602 -0.400194308172 -4.988497296127
C 2.221621157987 3.833430111062 -3.853848295512
C 1.956179804453 3.439986095134 -1.390032394589
C 3.901781425713 2.446975337136 -2.611002332388
H -0.597166683173 2.497784836080 -3.933294663010
H -1.074345654185 0.860803574638 -3.433138409476
H -0.815397243653 2.114194587848 -2.212180496210
H 5.511958913637 -1.661213880101 -1.667748662350
H 3.943609617392 -0.890054521411 -1.303915414013
H 4.729290450616 -1.953923553855 -0.102683339856
C 5.730461287095 -5.012191782978 -2.238109821161
C 4.337275963518 -5.302042409787 -0.187185023096
C 3.416520467559 -5.988858479225 -2.410273236720
H 4.972029091155 -2.819703692749 -4.050943009132
H 3.453954944693 -3.571622259391 -4.574450387575
H 3.505351215926 -1.842571324069 -4.174175545507
H 2.811175040620 4.746576220828 -3.656557715887
H 2.551903560826 3.435905910914 -4.822795904348
H 1.173009666902 4.141617552803 -3.959775500989
H 2.547365665077 4.346437716317 -1.168163049006
H 0.899876012752 3.738144856786 -1.420080506974
H 2.080050314068 2.746627863242 -0.549815926345
H 4.505925130140 3.343550491385 -2.385126005618
H 4.070970433172 1.711227969082 -1.816487172044
H 4.287950930660 2.019515921990 -3.546553499662
H 3.832610816824 -6.997081902282 -2.252915831990
H 2.385579645741 -5.983912170533 -2.043440565887
H 3.372330398315 -5.816076282631 -3.492198366889
H 6.164093687820 -6.000824745917 -2.020223166904
H 5.768412616022 -4.875878386521 -3.325085033616
H 6.386453317278 -4.260419406437 -1.778251397270
H 4.807424903951 -6.290805345878 -0.061448671613
H 4.931206538619 -4.582962231618 0.392227195470
H 3.339498127121 -5.349848892970 0.257710684247

E(M06-2X/6-31+G*) = -4074.59323421

Sum of electronic and zero-point Energies= -4074.030639
Sum of electronic and thermal Energies= -4073.993796
Sum of electronic and thermal Enthalpies= -4073.992852
Sum of electronic and thermal Free Energies=-4074.097329
C 0.010941935832 -0.007033799620 -0.004350941909
C 0.006840483013 -0.005275887565 1.421196006359
C 1.362945561126 -0.005722855820 1.922287309946
C 2.186055873778 -0.052753701736 0.736745971739
C 1.366442633743 -0.037407298568 -0.428814452295
Fe 0.927386549958 -1.752689328525 0.696229701800
C 1.155891587973 -3.635949624779 -0.309060197690
C 2.046217036168 -3.595918830891 0.794637561083
C 1.278498643008 -3.413330175924 1.980992330114
C -0.095113444874 -3.343689516675 1.590717248751
C -0.168269681468 -3.491365668965 0.180225695467
N 1.750500058529 -3.259002146962 3.316034404214
P 3.320762436036 -2.970572933648 3.820831394778
N 1.762754421129 -0.071267052467 3.230096626037
Si 1.766813925490 1.261367723210 4.247358058303
C 3.133640067208 2.560292425304 3.813030560557
C 2.724091036843 3.293757536798 2.528459474201
C 0.121776957367 2.239956117504 4.278331528462
C 2.065837858442 0.700406192886 6.035562623707
Si 0.556984757012 -3.330463861940 4.674551868995
C 1.498667438665 -3.035402945888 6.280152606953
C -0.741352386361 -1.983308833478 4.540229168716
C -0.172052258059 -5.105271446911 4.777191397913
C 0.958363702033 -6.125221259511 4.587883233479
Cl 4.364109743362 -1.976539352259 2.319409144662
Cl 4.234573562007 -4.916426786228 3.397979757579
C 3.348347170030 3.590232324809 4.927040964082
C 4.449741475045 1.817421327463 3.556573943443
C -0.766680867469 -5.265577947957 6.188953921082
C -1.285752823659 -5.416690614651 3.767581408826
H 1.449336939535 -3.735795659324 -1.345721560501
H -1.073405650892 -3.452529140209 -0.411166420846
H -0.935556263807 -3.147593479802 2.238852625117
H 3.121591425800 -3.665942428408 0.738116165860
H -0.860074870598 -0.017408754951 -0.648829950025
H 1.712761501434 -0.069718209738 -1.454899920225
H 3.265664723843 -0.106381728695 0.745427667798
H -0.872932656956 -0.024683599344 2.055172404484
H 2.105491046801 1.546100166825 6.733396157211
H 1.243198461234 0.046638781216 6.352941702459
H 3.001517229650 0.134009135358 6.128247020085
H 0.179676700468 3.170310757018 4.859548676067
H -0.192320009117 2.495826975172 3.258425797397
H -0.669465314977 1.617695610829 4.717966194300
H -1.024231454853 -1.654174338958 5.548051927824
H -0.253505131940 -1.138864578596 4.030761330955
H -1.655013734686 -2.262144472521 4.006464366478
H 0.760774283614 -2.983330628370 7.090526943804
H 2.217545415779 -3.825701575362 6.523994640169
H 2.033484305421 -2.082524852995 6.259195594002
H 0.575632357413 -7.145904423718 4.742997826518
H 1.385625990149 -6.068475519708 3.580528840957
H 1.781315396702 -5.968560812658 5.296600576442
H -1.724559014171 -6.398970872224 4.000931494405
H -2.097616259372 -4.678381101415 3.806098900938
H -0.909957861658 -5.455190485545 2.741757362078

H -1.240942763678 -6.253841233494 6.281198328127
H -0.001779764910 -5.193685590153 6.969624002519
H -1.538245834949 -4.511582645098 6.398688607380
H 4.082060356795 4.353322933270 4.616171543111
H 2.418815747911 4.115706640500 5.184629559261
H 3.731809848265 3.121281003938 5.842006016091
H 5.251622142570 2.525684367723 3.286364014292
H 4.781625143957 1.261021667353 4.443977040991
H 4.338351877058 1.088907113171 2.746118741260
H 3.528962886384 3.970167640703 2.193403588909
H 2.515200043877 2.590898479777 1.711733190439
H 1.824263521094 3.903430848940 2.683135530184

**deprotonated TS(10c/2c)**

E(B3LYP-D3/6-31+G*) = -3415.27380044
Sum of electronic and zero-point Energies= -3414.808092
Sum of electronic and thermal Energies= -3414.779531
Sum of electronic and thermal Enthalpies= -3414.778586
Sum of electronic and thermal Free Energies=-3414.866369
C 0.000000000000 0.000000000000 0.000000000000
C 0.000000000000 0.000000000000 1.437786000000
C 1.377594522885 0.000000000000 1.937583508364
C 2.159014307525 -0.328056070248 0.752586477493
C 1.353367280283 -0.190419981045 -0.424928532214
Fe 0.696512501440 -1.794602775405 0.606867052540
C 0.609436360771 -3.456374028695 -0.632307998060
C 1.681270362359 -3.570342568714 0.303344399924
C 1.126109417140 -3.521396140013 1.626780160377
C -0.296805849742 -3.358958660569 1.489160099839
C -0.611331963430 -3.325619657803 0.096176730124
N 1.840244306200 -3.609653764520 2.861135960114
P 3.428174344879 -4.054769871424 3.109476847878
Cl 4.703033180141 -2.900390543847 1.757666416029
N 1.862014200908 0.139187126321 3.162511079762
C 0.918078382860 0.511783580065 4.181856610465
C 1.620718315286 1.079964499424 5.446005643704
C 2.606244182529 0.045001698302 6.017528287638
C 1.201983999213 -2.962001853115 4.040479710478
C 0.552694085342 -3.916828083013 5.082319139340
C -0.370029777704 -3.047725174331 5.961048069136
C -0.268222190046 -5.038634105277 4.422081871303
C 1.627903048569 -4.559127587183 5.981870950316
C 2.390583487359 2.357464073543 5.067504267119
C 0.557089551700 1.412967151015 6.507282562010
Cl 3.522942652171 -5.913812761589 2.028607845382
H 0.718720653798 -3.433866906013 -1.709821384682
H -1.600315026207 -3.185727824868 -0.322937038482
H -1.013872843096 -3.252129787151 2.289100180034
H 2.727757843137 -3.654167706481 0.055456828396
H -0.866811820139 0.124572217859 -0.641080547224
H 1.700278047412 -0.251516487941 -1.451082064360
H 3.223957664817 -0.522868536159 0.773785491959
H -0.885392122686 0.103194889856 2.054269476010
H 0.199264319873 1.286038326386 3.834053309236
H 0.278157536117 -0.336096512679 4.518809207009
H 0.466511819461 -2.271383500216 3.627505806874
H 1.935700682747 -2.319676292553 4.533433304759
H 1.155328629515 -5.133859780643 6.790048437023
H 2.268470130987 -5.248039644346 5.419499636514
H 2.272897592935 -3.796825527154 6.436585087480
H -0.618785478240 -5.746442440461 5.185502199575
H -1.148909439533 -4.648602289804 3.902354443891
H 0.334349548526 -5.589394286799 3.691834396305
H 0.185791492826 -2.236079742423 6.445410183766
H -1.167606441674 -2.589119112336 5.363455629397
H -0.838770766012 -3.655199131022 6.746791518607
H 3.151583170025 0.453746377854 6.880914862464
H 2.076927643217 -0.855805390693 6.357014374521
H 3.324930272476 -0.250798982465 5.246853243641
H 2.917014329388 2.777389665050 5.937677789225
H 3.118045125214 2.131921578723 4.281173704478
H 1.704669277139 3.124843374983 4.681691134807
H 1.020480943020 1.815483850234 7.419574467413
H -0.155821507739 2.160974696275 6.133255461315
H -0.015078233032 0.517582243655 6.788389003896

E(M06-2X/6-31+G*) = -3414.56969178
Sum of electronic and zero-point Energies= -3414.100867
Sum of electronic and thermal Energies= -3414.073313
Sum of electronic and thermal Enthalpies= -3414.072368
Sum of electronic and thermal Free Energies=-3414.157036
C 0.113684148619 0.109461447235 0.012719484761
C 0.150551063838 0.113631880196 1.437591687665
C 1.505364216595 -0.021338149461 1.840827217016
C 2.296684467687 -0.104188854065 0.652693471398
C 1.454756070138 0.038515155843 -0.519315944952
Fe 0.914498293143 -1.704130225734 0.762365990745
C 2.029932620314 -3.480578901258 0.650417949589
C 1.154800413761 -3.568341433594 1.765132915335
C -0.176378644764 -3.484355512153 1.282279697437
C -0.128623484343 -3.352193686343 -0.130387558949
C 1.236740126505 -3.331113836650 -0.532338761479
N 1.744075998438 -3.057727581414 -1.826065478882
P 0.969699136140 -2.372133851407 -3.165265458878
Cl -0.856085830454 -1.476123083604 -2.664439605283
N 1.814482088130 0.055046886976 -1.833040718602
C 3.160557422011 0.527185877759 -2.040579118997
C 3.340311331779 1.247029346268 -3.396827153347
C 2.440212715976 2.484430587289 -3.433705957196
C 4.805383372600 1.668286226586 -3.541052163145
C 2.963856293633 0.318647415272 -4.551971880008
C 3.194974049678 -2.837276179960 -1.931267160289
C 4.022091021214 -4.069727903627 -2.354932247209
C 3.740535613413 -5.297660630676 -1.485261970335
C 3.708068725544 -4.417266944581 -3.814633816964
C 5.497050591186 -3.669701257763 -2.235467116049
Cl -0.062997053842 -4.238967004932 -3.829459498243
H -1.079201443539 -3.500306055830 1.878385029336
H 1.462028922279 -3.659541999622 2.798715920164
H 3.107818561882 -3.466411341292 0.711446324133
H -0.981947653701 -3.238835233524 -0.780178063107
H 1.870950224241 -0.070640469159 2.859446106721
H -0.708735013107 0.183605226301 2.093786955636
H -0.779067624223 0.182335419209 -0.590711901252
H 3.369810016915 -0.258146237044 0.627744220602
H 3.452175507314 1.260029371557 -1.259931902240
H 3.953465041830 -0.257046031420 -1.992064382151
H 3.554224840892 -2.409561711247 -0.987632987313
H 3.364942446387 -2.056869287914 -2.679598552773
H 4.354404972102 -5.235003699587 -4.158471134848

H 2.667423732126 -4.737824785492 -3.931303663396
H 3.874636264192 -3.553259503798 -4.471165756466
H 4.293699976576 -6.162875710835 -1.873500949478
H 4.049572942456 -5.141760846079 -0.446207414847
H 2.672599529321 -5.541128812797 -1.490904796579
H 5.716470559693 -2.788150499872 -2.851729781676
H 5.757949387275 -3.426833122701 -1.197692581778
H 6.148439183207 -4.487398821703 -2.567757461499
H 3.137371618023 0.809130729246 -5.520201406178
H 3.562357715103 -0.603681998570 -4.530085317692
H 1.909566381188 0.037005096167 -4.482024608632
H 2.510075354965 2.995088399336 -4.404439408427
H 1.402993775629 2.185438710189 -3.253676643047
H 2.729099664548 3.197335310890 -2.649895618596
H 4.968858269718 2.208745526637 -4.483075549786
H 5.109280121843 2.326177374124 -2.716277971501
H 5.468023020428 0.792316850439 -3.535050704242

**deprotonated TS(10d/2d)**

E(B3LYP-D3/6-31+G*) = -3100.71281820
Sum of electronic and zero-point Energies= -3100.474307
Sum of electronic and thermal Energies= -3100.456733
Sum of electronic and thermal Enthalpies= -3100.455788
Sum of electronic and thermal Free Energies=-3100.519690
C 0.025783980872 -0.110555350721 0.008854177322
C -0.018642783150 -0.136824539992 1.443132215305
C 1.345039398928 -0.168093663291 1.912815679568
C 2.210304582289 -0.147918099616 0.777196822627
C 1.395250978105 -0.113613636060 -0.394184845790
Fe 0.950006372791 -1.801975883383 0.739501251724
C 1.166850855637 -3.486829853840 1.950752511754
C -0.262734847468 -3.526087809324 1.627982564067
C -0.280543065324 -3.371723786977 0.179588001349
C 1.040898127597 -3.503527198169 -0.355030788949
C 1.949373135893 -3.562596909424 0.749199545456
N -1.332756655303 -3.555193453337 2.417061966513
C -1.044633001982 -3.791632914717 3.813173678503
N -1.152002994780 -0.190299074632 2.290423957469
C -0.851994199354 -0.227398256944 3.729132553968
P -2.795025065870 -0.284475131997 2.003845251128
Cl -3.079595164263 -1.233846739739 0.146389556783
Cl -3.256567310430 1.813200605386 1.236680172075
H 1.744012375593 -0.114612013673 -1.419753701204
H 3.292573733701 -0.179425867424 0.809471771905
H 1.669715764989 -0.223830227095 2.942359930496
H -0.823899848370 -0.102608118433 -0.654631901583
H 3.028801431748 -3.657944739124 0.690755141337
H 1.305990415757 -3.529623130641 -1.406743390390
H -1.188077526284 -3.266435172283 -0.399610847687
H 1.578247588911 -3.484450791223 2.953282585667
H -0.383687174601 -3.037335480474 4.296499405506
H -1.983253880079 -3.795323442154 4.385983762324
H -0.547929699238 -4.769860256090 3.996063555205
H -0.202529584431 -1.078866034979 3.946538962516
H -0.367385587213 0.707771095215 4.036898681338
H -1.776700749450 -0.352947967929 4.299618803664

E(M06-2X/6-31+G*) = -3100.19981869
Sum of electronic and zero-point Energies= -3099.958467
Sum of electronic and thermal Energies= -3099.941438
Sum of electronic and thermal Enthalpies= -3099.940493
Sum of electronic and thermal Free Energies= 3100.002320
C -0.064216625816 -0.291468713494 -0.168640564687
C -0.052886499923 -0.180341805871 1.275967572631
C 1.285462716085 -0.049979133669 1.752348445375
C 2.158243148143 -0.179626121775 0.639990306011
C 1.344940808489 -0.369742153416 -0.523697588528
Fe 1.066634937842 -1.930847463383 0.907528736071
C -0.006561506206 -3.680501958669 0.398523437855
C 1.351777763785 -3.814608396462 -0.027783564541
C 2.183600029972 -3.748571387167 1.119872689119
C 1.346481478891 -3.583731443836 2.255324520175
C -0.002148261149 -3.546911124080 1.815233671717
N -1.099532536909 -3.561308113128 -0.491382017441
P -2.707411202892 -3.218903771756 -0.217499592312
Cl -3.280535086547 -5.048516223476 0.817048025662
N -1.159283655505 -0.397151814167 -0.941833550474
C -0.902859728885 -0.146285362083 -2.335597872918
C -0.711459761306 -3.385091861852 -1.892841555515
Cl -2.900713338859 -2.024698806688 1.491511196197
H 1.671617625056 -3.475899755087 3.281770932569
H 3.264775877863 -3.791924669272 1.117297450802
H 1.695516490179 -3.893648421389 -1.049319810073
H -0.866840727803 -3.392049965878 2.442210405422
H 3.240965221589 -0.140987740367 0.665850876644
H 1.582176322451 0.086913504923 2.785547567457
H -0.945622558018 -0.153093133929 1.885323614874
H 1.728060435674 -0.517806954147 -1.527099690534
H -0.200192130852 -0.845063867247 -2.846439410956
H -1.847078303017 -0.203560917048 -2.895873603175
H -0.477481758762 0.863373886513 -2.519953429246
H 0.048314306204 -2.603246016255 -1.964412084407
H -0.325296592124 -4.332554489081 -2.289042940995
H -1.575398807366 -3.072161636715 -2.483670846227

**TS(10a/4a) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -5736.59038727
Sum of electronic and zero-point Energies= -5736.057908
Sum of electronic and thermal Energies= -5736.014555
Sum of electronic and thermal Enthalpies= -5736.013611
Sum of electronic and thermal Free Energies=-5736.133930
C 0.384410379460 0.255331258464 -0.301712296269
C 0.109622836469 -0.029096693874 1.068852355432
C 1.357853046920 -0.097577141013 1.791649275701
C 2.385223212472 0.198761770539 0.836716021515
C 1.791378051539 0.406757333764 -0.441547662012
Fe 1.044382902898 1.798688813963 0.877580033101
C 1.955294323156 3.667966175829 1.275284856780
C 0.959503694201 3.326992635224 2.251350274804
C -0.292082160176 3.182371551739 1.576388122605
C -0.061417608394 3.383319661301 0.182275504645
C 1.323465454366 3.669008285909 -0.006541015270
N 3.268710273036 4.122529884244 1.621304031197
Si 3.271773989890 5.456376199418 2.880695313427
C 2.025174853847 6.737833145049 2.306773775875
N 1.490807100705 -0.567770800568 3.123937938118
Si 3.095507403134 -0.417235809577 3.913810023976
C 2.883115117152 -0.380339062010 5.796915585207
C 4.254921987719 -1.815123890936 3.413946776976
C 3.925375463676 1.232909328749 3.477092699330

P 4.647353224731 4.149703510304 0.646119012570
Cl 4.548174216535 2.376842957202 -0.474814456319
Cl 4.119141471732 5.568384231571 -0.924849298931
C 2.828372939672 4.777429315053 4.588318383249
C 4.996459103213 6.209917300946 2.992642214548
P 0.424532263082 -2.374084627672 2.942418495785
Cl 1.227116358961 -3.273275510426 4.709194425542
Cl 1.600590593551 -3.345432238967 1.489657760292
Cl -1.630854398381 -3.810123064475 3.039850004103
N -0.749074696265 0.208406811708 4.706940519496
C -1.998687972285 0.130631691678 3.886956726432
C -0.827571653977 -0.745301994293 5.859180952898
C -0.496675565923 1.600581639871 5.172901463562
H 0.109002113916 -0.066860408416 4.088158096584
H -2.849092849958 0.400664732012 4.519388420130
H -1.070463007339 -1.740379887170 5.484448382193
H 0.452663105065 1.628364723868 5.709360937520
H 1.141341979980 3.219634041368 3.308722532196
H -1.244130233968 2.939621110300 2.031789743636
H -0.800169620236 3.298354990993 -0.604056412297
H 1.814840900388 3.858959753883 -0.949105009905
H -0.355621348882 0.374254088269 -1.082536232861
H 2.318797106519 0.672295369235 -1.347589229849
H -0.878022322690 -0.185579969876 1.473878202272
H 3.441894184058 0.250082549689 1.042994332944
H 0.137189516025 -0.767925816393 6.364387393753
H -0.446580768949 2.254016639769 4.303532885851
H -1.309640602531 1.915572824225 5.832615175679
H -2.120970801537 -0.890564099000 3.515731925052
H -1.914190483275 0.831244497372 3.056049635710
H -1.609629639316 -0.402523795430 6.542533484142
H 4.380200219599 1.669073383407 4.376126499632
H 4.726275182364 1.103449652995 2.739897768025
H 3.224493095379 1.955244191951 3.056247517599
H 3.884501267998 -0.318602514759 6.244196760559
H 2.339074207939 0.513147657745 6.132057958087
H 2.396898019906 -1.268389172713 6.207704357336
H 5.251691176511 -1.641535602163 3.841819728157
H 3.901075600397 -2.793312783225 3.751358137766
H 4.358960510293 -1.861459077994 2.323552712480
H 4.952297342816 6.983537844683 3.772254841947
H 5.762509421048 5.485387628066 3.290548209252
H 5.324428072148 6.697789449788 2.068478615242
H 3.284418262679 5.422169724273 5.350831333271
H 1.747365023645 4.776643138850 4.764946237302
H 3.210371644892 3.762752093015 4.739877928573
H 1.980475545321 7.577671956039 3.012200565316
H 2.308281588867 7.130211679494 1.323176815122
H 1.020374134584 6.309500123155 2.221259156043

**TS(10a/4a) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -5115.76847730
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5115.78427241
Sum of electronic and zero-point Energies= -5115.298679
Sum of electronic and thermal Energies= -5115.264420
Sum of electronic and thermal Enthalpies= -5115.263476
Sum of electronic and thermal Free Energies=-5115.363279
C -0.046586874825 0.000408454371 -0.136217559976
C -0.151178035565 -0.011998189178 1.284811903993
C 1.175513390303 -0.091072836888 1.824565967825
C 2.096134943684 -0.120543035557 0.728773247232
C 1.337833033050 -0.058630200064 -0.477588053948
Fe 0.969482968722 1.612493890757 0.662623383586
C 0.177673196494 3.295913774178 -0.228659766397
C 0.147577949173 3.438920358398 1.200412255023
C 1.489880809872 3.355647871887 1.680545028975
C 2.342489081443 3.155654052662 0.560548653286
C 1.535878432695 3.125690432765 -0.615330415305
N -1.023066285769 3.819224791714 1.981657140843
C -2.219904263865 3.013505437199 1.596642544819
N 1.491986466350 -0.204061954306 3.213511502603
C 2.785207564002 0.359918255750 3.627186714452
P -1.179950660671 5.704062733934 1.609966422958
Cl -2.799092368273 6.043899598771 2.936717679992
Cl -2.553634041692 5.443652069397 -0.312367520995
P 0.836259011348 -1.624270803150 3.885847541936
Cl 2.464181203988 -3.020608845762 3.778308291135
Cl 0.936422151589 -1.141014747782 5.944801702227
Cl 0.623224022900 6.139908962054 3.211860931247
N -0.892620104111 3.101359632675 4.589176479113
C -1.289642159837 1.652025184998 4.503695463279
C -1.810939618867 3.843366067901 5.517158460890
C 0.541744713980 3.163952642609 5.028120071295
C -1.352944751523 5.229448908672 5.963252378977
H -2.767074350559 3.933525844127 4.996343972392
H -1.975775942263 3.214212722076 6.402515492514
H 1.088412101841 2.524227217914 4.331412071642
C 0.857257292900 2.711828732991 6.458364153272
H 0.872414324601 4.190483003910 4.866766595400
H -0.779366556252 1.261551881011 3.620915146161
C -2.787443691114 1.342280512347 4.464372272077
H -0.866643422037 1.121309822341 5.361318384320
H -0.909501839681 3.592964812156 3.259101523059
H -2.027904772578 1.984465864372 1.891960666939
H -3.091172334107 3.411655414834 2.116269454984
H -2.407816769883 3.054091964845 0.526920099199
H -0.872159639872 0.081795782327 -0.830814150638
H 1.747170694546 -0.021405084600 -1.478775799128
H -1.066602469848 0.003744210384 1.858683750049
H 3.174035872851 -0.154576759348 0.806971787196
H -0.675424680177 3.333239811065 -0.889430886202
H 1.886240284897 2.959946142878 -1.625736143419
H 3.416118397819 3.025897031466 0.601296841723
H 1.800610473437 3.490190411244 2.701321938977
H 2.890269026483 1.339755380684 3.156201457379
H 3.620218190649 -0.282297732983 3.320715984482
H 2.804889619199 0.471961364678 4.712549120178
H 0.313464225269 3.285777009417 7.213251790174
H 0.661340543817 1.649656556980 6.625307293279
H 1.927009809769 2.874662660494 6.634172061603
H -2.909817554932 0.280622511327 4.219474247346
H -3.261903784396 1.506128078235 5.435945550517
H -3.337680067887 1.921433780646 3.721570757718
H -2.172348217001 5.684306781153 6.531853319585
H -0.476850142458 5.194114481818 6.616498295942
H -1.118350197249 5.879322509243 5.123170829167

**TS(10b/4b) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -5972.47089377
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5972.48678774

Sum of electronic and zero-point Energies= -5971.766353
Sum of electronic and thermal Energies= -5971.716759
Sum of electronic and thermal Enthalpies= -5971.715815
Sum of electronic and thermal Free Energies=-5971.845352
C -0.007139454650 -0.005743751135 0.003335184717
C -0.004308162489 -0.003890374341 1.427183061461
C 1.359807406743 -0.001593020503 1.878373229030
C 2.183925333368 -0.082021184265 0.706069375640
C 1.343546063352 -0.059903063561 -0.439084765153
Fe 0.865732684229 -1.720817569658 0.695677773568
C -0.532019452646 -3.006476163911 -0.065311977408
C -0.401774635757 -3.206030926012 1.339316449783
C 0.943389156432 -3.603924040727 1.597045719870
C 1.635592259195 -3.715186212199 0.339551719683
C 0.725656042977 -3.289030849977 -0.676035689116
N 2.869511320386 -4.440119844990 0.164646930468
Si 4.247312303652 -3.933608774706 -0.941692690851
C 4.228754836053 -2.063431194363 -1.061711469867
N 1.885728537308 0.369100173036 3.213598630503
P 2.821672255062 2.007910878374 2.758210474779
Cl 3.872459925277 2.276396902851 4.558003783151
Si 0.503010225446 0.363092516741 4.562096451989
C 0.018622128750 -1.465639490523 4.583099250817
C 0.908827557907 0.906835039761 6.373821983641
C -0.339137399693 0.404193600972 7.161151386203
C -1.022370967805 1.362109535674 4.031313702293
C 2.144891206360 0.240856675999 7.004172608266
C 0.994209669709 2.435088532130 6.578202448579
P 2.671705137401 -5.876129695114 1.082324072868
Cl 4.021057739728 -7.264437621442 0.241173704228
Cl 3.784774713550 -5.502456756281 2.915443014299
Cl 1.210958408402 3.515763284770 3.211143528508
C 4.102014019355 -4.601519454309 -2.750750179032
C 5.458392485287 -4.274321269761 -3.429069949484
C 5.856825447741 -4.484281540663 -0.133390002801
C 3.863741918519 -6.117842506630 -2.871185548723
C 2.980796694527 -3.881082731103 -3.532182802227
N 3.799026715162 -1.447091112600 3.852799341471
C 4.264104731591 -2.040712738943 2.574449502716
C 3.202198437844 -2.506617663078 4.691147053264
C 4.969462740908 -0.872425653725 4.565160725404
Cl 5.175888250809 1.138017467246 1.674001660436
H 2.796194938624 -0.448774966954 3.536550826663
H 5.421289095002 -0.096368448465 3.948456222276
H 4.647124421963 -0.445418721013 5.515324332835
H 5.704883145957 -1.666048009695 4.760701902189
H 3.407241466807 -2.413388011745 2.014828516515
H 4.952091341219 -2.870676013288 2.772258231331
H 4.773327757007 -1.266192669599 2.004836265590
H 2.358839585844 -2.957560989384 4.171935189712
H 2.863828420081 -2.079044002584 5.634262003493
H 3.938644898653 -3.292615076299 4.899621934670
H -1.174212328030 -3.052968819794 2.080825068232
H -1.416884571206 -2.653936688351 -0.579666487092
H 1.362436116582 -3.838298291128 2.564643671252
H 0.948703898153 -3.215556990614 -1.729619985367
H -0.893235930297 -0.026822406917 2.033542602028
H -0.890061141784 -0.020595280566 -0.622408661162
H 1.676575482049 -0.093052664638 -1.467406567378
H 3.261554121661 -0.074860880779 0.701995739527
H -1.226467550384 2.140225089621 4.771385270567
H -0.927079512896 1.868063375096 3.072654866832
H -1.893924150832 0.695466460059 3.995777940696
H -1.058045171827 -1.543340861560 4.774773308088
H 0.222970598365 -1.937256215394 3.620605746210
H 0.531456802682 -2.032512398981 5.363557535784
H 4.880373256736 -1.758040646211 -1.888648220488
H 3.230548738631 -1.674554781714 -1.261972166799
H 4.610747650662 -1.580547632701 -0.160346647553
H 6.648501713822 -3.787516270950 -0.435865375455
H 5.784481740104 -4.454914540680 0.958647101636
H 6.162359657913 -5.493600051346 -0.420544939585
H -0.235152385759 0.708095878756 8.211907093186
H -1.277562733534 0.837461468964 6.795756090583
H -0.437892175571 -0.686808225822 7.149611466764
H 2.228455489200 0.543270383014 8.057866119629
H 2.073735214376 -0.852649610856 6.996435881074
H 3.070132269593 0.537843956473 6.507547652482
H 1.066966337407 2.646490545390 7.654894070994
H 1.862718241086 2.876535277644 6.092027317962
H 0.109669673968 2.958083288885 6.202650670826
H 3.043527345059 -4.143713993066 -4.598229098362
H 1.988151622339 -4.194386608826 -3.189648241347
H 3.043082317383 -2.788558656672 -3.463600358966
H 5.437064813166 -4.612136668578 -4.475252928099
H 5.678024369851 -3.200264322019 -3.443666976930
H 6.297342637581 -4.784192500830 -2.940665885763
H 3.795853140648 -6.396939923742 -3.933366889059
H 4.678216888828 -6.700605996148 -2.430671113968
H 2.931280784028 -6.429314384395 -2.387613889640

**TS(10b/4b) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -6090.41072896
E(PCM-B3LYP-D3/6-31+G* (ether)) = -6090.42626236
Sum of electronic and zero-point Energies= -6089.619392
Sum of electronic and thermal Energies= -6089.566053
Sum of electronic and thermal Enthalpies= -6089.565109
Sum of electronic and thermal Free Energies=-6089.701484
C 0.000515383614 -0.215478802632 -0.460631807399
C -0.375497089548 -0.187691755510 0.914026583946
C 0.802309919096 0.011424139961 1.693634944358
C 1.913607267107 0.146491798373 0.801411747638
C 1.412794940938 -0.041331692782 -0.529532968309
Fe 0.907370427301 -1.752724278814 0.574498238541
C 2.020303914918 -3.512846866495 0.583290570484
C 0.963989701481 -3.644323587105 -0.382823509238
C -0.271350100408 -3.450710315652 0.328936746245
C 0.027480491993 -3.250483583279 1.699755577724
C 1.436561117678 -3.298647064455 1.859025750568
N 1.114494288427 -4.300766388821 -1.698372296035
Si 0.011614037154 -3.547188060235 -3.112148633758
C -0.317823731800 -4.543540045836 -4.759009816609
C 0.922424297701 -5.150209972348 -5.442820476998
N 3.184846393290 0.789868907484 1.075472750030
P 3.037899576169 2.272530057409 0.227743539022
Cl 4.258199188393 3.625768333814 1.311288867630
P 0.724105608127 -6.087194897479 -0.977769187671
Cl 1.082138876512 -7.312089303946 -2.660919892654
Cl -1.675725618765 -6.081334226509 -1.275221612000
Si 4.420286212289 0.275028708253 2.317505113694

C 3.847586216429 -1.376204243041 2.994995934383
C 6.179901412573 0.056526933761 1.579536425373
C 6.869370471600 1.377994964681 1.181930583126
C 4.424532361507 1.466233649825 3.784541247623
C 6.137353377647 -0.877417483405 0.354601685246
C 7.035688548448 -0.611398685558 2.687190245634
C -1.665544695058 -2.934116938458 -2.497922779127
C 0.873564487710 -1.943226433498 -3.634148673593
Cl 4.320220063408 2.011254344970 -1.508527167915
C -1.402019962838 -5.631610770223 -4.605222267868
C -0.882651888106 -3.484615590157 -5.754505254374
Cl 2.922097835858 -6.552715749289 -0.069385110188
N 3.748034144762 -3.876452858656 -2.326341517387
C 3.853160422531 -4.199496699108 -3.783629412552
C 4.067346161852 -5.681141681268 -4.084242849056
C 4.854610375331 -4.525821820801 -1.551194417943
C 6.269968797984 -4.050815945967 -1.886832408206
C 3.733467699817 -2.389514033442 -2.057915460615
C 4.423337557099 -1.463045675634 -3.057887544016
H 2.422166639250 -4.235056899167 -1.977195718021
H 5.094281928504 -5.994869926299 -3.873667006643
H 3.391223259152 -6.319897220018 -3.513815730370
H 3.882203520021 -5.853055267297 -5.149629897285
H 6.433713453788 -3.001679913486 -1.624960320551
H 6.521552681233 -4.186221745141 -2.944241605530
H 6.978412178584 -4.648737738950 -1.302161662340
H 4.699955394204 0.908107021419 4.688604219637
H 5.125793639431 2.296407214841 3.670972494072
H 3.428975810497 1.895457740938 3.946368760235
H 4.498425341275 -1.648029334518 3.833905866140
H 2.826164059420 -1.308461271523 3.377578552352
H 2.928848121980 -3.850928984849 -4.242213156679
H 4.666634608674 -3.623161680115 -4.233065569125
H 4.650474755744 -4.354415315394 -0.493730088866
H 4.765006183509 -5.599792349328 -1.687319889171
H 2.693728071940 -2.097200950266 -1.950835640228
H 4.176470533762 -2.248394977489 -1.072628987370
H -0.661825056558 -0.354632741151 -1.302561053181
H -1.373796827601 -0.339985151042 1.304574350765
H 2.016553184133 0.018953968489 -1.423723383205
H 0.852837234278 0.076716780934 2.772597260920
H -1.260459831721 -3.506849639763 -0.089157739043
H -0.698211066328 -3.053199147588 2.478080646311
H 1.967673560317 -3.186478897561 2.789671287245
H 3.069366190124 -3.644207696024 0.389102823989
H 4.362281631736 -0.443008408496 -2.669019335434
H 5.481622271876 -1.699191366663 -3.197587984953
H 3.938095230223 -1.464674734474 -4.038064291200
H 0.141246041940 -1.387391129720 -4.230221814589
H 1.119560268415 -1.315508618624 -2.779861631667
H 1.767557832388 -2.065029672893 -4.249528117743
H -2.134282897929 -2.428698260939 -3.350730714715
H -2.329444655546 -3.730587814173 -2.162758451800
H -1.566705092855 -2.191979362216 -1.704980841439
H 3.885661672245 -2.180963019897 2.258303793251
H 7.156894758746 -1.060190379037 -0.015896332291
H 5.704261788833 -1.855270483214 0.600444257713
H 5.562116610558 -0.436877673883 -0.465241465354
H 8.069270997629 -0.728942312979 2.331267777593
H 7.076718142385 -0.005529087230 3.601561699567
H 6.671378721924 -1.609566019009 2.955066856522
H 7.905181247867 1.170492150053 0.874666786916
H 6.375048006767 1.871641509390 0.342861859139
H 6.910645189766 2.089783261854 2.013844530707
H 0.613423418533 -5.653848497862 -6.370098456558
H 1.649306161134 -4.381354462507 -5.730427616935
H 1.423392892407 -5.891177722008 -4.822257676292
H -1.163607855631 -4.002933112372 -6.681667775145
H -1.785031024465 -2.983398651325 -5.389085532406
H -0.147543122328 -2.720149538590 -6.027628811312
H -1.658311784402 -6.021226097236 -5.601594415148
H -1.075199639441 -6.469200511426 -3.991733302843
H -2.319141639143 -5.239239777656 -4.155049551438

**TS(10c/4c) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -5312.33242427
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5312.34807654
Sum of electronic and zero-point Energies= -5311.721818
Sum of electronic and thermal Energies= -5311.680797
Sum of electronic and thermal Enthalpies= -5311.679853
Sum of electronic and thermal Free Energies=-5311.794691
C -0.043757933041 0.024917346063 0.028605620703
C -0.028992523736 0.021743712089 1.448057220477
C 1.336442707300 0.005372782734 1.881030857091
C 2.161161015537 0.001916028616 0.699804097120
C 1.304626879103 0.008408138370 -0.432573633947
Fe 0.983159963744 1.687362878935 0.721649693962
C -0.110495588687 3.442903379269 0.863174261131
C 0.443413548913 3.308718066874 -0.451908549191
C 1.861590757900 3.225641944006 -0.329641927706
C 2.198280029244 3.319876100324 1.051078799381
C 0.983962036879 3.442887423936 1.790117676458
N -1.492536557814 3.644873206255 1.201721960389
P -1.611730641773 5.061402914223 2.145420000989
Cl -2.883594809054 4.492667447940 3.768254025940
N 1.797173411512 -0.222498206668 3.265466074795
P 1.824122122864 -2.143928812869 3.148784638871
Cl 2.379224799948 -2.669355245832 5.116447156045
C 3.048274751985 0.641976401010 3.485329890686
C 4.048759447924 0.617915440571 4.695464911970
C 4.728231522230 2.010071579079 4.593148442288
C 3.464855681893 0.483379675919 6.110808198651
C 5.160225542876 -0.439956066046 4.537802145983
C -2.449889592614 3.109169476008 0.186640787793
C -3.800331596232 2.466271195208 0.602821486312
C -4.259440054731 1.690679357879 -0.655756232779
C -3.624592183619 1.472998328048 1.759542625424
C -4.894399974751 3.495135856590 0.942899658705
Cl 3.936975501120 -2.296356584051 2.187799530086
Cl -2.943414892194 6.289447814091 1.033458514960
Cl -0.648808351423 -2.298690466900 3.713768871961
N 0.003166545180 0.857825879906 4.967179331643
C -0.089617486849 0.008427412114 6.186477965566
C -1.341006637630 0.986286776829 4.346939713534
C 0.444587837423 2.224155240995 5.336966307846
H 0.881689080676 0.246725187732 4.100353515688
H -0.383180323763 -0.998457570539 5.890852538992
H 0.879350229642 -0.024620985588 6.681350303472
H -0.832412405304 0.432766472623 6.875013114210
H -1.256428164215 1.600857273770 3.450648566849

H -2.027577430842 1.480172782092 5.046249967573
H -1.717139465406 -0.004164136717 4.095033260811
H 0.367664124385 2.873380177806 4.467524359205
H 1.472065351197 2.215754384786 5.688935025714
H -0.203250936787 2.629829474673 6.124747539598
H 2.614946800554 1.644815108442 3.421857243149
H 3.672349819778 0.513461979168 2.602618882214
H 3.192784058317 3.263310162791 1.473756460903
H 2.555213832807 3.070273437495 -1.145961006547
H 0.906410035452 3.543951353962 2.860172384124
H -0.113902844496 3.244500483816 -1.375985144931
H 3.238445785813 -0.020160269949 0.665236532259
H 1.629312070723 0.039423313425 -1.464550335087
H -0.931388887075 0.053352112780 -0.589619248881
H -0.890990526207 -0.027043410253 2.084793923618
H -1.877682593962 2.321969264906 -0.306643664604
H -2.645018628695 3.894387107643 -0.555669513058
H 5.939804163072 -0.252900286927 5.287117627748
H 4.791991832030 -1.454603058276 4.682930973680
H 5.621818099271 -0.395087798595 3.547090337664
H 4.290848112005 0.432344546287 6.829998300310
H 2.856598332747 1.341780634113 6.403085511731
H 2.880028541472 -0.427457722077 6.227392583547
H 5.518474488618 2.097389623157 5.347023155955
H 5.191838383251 2.161002111382 3.609742764397
H 4.013517145349 2.826610322120 4.761728847490
H -5.849061112165 2.977485134258 1.098263618098
H -4.676353291712 4.056385865537 1.851751480102
H -5.028517450938 4.214150630393 0.126579792648
H -4.564364170311 0.939825240241 1.946368927153
H -2.860821080929 0.723433324844 1.526428516052
H -3.342196685891 1.985184454090 2.680830131902
H -5.243534950252 1.240049211850 -0.484980306974
H -4.343499702415 2.352499788141 -1.527576405602
H -3.562561750160 0.880830415237 -0.907467504762

**TS(10c/4c) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -5430.28203731
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5430.29718895
Sum of electronic and zero-point Energies= -5429.584426
Sum of electronic and thermal Energies= -5429.539844
Sum of electronic and thermal Enthalpies= -5429.538900
Sum of electronic and thermal Free Energies=-5429.658803
C -0.120641745936 -0.247768421590 0.024739986857
C -0.023940470326 -0.241575726776 1.441173581939
C 1.325915220644 0.073309969493 1.797385804136
C 2.064022244098 0.251878327693 0.581623277939
C 1.169335891845 0.050497924790 -0.504532097293
Fe 0.509236031517 1.620724308085 0.651409847618
C -0.827882887251 3.162300138114 1.090393183253
C -0.748202099795 2.951910406908 -0.323088183435
C 0.602868026639 3.151769763746 -0.723959673990
C 1.368274713139 3.494368864139 0.428400116469
C 0.496125472370 3.489622511638 1.552380034053
N -2.010111287340 3.193209279640 1.902958172499
P -2.156699894149 4.706071643192 2.646536100809
Cl -3.585992495483 5.818526017192 1.462148069425
N 1.842748083981 -0.057853307665 3.156670534234
P 2.509361805539 -1.854671807012 3.127960024932
Cl 3.271373796209 -1.827802959709 5.103166869287
C 2.595039184645 1.151502687645 3.727774506602
C 4.057331578235 1.684092909127 3.550176637741
C 3.964079250849 3.089163839441 4.212903008856
C 4.524228133392 1.901778972822 2.104258668032
C 5.108817108720 0.888979016976 4.344781663876
C -2.867096032781 1.983868151954 1.985216124648
C -4.233155449986 1.896004942533 1.249908404258
C -4.139606031901 2.374601923284 -0.205462935264
C -5.343536696802 2.668646247900 1.985595693690
C -4.597040931119 0.393880559781 1.272611335678
Cl 0.302805772590 -2.850744925489 3.651217160580
Cl -3.350741330270 4.215216002072 4.324986348919
Cl 4.558924253768 -1.546669294928 1.972978375278
N -0.189780446524 0.434781028911 4.950451724441
C 0.285678447903 0.244104778200 6.363228715560
C 0.297477672164 -1.202008676477 6.854005193304
C -0.436945923313 1.889057381594 4.609734225670
C 0.293046527043 2.965558844867 5.412830381790
C -1.481123589413 -0.302790224042 4.718100551338
C -2.642654174003 0.031359875655 5.661299692882
H 0.822574153772 0.004272947023 4.001858390804
H 1.422966124383 0.148481647821 -1.552019856587
H -1.020647325722 -0.431501749204 -0.547275919696
H -0.801222632410 -0.508034492337 2.135164529722
H 0.768641220865 3.731784312788 2.569650845477
H -2.222307489445 1.190602218088 1.605283073917
H -3.862527389007 -0.209029879391 0.723212396170
H -1.783958852746 -0.073577560554 3.695189080080
H -1.256049445552 -1.365848111453 4.744617343238
H -2.951876126817 1.081224753573 5.621586856190
H -3.504786937163 -0.572891040978 5.356555493788
H -2.424240280536 -0.218334229831 6.703385625852
H -0.341052235606 0.847995159410 7.030721241453
H 1.296318826284 0.654722163446 6.416920730679
H -0.218993384940 1.979539100308 3.545304518335
H -1.501968079557 2.092023833407 4.717836683972
H 1.940758126596 1.958471756966 3.400891276601
H 2.473564830842 1.023890491418 4.802804758476
H 2.429826063751 3.696079096505 0.448828738405
H 0.988376557128 3.026470316548 -1.727468835372
H -1.566053789262 2.673387365437 -0.968110668198
H 3.112363814943 0.475431600620 0.501109879250
H -3.046259060575 1.781749454893 3.045962277174
H 0.046613160312 3.936974303819 4.968675377493
H -0.044627967566 3.000429121555 6.452252866384
H 1.378072300184 2.867121152691 5.408530849029
H 0.857342441273 -1.239370653281 7.795260202414
H -0.709038627384 -1.580587829678 7.052544816983
H 0.773986971821 -1.877057378517 6.145340999221
H 5.435123196710 2.512755282118 2.105774917983
H 4.764080765915 0.959429292159 1.613048141281
H 3.766723310123 2.432276768816 1.520193193945
H 4.949411113919 3.567081704834 4.195000807657
H 3.264218267746 3.749157836158 3.683850082994
H 3.652368557268 3.028611415682 5.263295895350
H 6.064620634716 1.427272798333 4.316853181262
H 4.812024769120 0.785391194420 5.395268538840
H 5.274393447722 -0.105063806389 3.935722082304
H -5.121747371093 2.307430192887 -0.688300156462
H -3.808833330266 3.416628345843 -0.260861652189

H -3.447709174343 1.750203273646 -0.783495728295
H -6.310441526570 2.474950761949 1.504891736804
H -5.418209167317 2.352022357876 3.032421850184
H -5.180089084583 3.747195720560 1.970667713726
H -5.577034222816 0.230683567747 0.809590062528
H -4.648693032894 0.009740872882 2.299885073910

**TS(10d/4d) with $NMe_3$**

E(B3LYP-D3/6-31+G*) = -4997.82383342
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4997.84010789
Sum of electronic and zero-point Energies= -4997.440581
Sum of electronic and thermal Energies= -4997.410149
Sum of electronic and thermal Enthalpies= -4997.409205
Sum of electronic and thermal Free Energies=-4997.501182
N 0.003734191021 -0.020233280600 -0.007465446546
C 0.001892210935 -0.049859319060 1.477459937283
H 1.030588148325 -0.091865462950 1.833598174346
H -0.467182800932 0.860166678665 1.855412782030
H -0.560701990834 -0.925113680787 1.830074798964
C 0.628083765848 -1.255849661743 -0.541674311193
H 0.577828483952 -1.230016120266 -1.630531794514
H 0.080770630034 -2.138854833119 -0.188649390702
H 1.664542662685 -1.297297709415 -0.206813075872
C -1.390192819814 0.071435565147 -0.499282010570
H -1.384423530059 0.097584261766 -1.589068293670
H -1.860794167978 0.977211004022 -0.110817519149
H -1.970475982948 -0.802308945825 -0.175955531372
H 0.718309866691 1.073104402496 -0.445275255944
N 1.183648362431 2.189278275521 -0.901793695145
P 2.561132866214 2.879832445769 0.236862916305
Cl 3.313769216575 0.544268776951 0.663335641412
Cl 2.215964626453 5.118547776783 -0.381491786175
Cl 1.403938163607 3.006374021571 2.003912612490
C 1.871766587642 2.021672999109 -2.172153348995
C 2.544350136242 0.833347946367 -2.595739562901
C 3.244752008465 1.138025150602 -3.795820960995
C 3.014164875376 2.510276736919 -4.113062743442
C 2.162669250004 3.062469391140 -3.115971260269
Fe 1.226652395852 1.488160709502 -4.065873947820
C -0.814033629930 1.182286119224 -4.165917375790
C -0.117166966247 0.009380678481 -4.608300491814
C 0.696370534701 0.376913014310 -5.727144954856
C 0.500345104818 1.769060043795 -5.969572400423
C -0.436889997292 2.263976053574 -5.014589765249
N -0.262831161091 -1.296873730874 -4.052097150641
P -1.867867144198 -1.858194225215 -4.077897226180
Cl -1.788398967876 -3.264427752380 -2.495476076891
C -0.048613767776 3.022776466738 -1.024705551676
C 0.904010850995 -2.183926087876 -4.167760974385
Cl -1.892080122774 -3.213571372739 -5.737330344727
H -0.730770356744 2.494893582221 -1.690786840486
H -0.491290211755 3.138654221694 -0.034372865517
H 0.167846380627 4.009422215031 -1.429548070886
H -0.772631685536 3.288222107172 -4.920291904891
H 1.007137399411 2.354878037815 -6.725408236026
H -1.521221421550 1.228888551882 -3.351029016216
H 1.365335630037 -0.277542123889 -6.268679892202
H 1.814589984802 4.083035858996 -3.064340156100
H 3.387439161623 3.034896200275 -4.982856378135
H 3.829506644478 0.439512775540 -4.379961393377
H 2.556119727358 -0.102241599574 -2.062412908353
H 1.788623541087 -1.622522418597 -3.857717137984
H 1.035904082004 -2.537752441933 -5.197404456740
H 0.773352387668 -3.047350481937 -3.513182374619

**TS(10d/4d) with $NEt_3$**

E(B3LYP-D3/6-31+G*) = -5115.76847730
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5115.78427241
Sum of electronic and zero-point Energies= -5115.298679
Sum of electronic and thermal Energies= -5115.264420
Sum of electronic and thermal Enthalpies= -5115.263476
Sum of electronic and thermal Free Energies=-5115.363279
C -0.046586874825 0.000408454371 -0.136217559976
C -0.151178035565 -0.011998189178 1.284811903993
C 1.175513390303 -0.091072836888 1.824565967825
C 2.096134943684 -0.120543035557 0.728773247232
C 1.337833033050 -0.058630200064 -0.477588053948
Fe 0.969482968722 1.612493890757 0.662623383586
C 0.177673196494 3.295913774178 -0.228659766397
C 0.147577949173 3.438920358398 1.200412255023
C 1.489880809872 3.355647871887 1.680545028975
C 2.342489081443 3.155654052662 0.560548653286
C 1.535878432695 3.125690432765 -0.615330415305
N -1.023066285769 3.819224791714 1.981657140843
C -2.219904263865 3.013505437199 1.596642544819
N 1.491986466350 -0.204061954306 3.213511502603
C 2.785207564002 0.359918255750 3.627186714452
P -1.179950660671 5.704062733934 1.609966422958
Cl -2.799092368273 6.043899598771 2.936717679992
Cl -2.553634041692 5.443652069397 -0.312367520995
P 0.836259011348 -1.624270803150 3.885847541936
Cl 2.464181203988 -3.020608845762 3.778308291135
Cl 0.936422151589 -1.141014747782 5.944801702227
Cl 0.623224022900 6.139908962054 3.211860931247
N -0.892620104111 3.101359632675 4.589176479113
C -1.289642159837 1.652025184998 4.503695463279
C -1.810939618867 3.843366067901 5.517158460890
C 0.541744713980 3.163952642609 5.028120071295
C -1.352944751523 5.229448908672 5.963252378977
H -2.767074350559 3.933525844127 4.996343972392
H -1.975775942263 3.214212722076 6.402515492514
H 1.088412101841 2.524227217914 4.331412071642
C 0.857257292900 2.711828732991 6.458364153272
H 0.872414324601 4.190483003910 4.866766595400
H -0.779366556252 1.261551881011 3.620915146161
C -2.787443691114 1.342280512347 4.464372272077
H -0.866643422037 1.121309822341 5.361318384320
H -0.909501839681 3.592964812156 3.259101523059
H -2.027904772578 1.984465864372 1.891960666939
H -3.091172334107 3.411655414834 2.116269454984
H -2.407816769883 3.054091964845 0.526920099199
H -0.872159639872 0.081795782327 -0.830814150638
H 1.747170694546 -0.021405084600 -1.478775799128
H -1.066602469848 0.003744210384 1.858683750049
H 3.174035872851 -0.154576759348 0.806971787196
H -0.675424680177 3.333239811065 -0.889430886202
H 1.886240284897 2.959946142878 -1.625736143419
H 3.416118397819 3.025897031466 0.601296841723
H 1.800610473437 3.490190411244 2.701321938977
H 2.890269026483 1.339755380684 3.156201457379

H 3.620218190649 -0.282297732983 3.320715984482
H 2.804889619199 0.471961364678 4.712549120178
H 0.313464225269 3.285777009417 7.213251790174
H 0.661340543817 1.649656556980 6.625307293279
H 1.927009809769 2.874662660494 6.634172061603
H -2.909817554932 0.280622511327 4.219474247346
H -3.261903784396 1.506128078235 5.435945550517
H -3.337680067887 1.921433780646 3.721570757718
H -2.172348217001 5.684306781153 6.531853319585
H -0.476850142458 5.194114481818 6.616498295942
H -1.118350197249 5.879322509243 5.123170829167

**TS(4a/2a)**

E(B3LYP-D3/6-31+G*) = -5101.25793608
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5101.26671823
Sum of electronic and zero-point Energies= -5100.862328
Sum of electronic and thermal Energies= -5100.828643
Sum of electronic and thermal Enthalpies= -5100.827699
Sum of electronic and thermal Free Energies=-5100.923280
C -0.007064358067 0.019068004207 -0.006021939728
C 0.006072976627 -0.005282782016 1.418546537760
C 1.362135142875 -0.022847251850 1.848440144879
C 2.206411868186 0.004192165580 0.678215381267
C 1.337806902753 0.020099697410 -0.469645260678
Fe 1.044786104424 1.651275422391 0.716699792705
C 0.226426823866 3.453548232240 1.358765582888
C 1.525154163242 3.256256569107 1.906561634396
C 2.443502429546 3.076418891943 0.813758856066
C 1.698278481254 3.226280039191 -0.407037848472
C 0.332012667326 3.437873505795 -0.064941898668
N 3.854450892646 2.828465632082 0.890316713060
Si 4.892221377541 4.302422370766 0.531046705174
C 3.904697433768 5.761662125813 1.196181432431
N 3.674965537526 -0.050793547386 0.722683761728
Si 4.191105508815 -1.730205623748 1.563098400605
C 5.827026275952 -2.283986991116 0.814378954257
P 4.598997814382 1.498605660945 1.580277061210
Cl 3.707110313072 1.496976928862 3.579973199646
C 5.149063405389 4.456134502596 -1.319253442328
C 6.519145334096 4.157985071667 1.460997173538
C 2.792045824447 -2.947432582658 1.291292531302
C 4.473760772802 -1.588094308894 3.413055245593
P 4.674061948874 -0.254942893995 -1.114049185728
Cl 6.727670240744 1.135254476018 -0.594983626385
Cl 3.385199699083 -1.939560821836 -2.010620015152
Cl 3.850371086631 1.290593114090 -2.241348197364
H 1.628302737011 0.055899490195 -1.503956571700
H -0.883033014688 0.064406921734 -0.639597028335
H -0.857784209965 0.016700948155 2.069920508012
H 1.699292887233 -0.014885492637 2.872413111509
H 2.100831257406 3.130864328631 -1.403140382072
H -0.486017331651 3.533879783870 -0.767008958796
H -0.686418097269 3.569018176296 1.928762613234
H 1.773407474528 3.196548427881 2.954071166053
H 6.207353250751 -3.064083888577 1.489520690581
H 5.735310225517 -2.731439172036 -0.179935422977
H 6.579042870627 -1.487606255918 0.778173478072
H 4.747861579860 -2.609384625935 3.717208954973
H 5.294180486899 -0.924540773585 3.698324490541
H 3.583542276318 -1.299077577206 3.975781308913
H 7.088583455237 5.082577840324 1.293467586178
H 6.366670675530 4.057257117740 2.542551217305
H 7.129298535657 3.321188095765 1.108229812795
H 5.714598895187 5.372146383206 -1.536916654012
H 5.712809525618 3.600946081931 -1.702926106792
H 4.196426320079 4.516390924245 -1.857953279298
H 3.197639945579 -3.956074896378 1.449701326005
H 1.989065720500 -2.785852480763 2.017614796085
H 2.368358741770 -2.907684292902 0.286942202234
H 4.488321253331 6.682903961261 1.068572584382
H 2.951390830213 5.891224401565 0.672469494306
H 3.688618620827 5.644474125473 2.264693146793

**TS(4b/2b)**

E(B3LYP-D3/6-31+G*) = -5337.14249940
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5337.15084441
Sum of electronic and zero-point Energies= -5336.573517
Sum of electronic and thermal Energies= -5336.532578
Sum of electronic and thermal Enthalpies= -5336.531634
Sum of electronic and thermal Free Energies=-5336.641577
C -0.021556288622 -0.010707898984 0.024892077632
C -0.002920198459 0.016918101729 1.465593734234
C 1.353612850436 0.024119437683 1.893191184501
C 2.189949903786 0.011847283209 0.739703265115
C 1.352490251304 -0.006889482054 -0.410848644584
Fe 0.931654897610 1.652875647946 0.690537346314
C -0.238659676742 3.259502966071 1.169698225477
C 1.056190827381 3.446686450358 1.730341569169
C 2.009855687287 3.424364340410 0.668384309506
C 1.311353533599 3.225227415815 -0.555881722159
C -0.090191657024 3.095708025358 -0.250825567718
N -1.165578958512 2.868444602768 -1.173331551028
Si -2.243897708818 4.325097682373 -1.541854809160
C -3.476178094661 4.515025612838 -0.138866852069
N -1.178644129287 -0.070528831434 -0.880841984752
Si -1.212743350316 -1.743013834941 -1.949697158280
C 0.045201214524 -3.124625332789 -1.425594133029
C 0.265583879043 -3.337294515904 0.084887431192
P -1.375685959157 1.517561148986 -2.138588250844
Cl 0.544240529226 1.456248637328 -3.196791426496
C -3.112934151151 4.009564597389 -3.183725521794
C -1.164650745175 5.907872865422 -1.727648248111
C -0.051147486994 5.705251716104 -2.775491245179
C -2.112940960729 7.024978341505 -2.237578193273
C -0.546923593274 6.390066619346 -0.396807206866
C -0.937284414180 -1.361977411835 -3.774434331532
C -2.985682011854 -2.400602848979 -1.923988823885
C -0.580758897213 -4.432351879196 -1.990576079319
C 1.417494397845 -2.943116617417 -2.115879352883
P -3.048471476342 -0.229457661096 0.046002131587
Cl -2.559114491568 -1.883558866297 1.592297571256
Cl -3.030957798941 1.362708240322 1.392954445731
Cl -4.397300161871 1.081235993842 -1.623775230195
H -0.847256623854 0.043761813769 2.129011703541
H 1.680082510356 0.066034253011 2.923939350993
H 3.271403628936 0.047360221751 0.727346056575
H 1.686506561557 0.026449094286 -1.433310691988
H -1.167137545646 3.205606392852 1.714658510738
H 1.276441248461 3.551525990778 2.784662116253
H 3.083606126235 3.510402749919 0.773495430258

H 1.757516700695 3.127808683640 -1.532267104222
H -2.994240313348 -3.179152796762 -2.698541733405
H -3.305317525982 -2.868080125236 -0.989434392569
H -3.722107160813 -1.649736821473 -2.229779220610
H -1.143796801557 -2.311399812271 -4.287328863033
H -1.648554607653 -0.627160148939 -4.165149233673
H 0.069738409609 -1.045396535034 -4.041790405601
H -3.813183189782 4.836357288036 -3.358038436915
H -2.414003960815 3.984427995861 -4.027984380563
H -3.698484953417 3.087364152411 -3.181675106348
H -4.061810089752 5.432746495155 -0.275982654721
H -4.165793541845 3.665639457472 -0.129014138082
H -2.986045981948 4.573834600825 0.838563116217
H 0.922352271839 -4.208242218720 0.226755873969
H 0.745935311574 -2.482258267088 0.562975675061
H -0.669101732795 -3.535957470158 0.613559384943
H 0.129483667964 -5.256208366766 -1.835209605272
H -1.509684177935 -4.702305880805 -1.478292042629
H -0.780859480402 -4.383255324057 -3.068366696696
H 2.041601343262 -3.822788663059 -1.903888345594
H 1.334405413163 -2.861519671501 -3.205238889950
H 1.959910322712 -2.070926051829 -1.746131886434
H 0.512849526232 6.640379972143 -2.909361426645
H 0.661041609965 4.932297763492 -2.474933050023
H -0.455219071375 5.426062788984 -3.756036100622
H -1.549059196800 7.963723653610 -2.338231687372
H -2.538309856825 6.798200860137 -3.221631479264
H -2.940824614253 7.220026335566 -1.544263314530
H -0.064364683035 7.367275256425 -0.547847140094
H -1.307431803562 6.519325887706 0.383377767977
H 0.213716628453 5.705408375720 -0.015722872614

**TS(4c/2c)**

E(B3LYP-D3/6-31+G*) = -4676.99815020
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4677.00780504
Sum of electronic and zero-point Energies= -4676.522856
Sum of electronic and thermal Energies= -4676.490839
Sum of electronic and thermal Enthalpies= -4676.489895
Sum of electronic and thermal Free Energies=-4676.583556
C 0.077319271657 -0.018121350853 -0.028286176464
C 0.038390883009 -0.021997922284 1.412959499928
C 1.398109266302 -0.027709711208 1.877674461348
C 2.251949259994 -0.046299230311 0.739357318071
C 1.441060260847 -0.038691958685 -0.433073441992
Fe 1.037281176693 1.621701868024 0.742539927730
C -0.044535938584 3.116670302176 1.523626874916
C 1.291319760133 3.162367395517 2.051737730390
C 2.184217411887 3.334196492723 0.954828440711
C 1.411142014590 3.410658350811 -0.243604517039
C 0.033759985484 3.297146539647 0.101298257399
N -1.211716866040 2.899473925651 2.313263411380
P -2.310156756293 1.645395519842 2.204523333093
Cl -2.826396397847 1.641064649827 0.116113308316
N -1.183615541242 -0.053894896357 2.214312216108
P -0.912343507006 -0.548583696529 4.286813883983
Cl -3.044021444484 0.250016441064 5.009710781614
C -2.186416009124 -1.094548496802 1.709797559983
C -1.937572009915 -2.634338218561 1.761325771381
C -3.015036008305 -3.194166031544 0.797430226219
C -2.199233101115 -3.250605673450 3.152520427071
C -0.550084200954 -3.058795298563 1.251859050747
C -1.444726191180 3.814894988727 3.469226153982
C -2.121480422445 5.163575489643 3.130590869167
C -3.498003787105 4.928040931292 2.485887916190
C -1.245506048299 6.016505967592 2.194763295569
C -2.299646809985 5.901746206428 4.473407725077
Cl 0.117964179578 1.191678591721 4.836909555891
Cl 1.033815211573 -1.941698747301 4.484080093600
H 1.732246369758 -0.003499184666 2.899925316499
H 3.333362678879 -0.034329806329 0.772372112132
H 1.791963994589 -0.019764235118 -1.456564279780
H -0.773434609928 0.013954180750 -0.690656542377
H 1.565868305288 3.022582876907 3.087971579749
H 3.264210402726 3.357539458452 1.019114930258
H 1.802223126541 3.514911592810 -1.247377799217
H -0.800759121689 3.301775567797 -0.582317171710
H -2.299035382435 -4.338596552976 3.054837220707
H -1.375162703873 -3.084499798494 3.850088527267
H -3.124570126341 -2.866867666353 3.598137152946
H -0.495503914380 -4.154181614852 1.232013441951
H -0.363184117529 -2.693068800830 0.236727254073
H 0.252326178544 -2.701606829300 1.900939683666
H -2.968537607721 -4.288747494400 0.782684613588
H -4.026795232738 -2.907437506435 1.111813500118
H -2.862159083816 -2.839255470810 -0.229385650231
H -4.011729160740 5.883566813335 2.325854828619
H -3.406686877671 4.436135885565 1.510855835706
H -4.138794770928 4.306556322789 3.124529493593
H -2.777364168511 6.875419214071 4.312816416730
H -2.929154852690 5.329266866060 5.166111459840
H -1.333273410688 6.080948068904 4.962056341262
H -1.696867631212 7.006772279586 2.056648665052
H -0.239450093684 6.158935514327 2.608455753306
H -1.139474440225 5.558316197174 1.207212516705
H -3.115534910487 -0.881460945664 2.250418268364
H -2.352950991566 -0.833615255341 0.666107998632
H -2.058514223053 3.275658508296 4.199032399566
H -0.475522005704 3.988287917799 3.947072999582

**TS(4d/2d)**

E(B3LYP-D3/6-31+G*) = -4362.45373168
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4362.46332684
Sum of electronic and zero-point Energies= -4362.206027
Sum of electronic and thermal Energies= -4362.184194
Sum of electronic and thermal Enthalpies= -4362.183250
Sum of electronic and thermal Free Energies=-4362.255904
C 0.011566893983 0.030334193485 0.012037535463
C 0.015524016588 0.030207078330 1.437358979985
C 1.373653774488 0.018386741095 1.881020468416
C 2.221887178047 0.023055351753 0.735497456857
C 1.379636508673 0.000161561686 -0.427854167067
Fe 0.998642475218 -1.627672337224 0.669884512994
C 1.349643146728 -3.057042693055 -0.692008538182
C 0.000697893977 -3.173823464954 -0.208435802347
C 0.059653054746 -3.400257280906 1.194993487789
C 1.428708763787 -3.443839815236 1.590573173924
C 2.232733072148 -3.246513221341 0.434191329104
N 1.798590601227 -2.838944969208 -2.066668132566
P 2.702432062530 -1.244762254836 -2.546392095847
Cl 4.458732267020 -1.493533675631 -1.300592818286

N 1.786503590876 -0.066927784742 -1.792192734808
C 1.425166937197 1.103946681460 -2.625617642241
C 2.640957841879 -3.998552466393 -2.512362918293
P 0.227420083843 -3.002419616101 -3.709450546489
Cl -1.181295668922 -1.650001832697 -2.973405022940
Cl 0.981978591007 -1.418003030679 -5.371730955572
Cl -0.783435799733 -4.902512362183 -2.903498127615
H 1.913256720735 2.005435262953 -2.239824618252
H 2.044956176132 -4.909610373488 -2.428739198954
H 3.529265857867 -4.080333757604 -1.882668331081
H 0.339283145295 1.235854298971 -2.610927373770
H 1.726658516009 0.929296939711 -3.661188044656
H 2.951708611056 -3.847749769627 -3.551339002944
H -0.904181758249 -3.080544650929 -0.782169819366
H -0.798613129955 -3.493643235677 1.847196891295
H 1.801076196736 -3.574119770391 2.598217995144
H 3.310018819342 -3.195575716721 0.412143470737
H -0.855903832472 -0.002868228963 -0.631934192233
H -0.861470015675 0.004707468394 2.070806764939
H 1.705675588371 -0.011801952735 2.910632333034
H 3.300916221955 -0.011530689743 0.732306527667

**5a neutral compound (*trans*)**

E(B3LYP-D3/6-31+G*) = -6520.83678103
Sum of electronic and zero-point Energies= -6520.058400
Sum of electronic and thermal Energies= -6520.001400
Sum of electronic and thermal Enthalpies= -6520.000456
Sum of electronic and thermal Free Energies=-6520.150785
C -0.040107312854 0.013872965168 0.066967650664
C 0.007255367951 0.012765860478 1.493782836162
C 1.383281541877 0.006162846746 1.899220181777
C 2.182727253070 0.039254555861 0.708834825508
C 1.304251008235 0.043039714871 -0.415237909913
Fe 0.917931873262 1.687218558160 0.758829027302
C 1.994729031437 3.460356588014 0.638435466167
C 1.193512059831 3.454650784225 1.828083145665
C -0.172499341740 3.280651450425 1.426034599430
C -0.215897557189 3.215643375829 0.000576193642
C 1.124763067471 3.314095064423 -0.482741301279
N 1.595592892646 3.734532545684 3.162448391854
Si 0.819539796615 5.122337698978 3.999644082294
C 2.089422058178 6.067955160625 5.031415124497
N 1.810990508703 -0.172718655752 3.242933815381
Si 1.190197323560 -1.601367975812 4.138864781301
C 2.554494676464 -2.359258129399 5.204532439331
P 2.888390584334 3.012731702470 4.048023959730
P 3.015123967594 0.722487156223 4.094438992818
P 4.861050268015 0.797860188388 2.811939441751
P 4.734349466420 3.088107930777 2.765566968281
N 5.938462879573 3.983289851937 3.617123073129
Si 6.559245019760 5.411966887469 2.721222336962
C 5.194951456863 6.169792815706 1.655507485624
C 6.366132813367 3.804368972667 4.960845240046
C 7.742145088427 3.797773163791 5.366333071164
C 7.789456675772 3.796608073747 6.793149749322
C 6.445081896154 3.767382028301 7.275305066293
C 5.566645938116 3.771194440457 6.151200581710
Fe 6.831488730951 2.123268189950 6.101176571391
C 7.965366857523 0.594839806268 6.859350651656
C 6.624713904639 0.496331888377 7.342679108101
C 5.754739634951 0.350097168036 6.221505450194
C 6.555944114307 0.355874500755 5.031849691196
C 7.921954925020 0.529892510742 5.433890149587
N 6.153854855039 0.076030578915 3.697478628638
Si 6.929885333029 -1.311764096707 2.860244580700
C 5.659974604904 -2.257365207949 1.828492955686
C 7.996634491206 4.879187841620 1.621575081082
C 7.100226107906 6.709491970902 3.979105938383
C 8.303862833742 -0.670719812507 1.737550114701
C 7.605472999279 -2.489582549361 4.169754136593
C -0.554464573884 4.481307717886 5.122314206406
C 0.143985760648 6.300138243066 2.690101249718
C -0.247141535719 -1.068538999557 5.238553204845
C 0.649121009919 -2.898849984996 2.880981221513
H -1.015293550706 3.206905303693 2.101018295994
H -1.102114757150 3.063123687609 -0.602421653618
H 1.433602518764 3.250434117735 -1.518578025822
H 3.070430395746 3.550549295343 0.610877833760
H 3.261894852071 0.066379602501 0.682330444700
H 1.606352677834 0.097430973618 -1.453586624350
H -0.936472568763 0.043433832944 -0.539584499791
H -0.839903550300 0.021489801922 2.167276916922
H -0.706984630549 5.888672972326 2.138899442717
H 0.920799652856 6.553193483161 1.958114953583
H -0.181269924312 7.231154758763 3.172828877576
H 2.409114451235 5.516854081402 5.921390037179
H 1.643913599424 7.016627392458 5.362111360501
H 2.986660067100 6.306840241679 4.447310527988
H -0.241053444797 -2.605912930039 2.316128727462
H 0.426997167138 -3.839150150467 3.402619231419
H 1.449839399968 -3.095452415729 2.157464405000
H 2.810836578832 -1.740351935092 6.070103735661
H 3.473232711362 -2.522443438216 4.627841740696
H 2.214999732006 -3.336536460546 5.575322841194
H 7.990404400983 6.416613689285 4.543979147247
H 7.322308497368 7.649799807212 3.457463537618
H 6.299482058138 6.906058373907 4.702604008168
H 4.938648329820 5.550860310561 0.789942686485
H 4.276195461530 6.332960720676 2.232174437165
H 5.534425618929 7.147074114596 1.284706624922
H 4.487477894987 3.744040675440 6.177666203332
H 8.589329192845 3.789095292355 4.692870838554
H 8.456453272972 -2.078120957092 4.720943380028
H 6.828677528158 -2.742654205486 4.901754242299
H 7.930723573533 -3.420589438923 3.687004428457
H 5.340271461393 -1.706255519759 0.938527139020
H 6.105466612692 -3.206039841152 1.497781640080
H 4.762745228666 -2.496245064988 2.412613106294
H 8.764739219064 0.603686074398 4.758899185827
H 4.679040478334 0.259878463669 6.249068779143
H 8.851586763949 0.747356592156 7.462345316073
H 6.315884356944 0.559941008789 8.378521956888
H 6.142944228260 3.712935617690 8.313640454529
H 8.685800509725 3.767044069983 7.399733298992
H -0.629915537024 -1.906147798404 5.836453373595
H 0.076176766964 -0.280234070308 5.930075320612
H -1.079503783433 -0.669874510294 4.645391335635
H 8.379391690400 5.716808020274 1.023680027180
H 8.828996387072 4.480558613040 2.214760665089
H 7.673365531730 4.090866415042 0.930048487221

H -1.028270462673 5.295974019530 5.685713242038
H -1.336477788788 3.970061312442 4.547269684338
H -0.149154757567 3.762153606133 5.845296801464
H 8.777656576392 -1.485378287205 1.174129569326
H 7.898536738082 0.048444049043 1.014586402243
H 9.085888331841 -0.159480942384 2.312584708055

**5a neutral compound** (*gauche*)
E(B3LYP-D3/6-31+G*) = -6520.83852190
Sum of electronic and zero-point Energies= -6520.060510
Sum of electronic and thermal Energies= -6520.002680
Sum of electronic and thermal Enthalpies= -6520.001736
Sum of electronic and thermal Free Energies=-6520.151404
C 0.134903015355 0.022144751215 -0.080574288172
C -0.118619160183 0.085321625273 1.325941294399
C 1.148988188303 0.046946187890 1.999026039817
C 2.169613934831 -0.082652858333 1.012262493183
C 1.542681168409 -0.089738787908 -0.273297674424
Fe 1.132462980749 1.666558372506 0.713181894119
C 2.071543720966 3.301170480622 1.564149349028
C 0.667859925312 3.583071807479 1.464279684723
C 0.304831283511 3.465944091427 0.080593097640
C 1.478676472704 3.155763880365 -0.664539927175
C 2.571831600941 3.053759810846 0.252441235780
N -0.179133458965 4.068213466868 2.510922284792
Si 0.057889369341 5.808394420601 2.816426295189
C 0.010249711472 6.682109339594 1.144302969777
N -1.398588617753 0.080612767709 1.956698870129
Si -1.906247300772 -1.439665232696 2.737692437991
C -1.628093645482 -1.382240669231 4.602586917584
P -0.852854001009 2.798445118819 3.534667659179
P -2.101535474879 1.679336775910 1.992436590731
P -3.721528014959 1.596945948620 3.582175885346
P -2.881980457813 3.630030562644 4.170922810923
N -2.878434712007 3.541871952739 5.925338932989
Si -1.573379420670 3.210393345980 7.092415855866
C -2.237938706750 3.682063752188 8.794697362727
C -4.200404973314 3.505818511024 6.466773595529
C -5.036412209568 4.634551158168 6.740629197294
C -6.188691156392 4.175756296015 7.443459567473
C -6.082660860160 2.757718666780 7.594682979827
C -4.870009055054 2.339452990506 6.972859601892
Fe -6.113680590592 3.266096957983 5.603792952262
C -8.015463177088 2.801190198756 4.981110603302
C -7.096424939063 1.876603712361 4.404210050484
C -6.172479262753 2.609875404065 3.594537656971
C -6.506012512911 4.002551712649 3.711965003987
C -7.656571518409 4.115326380245 4.546384322188
N -5.184933169150 2.057365907005 2.725013333653
Si -5.485773186283 2.257376743903 0.980266542857
C -7.356717297869 2.394959911027 0.766567164735
C -1.090184041218 1.386404759810 7.087709779661
C -0.049206360125 4.273123822148 6.755895319941
C -4.667217307601 3.825448598014 0.312854816460
C -4.916791193928 0.732386244598 0.023766802765
C -1.266384031000 6.560041258678 3.926126232826
C 1.745101772542 6.117715591004 3.616443880492
C -3.713103194034 -1.821073196831 2.349450625317
C -0.842795104409 -2.805879522847 1.986889524785
H -0.696521869429 3.599893363518 -0.304836667703
H 1.528724119209 2.984545213557 -1.732536982612
H 3.590863009327 2.789511415881 -0.001555903826
H 2.633606190379 3.279077315823 2.488529219874
H 1.283347245784 0.106908921255 3.070982429931
H 3.235419479419 -0.122462159159 1.199024890434
H 2.053697237272 -0.132174210472 -1.227104114240
H -0.627162500469 0.063775151518 -0.847974979966
H -4.499170948152 1.326763323427 6.887922580729
H -4.813328471821 5.653462586930 6.451912189518
H -5.965504358454 4.810407813412 3.237149667093
H -7.078597415487 0.803600680714 4.544286513663
H -6.817372694395 2.111480212781 8.058293702806
H -7.021597227416 4.787178676488 7.767821081256
H -8.143048661764 5.036727653519 4.840812847898
H -8.821607412352 2.556586821403 5.661568662257
H -1.849199500524 -2.358382342300 5.055664170337
H -0.585910890172 -1.133564927966 4.837493598853
H -2.267943336295 -0.636109048765 5.083655329739
H -3.993119658866 -2.770762415109 2.825730705064
H -4.405159424504 -1.053734350769 2.710412572829
H -3.862252440503 -1.930070429271 1.268843165920
H 0.129869216706 7.764726567244 1.284643436731
H 0.808347509529 6.339278741240 0.476544579810
H -0.947981272907 6.510238360304 0.638825586664
H -0.976522554541 7.604116094190 4.111741795770
H -2.252841552836 6.560708560520 3.452347273106
H -1.359778981133 6.069754624748 4.899346194638
H -0.334204604052 1.182842416569 7.858406823702
H -1.957529278500 0.747694823272 7.294468772238
H -0.674556230399 1.084566061839 6.121210535483
H -1.436201489275 3.580700997610 9.538242930554
H -2.586653266268 4.721526479751 8.813570562371
H -3.072814335921 3.046379302668 9.107970269777
H -4.869372093132 3.942222331364 -0.760791923098
H -5.058543180894 4.713311551699 0.824882880336
H -3.581128454363 3.807736766017 0.452271754007
H -7.601647348121 2.405632756546 -0.303909903616
H -7.870926686658 1.539914317835 1.221683283065
H -7.764927108470 3.306138109539 1.216593038143
H -1.180475264607 -3.778981654607 2.367400244539
H -0.924604263257 -2.823688246873 0.893634882321
H 0.217279679831 -2.693637948907 2.238565610849
H -5.125617139286 0.881561482390 -1.044597387191
H -3.848967235146 0.516587665094 0.124019515430
H -5.472765409606 -0.153322681685 0.353209518259
H 1.885560980996 7.190720708681 3.805060126005
H 1.840019166267 5.597048480283 4.577043711127
H 2.563521884495 5.785650429183 2.967261235164
H 0.708160988888 4.052489360326 7.520788416640
H 0.405354267106 4.074906159371 5.781094040111
H -0.280918210273 5.342709581812 6.819327500194

**5a radical cation** (*trans*)
E(UB3LYP) = -6520.62270469
Sum of electronic and zero-point Energies= -6519.841604
Sum of electronic and thermal Energies= -6519.784689
Sum of electronic and thermal Enthalpies= -6519.783744
Sum of electronic and thermal Free Energies=-6519.932618
C 0.003545583794 0.005978426744 -0.026916948215
C 0.028876491361 0.000020564997 1.400221415173

C 1.393789621284 0.005432292279 1.811215551012
C 2.212077884584 0.036129448072 0.641633843137
C 1.355192850537 0.074307446874 -0.507934007985
Fe 0.993613997898 -1.662821911180 0.670576267760
C 2.124596260840 -3.421007742389 0.710602166343
C 1.265960461461 -3.461421722077 -0.437576951990
C -0.080122743610 -3.305820425026 0.038696553143
C -0.053384479715 -3.244479951962 1.464503404249
C 1.309838517227 -3.302565474918 1.877046158175
N 1.615310397551 -3.665387294858 -1.787189425844
Si 0.615682493937 -4.826504097559 -2.771079007909
C -0.046013027116 -6.141898301800 -1.597473352646
N 1.712692746435 0.206655509870 -1.864302182158
Si 0.771588889789 1.376774469409 -2.894201142665
C 0.178323236630 2.769185498787 -1.774085142766
P 2.911411625065 -2.931110475355 -2.668869235267
P 2.968969849263 -0.626381997631 -2.715373595864
P 4.829073865239 -0.647999050739 -1.464539908402
P 4.771025221721 -2.952695052251 -1.417343116852
N 6.027450949246 -3.786256802504 -2.267667906843
Si 6.968217634814 -4.955944971416 -1.236984580656
C 7.561497093839 -6.349040343102 -2.356244935867
C 6.385283223140 -3.654636333285 -3.624036364465
C 5.528689545913 -3.617322989648 -4.773848150946
C 6.347276699066 -3.587174597885 -5.943231608735
C 7.712084623617 -3.581253061091 -5.531885840979
C 7.737045620284 -3.586345125277 -4.104738768569
Fe 6.746845227639 -1.918153079804 -4.803486029327
C 6.430207995134 -0.279190887386 -6.010891718730
C 7.793479310736 -0.336775243738 -5.598450543604
C 7.820347810441 -0.274576814005 -4.172683451100
C 6.474286853442 -0.118946521747 -3.696360493707
C 5.615545075883 -0.160203138472 -4.844434477442
N 6.125076467303 0.085742849862 -2.346834917388
Si 7.124966598710 1.247223850221 -1.363633602016
C 7.786818400419 2.561841493634 -2.538014020299
C 5.834002071501 -5.678139083287 0.082097459338
C 8.393284590289 -4.031828164226 -0.422516191837
C 6.030189845943 2.078991991984 -0.076153420681
C 8.502269863959 0.285927855558 -0.510926701125
C 1.710709591765 -5.657294209377 -4.058975712522
C -0.761759351258 -3.865054156025 -3.623392798939
C 1.905467644824 2.099903944022 -4.213061950655
C -0.653474678255 0.452845484424 -3.708881884656
H 8.621664367404 -3.543025195480 -3.484711821189
H 8.576581304002 -3.534851335807 -6.181400298998
H 5.987314708820 -3.552163900148 -6.963369580573
H 4.449537024567 -3.620733631113 -4.752259974400
H 4.537951280918 -0.101695580646 -4.823969586766
H 6.067742571130 -0.337764938722 -7.029060139320
H 8.653793807232 -0.453031410113 -6.244762906060
H 8.702421579340 -0.336873477678 -3.550647964208
H 8.349365725910 -6.051537774592 -3.054689164203
H 6.730718546874 -6.758775085274 -2.943744818334
H 7.959577515680 -7.161316892292 -1.734617094496
H 5.597581249373 -4.963207061202 0.876280980567
H 6.343390040263 -6.535227830481 0.543196179911
H 4.890065919897 -6.041821437762 -0.341057756482
H 8.557935804177 2.196740873894 -3.222960455486
H 8.226080296570 3.377557980820 -1.949508755120
H 6.977224811389 2.988827657477 -3.142558458129
H 5.758675269219 1.409862760964 0.746217175056
H 5.105449389870 2.472497980507 -0.514730584201
H 6.582814958736 2.927229686848 0.350210614761
H -0.817189558081 -5.777277183931 -0.912339784358
H -0.485163704696 -6.957337759053 -2.186445206103
H 0.763619638370 -6.569124245886 -0.993152046072
H 1.982066478786 -4.987625189469 -4.880960898727
H 2.635541758704 -6.050815070596 -3.620607987091
H 1.158307498211 -6.505428091523 -4.485835694365
H 3.202186649239 -3.479633574837 0.690191824215
H -0.962112965742 -3.243000097471 -0.583399916660
H -0.609435487242 2.471249509024 -1.075701148407
H 1.009145127010 3.178666171448 -1.186468620953
H -0.219895779801 3.581768497998 -2.395223799490
H 2.141926409037 1.385469646915 -5.007680205960
H 1.395850554263 2.957153528183 -4.673607615401
H 2.849388347450 2.463534400385 -3.789824545148
H -0.881253036335 -0.036816094801 -0.646726631297
H 3.291225435940 0.039413807195 0.619778559750
H -0.835460875028 -0.046611963731 2.049931145410
H 1.754012067051 -0.030248898546 2.831238064145
H 1.672212581176 -3.244650188402 2.895285001608
H -0.913740454493 -3.128451896045 2.110801692761
H 9.088943509901 0.940806442479 0.145927992216
H 8.083456992614 -0.517108562904 0.108715768675
H 9.197113370882 -0.174196593879 -1.223437618993
H -1.348067099318 -4.519691874145 -4.280815719615
H -1.456921131917 -3.405647687772 -2.910731096778
H -0.343089482566 -3.061461101953 -4.242410181341
H 8.946405493948 -4.688302040196 0.261305107624
H 9.110081778885 -3.637127475798 -1.152313924405
H 8.016328742160 -3.183895729322 0.163267762359
H -1.206987966456 1.109618792999 -4.392096484723
H -0.276457138192 -0.394592901454 -4.295340953210
H -1.369932740484 0.057455964782 -2.979122708031

**5a radical cation** (*gauche*)

E(UB3LYP/6-31+G*) = -6520.56318569
Sum of electronic and zero-point Energies= -6519.779684
Sum of electronic and thermal Energies= -6519.722915
Sum of electronic and thermal Enthalpies= -6519.721971
Sum of electronic and thermal Free Energies=-6519.868224
C 0.128564713138 0.053419174902 -0.138526917060
C -0.110903530549 0.114527955654 1.270259625944
C 1.162002104964 0.096358212113 1.933925834728
C 2.171980910895 -0.005297716049 0.936548654473
C 1.534452990065 -0.025901589551 -0.341150897461
Fe 1.078890764162 1.704324540924 0.654519588354
C 2.047811921706 3.329877990703 1.449040366802
C 0.636032410930 3.586030050063 1.433007174618
C 0.195278221684 3.478979118229 0.070765986274
C 1.327585682419 3.189416057774 -0.739285321888
C 2.471477940706 3.099553047524 0.110226726871
N -0.153134422457 4.062374806818 2.531516413436
Si 0.202256625673 5.770117241548 2.947461837931
C 0.296945784003 6.707266872914 1.319989664919
N -1.387311110760 0.079138102588 1.917307386617
Si -1.911895556138 -1.498387589547 2.589102323521
C -1.599396472342 -1.575622850630 4.446636787245

P -0.778521865256 2.793938881294 3.557342142605
P -2.046971447209 1.668653370527 2.003159917238
P -3.611906724759 1.555852212935 3.637952467368
P -2.824957785465 3.612662581859 4.127805409741
N -2.956907905924 3.640060962334 5.912771512918
Si -1.693970445851 3.094078597595 7.105339625695
C -2.276328733735 3.490339659884 8.855476228310
C -4.213212246674 4.058894009270 6.321578564527
C -5.036193100559 5.081053158407 5.723277854127
C -6.232928857055 5.210555504700 6.497239909128
C -6.210313024553 4.217956539600 7.515756914573
C -5.007296547422 3.469647358893 7.363525407440
Fe -6.191399099531 3.354514496919 5.636476155709
C -7.583761526229 1.860636090789 5.634642724832
C -6.389544907983 1.385475613189 5.004794738026
C -6.185759424140 2.131382167771 3.787119141900
C -7.175154363730 3.174466608814 3.793076880497
C -8.071763792888 2.963969234852 4.880915757271
N -5.175128978100 1.968110329926 2.859110387135
Si -5.425332892502 2.344565075805 1.093075182154
C -7.278129192802 2.462879652677 0.752160285374
C -1.401970619925 1.251162473751 6.897560014651
C -0.124747457408 4.092903783742 6.829204373462
C -4.581577267537 3.973606752840 0.674551775449
C -4.817240969467 0.883960447650 0.075330944108
C -1.164314396079 6.513414199111 4.015516150781
C 1.843048582006 5.914833766319 3.867931088727
C -3.740684457012 -1.776961572007 2.220160898354
C -0.891049541022 -2.802844030971 1.701854825222
H -0.823361017508 3.616085069814 -0.262929532642
H 1.320254178223 3.032846188407 -1.809833293174
H 3.478559385989 2.860460405528 -0.205185616612
H 2.666871391375 3.314972198774 2.335575329467
H 1.308070112802 0.140695424500 3.004734210669
H 3.239261688625 -0.029007123633 1.112487068840
H 2.037562571326 -0.062232777117 -1.298400477780
H -0.640044906982 0.067702020304 -0.899464848724
H -4.724164909242 2.609472687406 7.950877731234
H -4.750703838448 5.698580649726 4.884037596530
H -7.242788709621 3.972693864449 3.069521079227
H -5.787377081749 0.550607727231 5.333339066563
H -6.980213849729 4.037435364425 8.253967978172
H -7.014541538903 5.939930073595 6.329516537428
H -8.946895144865 3.558785735539 5.105877024753
H -8.028634154923 1.447749626535 6.530538166475
H -1.780831789902 -2.591544111973 4.819772557262
H -0.560407003657 -1.317837998097 4.682799602042
H -2.251370212293 -0.894818397681 5.002167888588
H -4.060795858644 -2.722526349422 2.675915670633
H -4.395293682542 -0.989751038604 2.608443165185
H -3.911892552713 -1.853136862485 1.141004906961
H 0.472636272465 7.772719447594 1.512583253728
H 1.111368982777 6.342042421051 0.686245897932
H -0.636370594286 6.615385967413 0.753212959937
H -0.867240781196 7.540327215905 4.265249618571
H -2.116297098726 6.563094061055 3.477479089515
H -1.330803452883 5.988860133148 4.961688837254
H -0.682471760816 0.899244434691 7.647403297721
H -2.327380987026 0.679081194087 7.029833466497
H -0.993208233357 1.009908047537 5.912053801654
H -1.382611505280 3.528418457795 9.490658274530
H -2.767121711179 4.466906406775 8.929021049767
H -2.942779382331 2.736799826516 9.285936602987
H -4.728372679123 4.206675483909 -0.387729083109
H -5.012047754310 4.796858446447 1.256980433035
H -3.504746789051 3.953180155577 0.866130557244
H -7.426068568228 2.245642358186 -0.313153161679
H -7.857827699271 1.723043267089 1.315067162733
H -7.708885967640 3.451102980493 0.938223976384
H -1.226373363574 -3.802715674165 2.003336063407
H -0.999012479672 -2.724122318067 0.614792780260
H 0.174894085684 -2.719264852092 1.936398770087
H -4.902343797615 1.148363795422 -0.986622516499
H -3.784096947377 0.580538591839 0.255980880691
H -5.460785046374 0.015047396635 0.253136011356
H 2.028997010641 6.959968205374 4.145966295552
H 1.857798459149 5.322317851411 4.789478760506
H 2.681266507211 5.588651882468 3.243119804133
H 0.616851564562 3.783988231276 7.577240889939
H 0.323401903837 3.939808369118 5.845281483099
H -0.304568015681 5.164828964466 6.967278028852

**5a singlet dication** (*trans*)

E(B3LYP-D3/6-31+G*) = -6520.24152815
Sum of electronic and thermal Energies= -6520.238696
Sum of electronic and thermal Enthalpies= -6520.237751
Sum of electronic and thermal Free Energies=-6520.550077
C 4.628426229240 -2.502311564655 0.933501226166
C 4.099589806308 -2.004226829167 -0.291359796125
C 2.669414843050 -2.039635691857 -0.203360296506
C 2.328921000515 -2.554844654607 1.095963278114
C 3.538714569571 -2.840507418446 1.784137983415
Fe 3.461463711927 -0.845894337812 1.263967101229
C 2.488248205447 0.690932448805 2.219065402227
C 3.028401848823 1.158125712320 0.956259592768
C 4.443048023618 0.924286478767 0.992462907096
C 4.772333744127 0.372809060341 2.261373024595
C 3.571554635147 0.247596571117 3.019023121716
N 2.353950795388 1.867036473937 -0.054163706755
Si 3.180907176307 3.453849772419 -0.647428325249
C 1.816142540953 4.602113150127 -1.233385863619
N 1.784279445244 -1.636456332306 -1.232887346843
Si 2.198068462875 -2.056021891805 -2.995808693305
C 0.575194497369 -2.245234979114 -3.925231838357
P 0.886647000263 1.520269662349 -0.817644046515
P 0.416098232847 -0.672194721237 -1.011654488461
P -0.419856576133 -0.678571222167 1.013803955638
P -0.886267035769 1.515941765306 0.829792200298
N -2.351000304029 1.870898546064 0.065314082519
Si -3.175379381608 3.455755747392 0.666478649627
C -1.808625008291 4.599249327696 1.257164654752
C -3.025532018587 1.168297045062 -0.949591944276
C -4.440391396604 0.936794418745 -0.988311815953
C -4.769500122093 0.393228722651 -2.260670490085
C -3.568386314356 0.271312308728 -3.018408955537
C -2.485182637235 0.708805537239 -2.215248345173
Fe -3.460867456658 -0.832950262095 -1.269633462893
C -4.632020240138 -2.488482748499 -0.950210296738
C -3.542086705467 -2.824553055375 -1.801474846252
C -2.332523898393 -2.545979644570 -1.110140490443

C -2.673370929078 -2.036982978265 0.191576373894
C -4.103431410460 -1.998828347812 0.278190761876
N -1.788311214825 -1.644332604870 1.225547195392
Si -2.202324893002 -2.083198034973 2.983445993381
C -0.579544535530 -2.285945821420 3.910116086720
C -4.315576356015 2.965139841593 2.072096487725
C -4.033252774092 4.193119967062 -0.824734715147
C -3.188231699522 -0.636031915484 3.665670685190
C -3.132969005094 -3.706204188968 2.936278581663
C 4.322074191668 2.969923571380 -2.054569618151
C 4.038801392973 4.182514454248 0.848058281068
C 3.186222062486 -0.602438964113 -3.660899910124
C 3.125206141761 -3.681469724939 -2.967125001279
H 5.135453985490 1.125735661035 0.188014982767
H 5.762563916848 0.085781698823 2.588118373962
H 3.490775253488 -0.143009194656 4.024455873497
H 1.457364020956 0.758284583554 2.527793504049
H 1.332262518502 -2.733792024923 1.469023564775
H 3.615167083586 -3.230278892152 2.790304340722
H 5.677916891582 -2.583313687216 1.182203618948
H 4.677368000635 -1.635410856161 -1.126441303422
H 4.906612567583 3.608191584801 1.182230881059
H 3.347761480191 4.276847248024 1.693482006741
H 4.385767767227 5.191740967708 0.593977413657
H 1.302352315276 4.264888100134 -2.137811116016
H 2.282285090652 5.569471642226 -1.462697575908
H 1.070906204745 4.783061068877 -0.450860734616
H 4.139174220388 -3.604363472036 -2.566793035841
H 3.202534857084 -4.059874347274 -3.993840309603
H 2.585613213435 -4.432744457581 -2.379410416702
H -0.022921447307 -1.329180870358 -3.965917888289
H -0.042677615216 -3.045151668883 -3.501550562315
H 0.806215205062 -2.530870912495 -4.959410377439
H -4.901820329510 3.621601516859 -1.161764675011
H -4.378980478647 5.201380428832 -0.565193412084
H -3.342333843237 4.291183850235 -1.669841498289
H -1.295291578570 4.257208117955 2.160044674296
H -1.063183447587 4.782132454329 0.475273817946
H -2.272914284994 5.566481078515 1.490709822930
H -1.454111275823 0.777230464258 -2.523092153079
H -5.133025679820 1.134150071030 -0.183029303143
H -4.146747646908 -3.621762723891 2.536918542108
H -2.595308487758 -4.451950523212 2.339831689741
H -3.211055749524 -4.096202406335 3.958588136568
H 0.021573985973 -1.372221092342 3.958391831988
H -0.810685103276 -2.579908342787 4.941929779993
H 0.035328693411 -3.084206512002 3.478949139586
H -4.681297231153 -1.633614898226 1.114843744690
H -1.335810999806 -2.725624262252 -1.482814916453
H -5.681406194386 -2.565468456673 -1.200619672411
H -3.618329715670 -3.208091748603 -2.810048744877
H -3.487493624851 -0.113232701173 -4.026158072942
H -5.759843628784 0.109236550272 -2.589725921341
H 3.502458046061 -0.788001055567 -4.694194569304
H 2.577027718011 0.310140268544 -3.663400449222
H 4.087255771081 -0.402537122209 -3.070973196962
H -4.738327334988 3.866569392221 2.532257027738
H -5.155711343148 2.341460301358 1.749677569365
H -3.768642325658 2.422871321185 2.851738529791
H 4.746355542480 3.873819619864 -2.508476192372
H 5.161216954203 2.343503811331 -1.734899228010
H 3.775790360078 2.433126257103 -2.838369326299
H -3.501012336973 -0.831639917793 4.698170748855
H -2.579794435212 0.277019760081 3.674885101316
H -4.091444729355 -0.431229752326 3.080797359845

**5a singlet dication** (*gauche*)

E(B3LYP-D3/6-31+G*) = -6520.23118512
Sum of electronic and zero-point Energies= -6519.447809
Sum of electronic and thermal Energies= -6519.390917
Sum of electronic and thermal Enthalpies= -6519.389973
Sum of electronic and thermal Free Energies=-6519.534453
C 0.548396332459 -0.094070982749 0.245904730162
C 0.032426340350 0.089871245472 1.566330784559
C 1.146473226701 0.100832051880 2.478020858248
C 2.329740770034 -0.099066664838 1.714558523405
C 1.961959438059 -0.210587819095 0.341776287057
Fe 1.364627752705 1.611953685579 1.102672652039
C 2.318846915444 3.286183628149 1.875822330445
C 0.923526142889 3.547555565663 1.707578945175
C 0.602046361009 3.351395751378 0.318140264182
C 1.802999105296 2.995541407270 -0.355695804436
C 2.856119575124 2.947683247783 0.603937044642
N 0.026164572425 4.062382127512 2.700754357155
Si -0.168958242861 5.884431499293 2.698065692682
C -1.632440423747 6.318115294473 1.601568033276
N -1.350065093718 0.106211717968 1.947257625296
Si -2.026660915587 -1.512835634916 2.475358714755
C -1.837033325732 -1.650526760313 4.340089851165
P -0.697792691930 2.798751373446 3.582513701388
P -1.982516094602 1.685595443027 1.883299437501
P -3.612672305665 1.658087062636 3.453325179893
P -2.693644709049 3.670205108679 4.199353177914
N -2.871565958997 3.491600677637 5.911279646365
Si -1.610121425300 2.882508848269 7.136892115278
C -2.233820798033 3.266286004309 8.862115724901
C -4.146824495575 3.852739043568 6.366788806005
C -4.917170270455 5.005647681178 5.945856722543
C -6.104335838144 5.037487723129 6.724239263817
C -6.136657854036 3.875564551794 7.546314140097
C -4.953020788598 3.123203675254 7.302470263972
Fe -6.045381927381 3.337132457815 5.571164852295
C -7.608691063937 2.014325758051 5.397204615189
C -6.449019508762 1.500026852304 4.759247772920
C -6.113000772962 2.395438878960 3.670674987767
C -7.000463015683 3.519137280657 3.757099361420
C -7.940278099648 3.260880917187 4.794678094196
N -5.083396992073 2.220667771813 2.735983461641
Si -5.408125719136 2.612314989496 0.945530372599
C -7.257658748870 2.805321042499 0.711913068090
C -1.381340970306 1.044865425033 6.840880624413
C -0.042967035452 3.882177607366 6.860204318911
C -4.458013825813 4.175187434071 0.531364951937
C -4.858642565984 1.119447549983 -0.055145509876
C -0.436637146126 6.475104933452 4.462803135319
C 1.434213389742 6.561551457825 2.007676590609
C -3.831720328638 -1.620496818957 1.960580040242
C -1.003754901184 -2.801758117653 1.582237744192
H -0.373128315150 3.485605196783 -0.127631682131
H 1.893995522194 2.769619919128 -1.409775594093

H 3.883197975882 2.673533022016 0.403199134391
H 2.854143066451 3.331760885110 2.814603544685
H 1.080936999383 0.209062145094 3.551185084533
H 3.337770819398 -0.129554054568 2.106158783997
H 2.644653428567 -0.334831229528 -0.488185770854
H -0.045096165931 -0.125777804326 -0.657803670869
H -4.694106154139 2.177516616624 7.755204261856
H -4.590246313287 5.757210194503 5.241147627764
H -6.969168115598 4.397349586640 3.129350489062
H -5.961858401429 0.559050954136 4.972742970631
H -6.933956453734 3.598018853705 8.222624089755
H -6.870320352795 5.799675604375 6.669924993936
H -8.751655176925 3.912817876980 5.089226571333
H -8.126666995124 1.550935759137 6.226410648477
H -2.106730075768 -2.661752342492 4.668714074782
H -0.803227579817 -1.469980866393 4.655258375249
H -2.484938573072 -0.943068728277 4.867771931903
H -4.226568770646 -2.584187928759 2.306303273199
H -4.475905202584 -0.842188350688 2.383030379492
H -3.936514902480 -1.596427059795 0.871322621931
H -1.691112201719 7.405567329967 1.470121841769
H -1.535769881231 5.873737491640 0.604644948873
H -2.579279166258 5.981892763504 2.036529323952
H -0.576974441569 7.563170115529 4.439256224843
H -1.315726005309 6.051185761682 4.959493969539
H 0.439295809109 6.272204132941 5.087005548460
H -0.699466585791 0.635344678400 7.596518338155
H -2.327983641328 0.499357744030 6.924089613825
H -0.949803734827 0.831468174164 5.858132590954
H -1.364382168853 3.256489529098 9.531513024555
H -2.684369890750 4.262084009111 8.931362970765
H -2.949535477451 2.537410403153 9.251233818521
H -4.685952927074 4.479285306497 -0.497813737124
H -4.737924157597 5.006494152297 1.188042119844
H -3.374899471896 4.035263501250 0.600854047638
H -7.466568503975 2.663553060336 -0.355975266627
H -7.828806462000 2.046296796766 1.256959617299
H -7.643136615835 3.790056722493 0.988672089727
H -1.398693174097 -3.797244931777 1.819067178451
H -1.046880402819 -2.677479458251 0.495134949952
H 0.047920774484 -2.781830460390 1.885016261030
H -5.018479514338 1.363995872263 -1.113362110795
H -3.811186657703 0.826971206570 0.050176440481
H -5.484033859492 0.252468212132 0.180520346349
H 1.398130987859 7.657530821876 2.031856575253
H 2.300267991065 6.244778506740 2.598195602265
H 1.601732723584 6.258281403958 0.969378503784
H 0.712011150669 3.498145181473 7.558557172785
H 0.392237070835 3.830124872150 5.859371757761
H -0.214704660107 4.934741358287 7.107064157167

**5a triplet dication (*trans*)**

E(UB3LYP/6-31+G*) = -6520.34889218
C 0.032818022113 0.053473123202 -0.028974068418
C 0.039926987946 0.040029666444 1.398065410949
C 1.400809105511 0.020934053688 1.824037555786
C 2.230447787143 0.039714583281 0.660019333156
C 1.389315199684 0.119217358544 -0.499455063518
Fe 0.989411267413 -1.663071193962 0.703028085317
C 2.133020929163 -3.432988002845 0.734247652617
C 1.287270831975 -3.514747088863 -0.421707891515
C -0.062806335654 -3.353039426893 0.044013996096
C -0.053129807930 -3.279017806776 1.469179605575
C 1.307225542535 -3.318011539418 1.895471517711
N 1.648761420867 -3.689809495235 -1.757701508434
Si 0.629056988271 -4.825588827457 -2.800235029080
C -0.073363154659 -6.134114434341 -1.648819671548
N 1.758534713206 0.216496975296 -1.841261864637
Si 0.803112982651 1.362357425290 -2.932516070485
C 0.176558260852 2.756086570335 -1.838737342704
P 2.966965209622 -2.948314844914 -2.610304592608
P 3.031943773067 -0.633612736005 -2.659907542850
P 4.883497707296 -0.658566105525 -1.386891897791
P 4.818717294503 -2.973278453216 -1.337552409867
N 6.092046780556 -3.823185437975 -2.156533641818
Si 7.047564540873 -4.969312528723 -1.065626097448
C 7.673954698753 -6.362828923929 -2.159773176554
C 6.461116247809 -3.725589806511 -3.498348918587
C 5.619859119123 -3.645634665478 -4.657704686858
C 6.449367517744 -3.626652617307 -5.821817245515
C 7.810294231848 -3.646048961576 -5.396007047283
C 7.817565633385 -3.659879378802 -3.968974568271
Fe 6.861102813737 -1.943012962839 -4.700401949345
C 6.543608249451 -0.287706581874 -5.892439688627
C 7.903920751661 -0.327001415982 -5.466030738498
C 7.913474531435 -0.253356655712 -4.040842394890
C 6.563372369802 -0.091611010218 -3.575210726026
C 5.717720941977 -0.172922224334 -4.731266426192
N 6.201767920840 0.083142387054 -2.239199018377
Si 7.221389361435 1.218677828960 -1.196338513912
C 7.924003547442 2.527380160900 -2.347433114660
C 5.869978118014 -5.664802107021 0.223956496933
C 8.425296192711 -3.981954053851 -0.255536197650
C 6.086142102859 2.033029919786 0.061237023035
C 8.542265924987 0.190431524566 -0.343539845115
C 1.764175205287 -5.640135532906 -4.057795337862
C -0.691954014912 -3.797547703154 -3.653075677683
C 1.980842087268 2.057594664067 -4.222109360820
C -0.574501480822 0.374797265053 -3.742558225911
H 8.697298735826 -3.629823134396 -3.341205255185
H 8.683519900271 -3.626490181684 -6.035348530308
H 6.097431120574 -3.598380996463 -6.845085916962
H 4.540150264095 -3.632366842527 -4.649717282490
H 4.638984450605 -0.125076939745 -4.724145362272
H 6.189555223963 -0.339303991030 -6.914066616776
H 8.773981455518 -0.422653809383 -6.102825777939
H 8.790781275282 -0.306340861830 -3.411195175960
H 8.492238359049 -6.080142804057 -2.828905100611
H 6.866550331249 -6.784161400715 -2.770979770205
H 8.048679526549 -7.168590688236 -1.515687005907
H 5.607834673298 -4.938570872711 0.999453090606
H 6.367814256068 -6.510344073929 0.717183729708
H 4.943900044224 -6.046278981873 -0.222340954883
H 8.724134419195 2.171069595239 -3.003235466134
H 8.344466707051 3.337062127444 -1.737396835142
H 7.140852831403 2.967551929875 -2.976655577434
H 5.784451200563 1.356041795075 0.866343070610
H 5.182477563677 2.446755349999 -0.401956710133
H 6.631228250035 2.869327470091 0.518995109853
H -0.873450437196 -5.777741208318 -0.993001409102

H -0.493835894499 -6.943937569301 -2.258662007166
H 0.709881685358 -6.574118872829 -1.019597237007
H 2.065773299894 -4.963282624652 -4.863049694948
H 2.667896009695 -6.053777512351 -3.594638233840
H 1.219040423146 -6.476513629684 -4.515348939300
H 3.211761984946 -3.480729278112 0.727049643086
H -0.940184528364 -3.300327104121 -0.585555198508
H -0.641707824616 2.473478375448 -1.169548669810
H 0.983909242057 3.177653016513 -1.227621439533
H -0.198237522105 3.561647794981 -2.483032926671
H 2.243060281906 1.331208560030 -4.997435892895
H 1.483071597231 2.903046685780 -4.715556591771
H 2.906874915532 2.439147347290 -3.775781688463
H -0.846833776701 0.023143435189 -0.656845331786
H 3.310157691217 0.026550332068 0.652152968218
H -0.833368540173 0.020536469108 2.037313430921
H 1.752630937059 -0.007018525330 2.847354518975
H 1.661366445280 -3.266100232422 2.917051945267
H -0.923144836548 -3.183306018325 2.106028167036
H 9.154438012873 0.819541862352 0.314869586086
H 8.088125601167 -0.591119019207 0.278051041021
H 9.222853665833 -0.299485077887 -1.049862027139
H -1.304335043733 -4.426850545510 -4.311106517174
H -1.372327337095 -3.307315359972 -2.946766422037
H -0.237904153234 -3.016261517808 -4.275064830358
H 9.002253567953 -4.616292731294 0.429132954486
H 9.131181030881 -3.560940712353 -0.981196894101
H 8.016624802392 -3.150852420064 0.332424009627
H -1.151271888311 1.008929830820 -4.427575853465
H -0.165751177105 -0.456536496156 -4.330135292837
H -1.280572555771 -0.045915701077 -3.016904442608

**5a triplet dication (*gauche*)**

E(UB3LYP/6-31+G*) = -6520.35316149
C -0.090327614180 -0.132693773380 0.178139027905
C -0.070094437475 0.049677546250 1.591201106319
C 1.296370867031 0.069969377345 2.018055423678
C 2.133006309898 -0.178316803435 0.872829823455
C 1.261220992425 -0.209186401528 -0.268326351932
Fe 0.877887210251 1.638154441693 0.684130454794
C 0.755816025086 3.500002930198 1.676812029063
C 1.928756353547 3.581966403109 0.851773213975
C 1.507526456688 3.264073661374 -0.487890510305
C 0.082074632407 3.130270775727 -0.492664828756
C -0.382158938806 3.286023873023 0.845484095342
N 3.221887485356 3.848921730341 1.304146999805
Si 3.492495531543 5.148547637749 2.569189082754
C 4.899916472406 6.263792076681 2.010447385518
N 3.523191619373 -0.296918611624 0.835206223643
Si 4.300344004528 -1.538689333305 -0.267702784239
C 5.585622232002 -2.505204244215 0.707380303790
P 4.404470487778 2.765252132396 0.558398439111
P 4.302635608040 0.895103771841 1.884257798430
P 6.497991115273 0.806171075631 1.418978077629
P 6.335342811478 3.082205317382 1.661164944878
N 7.492615503081 3.693667874324 0.471393857681
Si 7.195076633980 4.201061052554 -1.265394638647
C 8.706857917339 5.147928563895 -1.863995226527
C 8.789678902453 3.717415844666 0.986305176785
C 9.211425142362 4.108212688803 2.306292553677
C 10.640015791421 4.032731653738 2.364090554245
C 11.107838846896 3.525397468064 1.117402387203
C 9.969406100893 3.273440781154 0.297500266555
Fe 9.893422997407 2.134202737255 2.076122081168
C 10.890333093804 0.331425571399 2.055366756395
C 9.526773395330 0.103177237684 1.683219897158
C 8.689398691410 0.424390644245 2.809565942980
C 9.553849271646 0.979602424811 3.813434183635
C 10.905842092587 0.864451615286 3.376783040496
N 7.302768153425 0.301464623589 2.910973683202
Si 6.552757885897 -0.262534053684 4.486379234714
C 7.906498518761 -1.051246380123 5.528341672712
C 6.891858823685 2.661455367951 -2.298171019659
C 5.753361200866 5.407685039790 -1.313127371967
C 5.789640579430 1.218943594604 5.353487882031
C 5.301496242165 -1.617539002788 4.118760775975
C 1.951051197590 6.225291506643 2.639130086523
C 3.830571748878 4.319320152874 4.220546457540
C 2.976746041741 -2.773669111876 -0.780787134118
C 5.028658987344 -0.650864902526 -1.754405812132
H 9.987517369255 2.830339670446 -0.688042313125
H 12.138468329655 3.330579296726 0.850442794693
H 11.251803686116 4.312431418875 3.212351752711
H 8.563398060161 4.461943765857 3.096685963236
H 9.228278060351 1.405277102115 4.751916293023
H 11.781972635082 1.163416585258 3.937527027127
H 11.754533447101 0.133088968095 1.434172683977
H 9.187266429587 -0.303983179527 0.740496122363
H 0.741317414611 3.596161968095 2.753143857572
H 2.152223535419 3.203314991528 -1.354171543362
H 1.581905123084 -0.288407972409 -1.297322409584
H 1.639890413367 0.185200973460 3.037116573544
H -1.409245798374 3.218415539772 1.180056455105
H -0.530039175606 2.941184260785 -1.365374914376
H -0.970057972867 -0.170294676223 -0.451207172299
H -0.933172321131 0.157239009616 2.235862185473
H 5.526259974762 0.955347023303 6.385975673354
H 6.491363946636 2.061122152062 5.396878576372
H 4.877476057890 1.566435877817 4.859433795034
H 4.793487777109 -1.868500875383 5.059636920843
H 4.527505033712 -1.365528041477 3.389388693419
H 5.812379501472 -2.522627420410 3.772197115280
H 6.922129209801 2.913339630846 -3.366121634542
H 7.661660479704 1.901168040370 -2.116675500414
H 5.917182061648 2.208388524624 -2.094177182780
H 5.528093895509 5.618670767524 -2.367188057579
H 4.827509329995 5.061904032302 -0.846458367139
H 6.036181567984 6.356305368648 -0.843632777968
H 3.785723226907 5.060162253282 5.029254820528
H 3.083290223169 3.546503521663 4.439408074281
H 4.818787228495 3.851378958563 4.257053083736
H 2.250296269073 7.187947794917 3.074275114048
H 1.537682522986 6.438199643087 1.646525519380
H 1.148017061724 5.829922596900 3.268162399533
H 5.308729779904 -1.378892543777 -2.526681563908
H 4.303516146337 0.040886872109 -2.200751066977
H 5.925988702707 -0.079167708867 -1.499802488876
H 3.494922684473 -3.691165680310 -1.089501693208
H 2.308860764306 -3.046343838238 0.044464696455
H 2.362976608577 -2.456475718237 -1.629052320229

H 7.411879050075 -1.715271962710 6.249476178386
H 8.588413926650 -1.673225907710 4.937090090040
H 8.504241451061 -0.342669543044 6.109307070810
H 6.107509030541 -3.170184047093 0.006134847714
H 6.346796419078 -1.907337709284 1.215026127310
H 5.097108058722 -3.138834720745 1.455823184505
H 8.384190915870 5.767257144937 -2.711300484551
H 9.108179727680 5.829261741590 -1.104932787305
H 9.524219462249 4.517414876648 -2.226308069030
H 5.110959814468 6.970072135567 2.824655542618
H 5.838609534028 5.759786538183 1.766756262712
H 4.594720243126 6.852699618726 1.138481413510

**5b neutral compound** (*trans*)
E(B3LYP-D3/6-31+G*) = -6992.40559204
C -0.179842576400 -0.048035770502 0.053181719207
C -0.143049360126 -0.046804349732 1.480503500514
C 1.229179295344 -0.009367424187 1.901025070643
C 2.035806414746 -0.024993311878 0.712820758103
C 1.167289574338 -0.046135690094 -0.418940130826
N 1.655285517860 0.175931617046 3.252796068881
Si 1.044956473696 1.632368215652 4.150258857131
C -0.292126534723 1.203696156034 5.474451667241
C -1.483939191221 0.444781491995 4.856074895064
Fe 0.809500099157 -1.708442042608 0.747929283209
C 1.077618248282 -3.341469589406 -0.482634988868
C 1.941214718462 -3.454398378969 0.647432298977
C 1.132482172054 -3.471533419256 1.834180013404
C -0.234716082847 -3.342148002643 1.415424086128
C -0.268343169274 -3.283561141741 -0.010788436518
N 1.545021639239 -3.731969325854 3.177719229842
Si 0.851731343772 -5.184343407135 4.019788364452
C -0.461006521613 -4.730841165097 5.359915401060
C -1.605991434097 -3.881279336375 4.771639278924
P 2.938397487887 -0.672064412032 4.062880805542
P 2.872757477676 -2.989294578633 4.018986433967
P 4.726610286427 -3.016251691319 2.701353046215
P 4.792289350880 -0.699026847158 2.745295992579
N 6.120043801593 0.043616256141 3.586566106718
Si 6.813320580216 1.496008507691 2.744519189926
C 8.126044359347 1.042535474004 1.404368962598
C 9.271055033091 0.192990840779 1.992620409235
C 6.532658713379 -0.216873757094 4.930072420119
C 7.899886751214 -0.346236431512 5.348737689196
C 7.933605890384 -0.404901764086 6.774944672055
C 6.587672757353 -0.347062844424 7.246878189262
C 5.724001557948 -0.234098122943 6.116871612543
Fe 6.855766676087 -1.980013530832 6.016206253984
C 7.808291136473 -3.641578296949 5.283429537508
C 6.436015868794 -3.679036668599 4.863061925735
C 5.629524080189 -3.663507879180 6.051360287474
C 6.498168720871 -3.642398263522 7.183022868387
C 7.845246948909 -3.640424385972 6.710747462656
N 6.009771629851 -3.864285410509 3.511325228425
Si 6.620054290184 -5.320670571915 2.613752281004
C 7.957005197762 -4.891887258087 1.289465991377
C 9.148820074971 -4.132927262422 1.907785118252
C 7.582823597255 2.617832350422 4.061694539213
C 5.425093819172 2.483870254908 1.916368743939
C 7.324177074882 -6.533114587411 3.886431684533
C 5.178584985368 -6.196395901892 1.751062743141
C 8.730910013765 2.355939941411 0.849796968039
C 7.486962903006 0.266153193941 0.232962251732
C 8.485405858776 -6.215499155616 0.683479643150
C 7.363877129448 -4.035365263610 0.150187501082
C 0.340993921136 2.844787845453 2.877466377819
C 2.486369168540 2.508084687303 5.013051736707
C 0.082241819953 -6.306197410295 2.702631705206
C 2.239950002764 -6.172191438862 4.847969623965
C -0.820500678644 2.527358320529 6.080351103569
C 0.300865799789 0.347182951858 6.613806884320
C -1.065908813471 -6.044229261976 5.914485898826
C 0.178066946496 -3.954465348141 6.531330307854
H 8.755539894146 -0.393669045311 4.690307100078
H 8.821328863525 -0.515683254851 7.385194812915
H 6.270330269252 -0.407096647089 8.280633405769
H 4.645636579259 -0.177218784611 6.144054414304
H 4.549640412780 -3.661769604275 6.078608409375
H 6.184714490249 -3.605290096615 8.219039559498
H 8.737747679680 -3.602542708109 7.322900881611
H 8.665178268852 -3.615771916736 4.625402222183
H 8.538447489703 2.252603872435 4.450102144705
H 6.907069272138 2.739307919237 4.916345047287
H 7.754583866078 3.612437792588 3.630474603572
H 4.972051261898 1.966953249819 1.065743557848
H 5.821580521063 3.442663661916 1.556728614171
H 4.625173291961 2.711267871505 2.629444426101
H 8.298390369322 -6.237007651496 4.287296168628
H 7.440278024344 -7.518744252492 3.417659135615
H 6.641847202232 -6.648775022822 4.736656941473
H 4.756383713280 -5.623177523533 0.920889803362
H 4.366379324447 -6.404511983386 2.456085431426
H 5.520306356088 -7.162037374016 1.355344214959
H 7.973786626982 3.000421585223 0.386425448375
H 9.476713375792 2.125468068704 0.074230202326
H 9.240668879768 2.938706775724 1.626914027517
H 6.700677074604 0.844911907810 -0.265996102162
H 7.043001174274 -0.680701901065 0.558958467303
H 8.250579631252 0.030079103035 -0.523828188330
H 8.910491372992 -0.769988085828 2.370754083563
H 9.791162398720 0.708773391749 2.810101349619
H 10.021503148102 -0.021064213265 1.216670054814
H 7.692543517514 -6.796946596528 0.197083863862
H 8.960525700097 -6.856217708881 1.436566027510
H 9.243477383719 -5.998591640049 -0.084066009074
H 6.545482012812 -4.548103792737 -0.368939499018
H 8.139884421488 -3.814775373106 -0.598628705491
H 6.975353672680 -3.077723067124 0.513339283083
H 9.638129960838 -4.708911453660 2.703791331511
H 8.844111275251 -3.166113755890 2.323400956740
H 9.910558087180 -3.932543680342 1.139221685699
H -0.633192753121 2.548700105746 2.476523519045
H 0.224884981491 3.830441327988 3.346187125064
H 1.023406311974 2.960388996209 2.027299161782
H 2.908443058615 1.934908689996 5.843318469921
H 3.298670598314 2.716108971303 4.308113291434
H 2.144645333499 3.473772180826 5.408656388959
H 3.115693792201 -0.026765701485 0.685694199929
H -1.000012584234 -0.072545450158 2.138433115065
H -0.873379152821 -5.940979944299 2.314206845735

H 0.758004857439 -6.427693033839 1.847991049402
H -0.089519948453 -7.300792162238 3.133875315390
H 2.692992183788 -5.655254113198 5.698582598319
H 1.843458675963 -7.130973366646 5.207635859030
H 3.039870875304 -6.399611666511 4.134900836697
H -1.090407934407 -3.294649684818 2.073799411626
H 3.019580745446 -3.511304837253 0.620325641741
H -0.027642501377 3.108778795547 6.566785442087
H -1.295528054775 3.168076245707 5.327205823272
H -1.578642394900 2.310520512972 6.847847118237
H 1.119249735780 0.859893787228 7.132978842762
H -0.475211242196 0.126663161235 7.362571592376
H 0.689362854021 -0.610494053387 6.250719632007
H -1.973159633211 1.020763082932 4.060011963498
H -1.179254896994 -0.522065704644 4.440520104989
H -2.245743738348 0.244470582571 5.624591310525
H -1.156024057710 -3.172785503697 -0.621100849176
H 1.395027054042 -3.281503871875 -1.516373747167
H 1.480861220844 -0.083313640374 -1.454918839602
H -1.072274717482 -0.085921085187 -0.559071409722
H -0.308803498133 -6.688729802353 6.377861050652
H -1.811708824581 -5.813736947336 6.690049893371
H -1.575680577758 -6.626984375258 5.137368264352
H 0.964327638479 -4.533240598431 7.030308863604
H 0.622059859886 -3.007623820995 6.205337792354
H -0.585561546617 -3.718369047397 7.288101775284
H -1.245400544091 -2.918315702815 4.393493419589
H -2.126104051648 -4.397062930972 3.954162316172
H -2.356442150463 -3.667193913165 5.547578794620

**5b neutral compound** (*gauche*)

E(B3LYP-D3/6-31+G*) = -6992.61772663
C 4.361110652360 -1.093904264776 -0.423790258370
C 3.540536837225 -0.734463650946 0.694290641297
C 4.267073661409 0.229879106451 1.471241163190
C 5.551638742839 0.401944021295 0.874738259245
C 5.603085769723 -0.405867526046 -0.304051222522
Fe 4.088666018314 0.972950277451 -0.438748444471
C 3.436410624406 2.934752220888 -0.334442072355
C 2.471493400958 2.214329411391 -1.116556906136
C 3.180592559326 1.598187644760 -2.200694392147
C 4.543205164783 2.017077885606 -2.144344779608
C 4.702261223816 2.841190816606 -0.985526285153
N 1.046527539510 2.223542497118 -0.962982488888
Si 0.207477930009 3.241633009438 -2.173640395445
C 0.526841234616 2.570286322803 -3.915881943960
N 2.267935426858 -1.299969231538 1.020605027050
Si 2.214148054459 -2.132685461588 2.600402436224
C 2.498897859595 -0.932426040534 4.042071292182
P 0.575756990609 1.331902259739 0.501416482999
P 1.150435812049 -0.756067776622 -0.218776283662
P -0.942407189174 -1.534150241665 0.210357762397
P -1.535009266135 0.635826062693 0.009379237233
N -2.553786170905 0.874519955669 1.417968547974
Si -2.275469558539 1.548547600994 3.036853670331
C -3.655623322839 0.916910723468 4.166890169149
C -3.859566063827 0.391123344811 1.086060897388
C -4.762609369377 0.960719071527 0.134121333859
C -5.974420969694 0.212904116301 0.169571184508
C -5.823945839094 -0.834177536319 1.134038530542
C -4.507142841045 -0.745803940353 1.677151825594
Fe -4.442729020919 -1.047590333557 -0.354972155703
C -5.114677362773 -2.757855072416 -1.249103397317
C -3.785136441828 -2.982390948517 -0.785184116413
C -2.916951274026 -2.060771042194 -1.451486178535
C -3.732477250060 -1.222919310228 -2.283531394213
C -5.081548804834 -1.676131372069 -2.186966243775
N -1.487820362629 -2.036443657607 -1.402710999107
Si -0.632187760902 -2.795554864647 -2.765883350970
C -1.929355210578 -3.135344789099 -4.098452441761
C -0.629690112807 0.938393557931 3.732595872207
C -2.354417828575 3.468734585069 3.024080033453
C -3.739914818560 3.911386276263 2.504557227731
C 0.679507084416 -1.673096018891 -3.543611467932
C 0.159215830793 -4.468645923036 -2.250907126382
C -0.935985537842 -5.440635261238 -1.763691552615
C -1.670955992858 3.258434143490 -1.976938589438
C 0.821772816259 5.076285823250 -2.111042690877
C 2.243901361724 5.237691230905 -2.692579539393
C 0.540528580826 -2.951808324941 2.889364237847
C 3.581183097347 -3.495497600150 2.658844597267
C 5.013225334488 -2.920954190138 2.729901275526
C -0.131120586834 5.948039907411 -2.965103862272
C 0.781620815592 5.603356883634 -0.663197999049
C 3.351587539361 -4.348263544399 3.931260161351
C 3.470173737386 -4.407728201550 1.422093683176
C -2.147618820873 4.006025403340 4.458031673069
C -1.266677822396 4.076749263221 2.120226624651
C 0.882148892956 -5.085487736923 -3.470211000490
C 1.188694293976 -4.278319599876 -1.122502165627
H 2.732949270100 0.939455739964 -2.931921157252
H 5.328812202044 1.723674449900 -2.828910760745
H 5.629522674754 3.283828414527 -0.643876543480
H 3.223553435591 3.474068541063 0.577846834734
H 3.899822512346 0.731918541962 2.354052955335
H 6.331915911690 1.065112232285 1.225393888565
H 6.429236406604 -0.460038012138 -1.001529793229
H 4.070398181285 -1.774141189036 -1.213044285072
H -4.061835428619 -1.395690690964 2.418379962680
H -4.537575660027 1.808485233909 -0.499732257514
H -3.356902856962 -0.410319625250 -2.890660058449
H -3.467112883317 -3.725501743752 -0.066774181487
H -6.560245660864 -1.589423985639 1.377177795970
H -6.844409985184 0.385623957353 -0.451433537710
H -5.934757274448 -1.249740701021 -2.699032098672
H -5.999361800673 -3.289072267970 -0.921019067572
H 0.251254523766 6.978844806240 -3.011761615942
H -0.211553657794 5.587175117682 -3.999031061678
H -1.141381246327 5.997152300895 -2.543406816359
H 2.549895614938 6.294060997600 -2.641099437176
H 2.990392119575 4.651672048121 -2.151479698211
H 2.284892059914 4.939026887898 -3.747256709501
H 1.089576797054 6.659711319451 -0.630780276519
H -0.227568805476 5.543294849821 -0.237193618822
H 1.449493764205 5.042549910317 -0.003892707331
H 1.342069584602 -6.045486102610 -3.190461814893
H 0.199168251082 -5.284297339757 -4.305596158312
H 1.686532238543 -4.435580011681 -3.839325172776
H -0.489523233284 -6.405274308020 -1.477668138343
H -1.461335378133 -5.046574930464 -0.885927855553

H -1.685773088506 -5.643770347877 -2.538390756836
H 1.671780979198 -5.236042520382 -0.878625031289
H 1.983309100615 -3.574594953696 -1.397123760793
H 0.725643598674 -3.909589928953 -0.200203736499
H -2.180389721626 5.106075055157 4.458236014451
H -2.925352676635 3.660007490949 5.149904025773
H -1.174024464072 3.709127560620 4.869689134079
H -1.345556879491 5.174627938091 2.114950461216
H -0.254116559234 3.823670627605 2.455703940131
H -1.363081536492 3.739129413461 1.084368083563
H -3.808857551360 5.009755179909 2.490020830061
H -3.922923614882 3.552872286182 1.484574712310
H -4.555299879433 3.540882929593 3.137817431138
H 4.144861366417 -5.105585637823 4.020404887554
H 3.379101607702 -3.742254559922 4.846786327720
H 2.395433215431 -4.883553205786 3.907392094494
H 4.216629936454 -5.214907679030 1.474489460595
H 2.483228508959 -4.878612283682 1.350032414460
H 3.641602212259 -3.852444029718 0.494148505362
H 5.735969475612 -3.746309166968 2.820861235273
H 5.281806437537 -2.347185691027 1.839537677268
H 5.153717783313 -2.271687743986 3.602516486511
H 2.104414301889 -1.373011852730 4.967021676163
H 3.559453632309 -0.715127200772 4.205339379670
H 1.976769358924 0.016436779834 3.882366999213
H 0.567930627649 -3.421813282614 3.880236267703
H -0.289873818666 -2.241006165414 2.887786879903
H 0.305568682276 -3.727106179821 2.153018676330
H -0.012412837121 3.193944537358 -4.641841755119
H 1.583729983366 2.572314511542 -4.198282948389
H 0.150919280132 1.545156957924 -4.018371445477
H -2.070566913823 3.885081745237 -2.784045196726
H -2.100836693393 2.260439272063 -2.081334986233
H -2.025882796742 3.679076576035 -1.030781584310
H -0.715817593945 0.775965391397 4.814400963119
H -0.357873973040 -0.019805823460 3.277057187010
H 0.196051458100 1.633297098926 3.559546817747
H -3.613290010611 1.447952185117 5.125344870644
H -4.654765516375 1.060247745500 3.743921447840
H -3.534038397112 -0.152232578509 4.376922077090
H 0.793608170423 -1.935819490493 -4.603731138536
H 0.363516880121 -0.625701741482 -3.486841159481
H 1.658566415601 -1.741460585196 -3.062775932819
H -1.465158871741 -3.692154633705 -4.921307373075
H -2.777454607159 -3.718483052371 -3.724530164285
H -2.328975243941 -2.202498610135 -4.511580981681

**5b radical cation (*trans*)**

E(UB3LYP/6-31+G*) = -6992.19973688
C -0.237297588021 -0.042653980919 0.066514827908
C -0.205103133399 -0.043534005731 1.492797741082
C 1.167355738823 -0.021058015438 1.907619566205
C 1.977948140606 -0.028397146279 0.722446551262
C 1.108417305964 -0.042489627806 -0.407179543515
N 1.619019980387 0.172011600286 3.257212639891
Si 1.037331320782 1.675651545782 4.162846495984
C -0.314476053603 1.249217070130 5.460033902567
C -1.521086453703 0.523320907205 4.830267241856
Fe 0.756377948996 -1.706983190083 0.768629636967
C 1.016323892264 -3.342179830882 -0.470537606153
C 1.881952838412 -3.448435612502 0.657171580047
C 1.070424029330 -3.455854904886 1.841701293699
C -0.297977681154 -3.340473855354 1.428897119729
C -0.327983235603 -3.284741741356 0.003650841039
N 1.508536702153 -3.725585123867 3.182586991139
Si 0.841417451549 -5.227278218542 4.030710765440
C -0.485912565552 -4.774729294918 5.344202524730
C -1.648632488150 -3.958204829347 4.743518445760
P 2.865200887865 -0.705527969486 3.997852831596
P 2.801569270668 -2.949033875723 3.955071928107
P 4.799708097029 -2.982879233099 2.766233195274
P 4.863362926373 -0.739380166506 2.809029608386
N 6.156367311910 0.037135732943 3.581593205533
Si 6.823586775722 1.538799711361 2.733499002653
C 8.151036810197 1.086192126189 1.420145106878
C 9.313710124280 0.269699678868 2.020962605351
C 6.594419050955 -0.232629317933 4.922488858339
C 7.962806301108 -0.347951105198 5.335352865019
C 7.992748260379 -0.403756080782 6.760597163378
C 6.648415478394 -0.346422425106 7.234725149866
C 5.782832802961 -0.240155621450 6.106980522416
Fe 6.908514191838 -1.981537381449 5.995483752556
C 7.870072890931 -3.644884515958 5.271190688605
C 6.497601294394 -3.667418929611 4.856416004871
C 5.687045674046 -3.660205663065 6.041613479587
C 6.556611099398 -3.646118702925 7.171212055793
C 7.902311601968 -3.645845706465 6.697473953553
N 6.045910589958 -3.860429491726 3.506824061683
Si 6.627808605274 -5.363886404740 2.601034721537
C 7.979682913944 -4.937037948934 1.304063450938
C 9.186152963895 -4.211197360702 1.934165965430
C 7.508207633499 2.667833309327 4.077960559996
C 5.379823227741 2.418195650465 1.886241810821
C 7.246766083063 -6.580215965725 3.900430487924
C 5.137302470486 -6.127448398741 1.722943883616
C 8.724141483365 2.412053698157 0.857638257228
C 7.530309610318 0.283221143002 0.256156269201
C 8.477325185801 -6.270657457290 0.690415509294
C 7.406255442960 -4.056259000779 0.172549951965
C 0.418463335730 2.891886420295 2.863319269143
C 2.528010647715 2.439124698439 5.040711444308
C 0.156670306044 -6.356293792272 2.686298309366
C 2.285275043835 -6.106680884061 4.877798748653
C -0.811948622430 2.583025569600 6.073411120099
C 0.258999180647 0.368684143216 6.591712311870
C -1.058981910407 -6.100610496127 5.906699765273
C 0.134915743894 -3.971820445903 6.508178511461
H 8.819728303048 -0.391252692170 4.678896029552
H 8.880203746766 -0.511024212210 7.371095328702
H 6.334521458380 -0.401632318407 8.269358927953
H 4.704541012055 -0.177316261562 6.137610829247
H 4.606900214782 -3.663724806217 6.071521113454
H 6.245755385012 -3.613385966986 8.207717177436
H 8.794044104979 -3.612034926327 7.310221466032
H 8.728414885155 -3.624338003714 4.615475168214
H 8.462840762407 2.329115860413 4.491535604808
H 6.804185187361 2.768588879884 4.911869150899
H 7.665345370738 3.668448056116 3.655722895432
H 4.931827843728 1.850173412520 1.065364126936
H 5.739275874116 3.367220738240 1.467969500402

H 4.585379219750 2.664269520471 2.598952985674
H 8.218602382979 -6.311742402572 4.325351075849
H 7.347734446865 -7.571203554656 3.440044823047
H 6.537528879272 -6.673049749933 4.730831565050
H 4.722331829809 -5.503911430221 0.925329634848
H 4.329950273791 -6.355786601430 2.427000846482
H 5.443022044340 -7.078332972732 1.267793483264
H 7.954831539388 3.035636627567 0.386447535238
H 9.476068808320 2.193003522259 0.086532901455
H 9.219638643806 3.011179798905 1.630963466491
H 6.736619264310 0.838720116925 -0.257088201447
H 7.109538670792 -0.673206142584 0.590272544302
H 8.300875906487 0.052628897335 -0.493393564601
H 8.979731065993 -0.706268455400 2.391996319114
H 9.812062837328 0.799547609903 2.842252438020
H 10.076049687614 0.080446847144 1.251915174654
H 7.674298271099 -6.831272388388 0.196885026753
H 8.937642802098 -6.925984003618 1.439519396597
H 9.240942628685 -6.065108635083 -0.072879016129
H 6.582732433554 -4.545887972225 -0.360380648255
H 8.189174230573 -3.841170628364 -0.568762805880
H 7.040107601133 -3.091019890410 0.543609474669
H 9.653298646887 -4.799613288059 2.733636108542
H 8.907461094424 -3.233029745152 2.343123138373
H 9.958463914474 -4.035633429554 1.171848530089
H -0.553438023999 2.623493923115 2.438497283263
H 0.317670346418 3.882956943741 3.323565309462
H 1.127662185868 2.984494338792 2.032859821983
H 2.942950196907 1.815640066389 5.838383372343
H 3.335341779948 2.667243534668 4.336558903787
H 2.222463725498 3.390120149635 5.495744463663
H 3.058094859162 -0.024942627393 0.692568813150
H -1.063467035434 -0.063988543967 2.148481310665
H -0.798011653878 -6.017580764627 2.272833340142
H 0.860603330400 -6.457029338545 1.852311992265
H -0.000411162235 -7.356916698862 3.108537673657
H 2.733341402693 -5.538681021919 5.698653425272
H 1.925878490204 -7.055726355146 5.296072378755
H 3.079654540083 -6.352715274997 4.165001893200
H -1.154865424826 -3.297087242086 2.085392713962
H 2.960239426876 -3.511335514667 0.626497133155
H -0.008849322956 3.143658221659 6.566803560575
H -1.272212461956 3.238241342695 5.324177671668
H -1.575570706150 2.377727317746 6.836768791690
H 1.082595613615 0.858397448464 7.124452818356
H -0.523866050056 0.153816298811 7.333145689685
H 0.625063810910 -0.596661379558 6.220853946992
H -1.988167238959 1.111492082504 4.030579644810
H -1.242580830614 -0.455063442827 4.421707046851
H -2.293394030654 0.348197257316 5.592689294344
H -1.215460589687 -3.177454876968 -0.606812356214
H 1.330172122183 -3.287044826923 -1.505189183391
H 1.419304542268 -0.075300752433 -1.443672802009
H -1.129012841244 -0.076445856460 -0.546258774827
H -0.289642520555 -6.724217801137 6.377810380098
H -1.810851308510 -5.881585273541 6.677868761601
H -1.554540570801 -6.699703627081 5.133387936805
H 0.928637589618 -4.527353140347 7.021338666829
H 0.555676341050 -3.015388155162 6.174068874222
H -0.635589636904 -3.741246826369 7.257796700989
H -1.314670755169 -2.982241629443 4.372458323010
H -2.147086204046 -4.488032647976 3.922276899219
H -2.410885458698 -3.768943049860 5.512649615872

**5b radical cation (*gauche*)**

E(UB3LYP/6-31+G*) = -6992.41575899
C -0.016140530101 -0.043786374158 0.007580544927
C -0.008042344793 -0.015370076460 1.449654409629
C 1.380090320390 -0.010236076684 1.833708253482
C 2.188355567591 -0.231195741505 0.678772591435
C 1.323896277040 -0.242861600338 -0.454032272167
Fe 1.233081038613 1.588562715727 0.470330411046
C 1.582474437645 3.450873331941 1.384301771616
C 0.418968908623 3.639438071323 0.551713079458
C 0.806168962546 3.234036272005 -0.773044524227
C 2.200702251777 2.937995197130 -0.781197297684
C 2.678909378176 3.063898741667 0.554682639791
N -0.862065450864 4.004597537498 0.965254265151
Si -1.857553565357 5.186067264501 0.001635104727
C -3.682321091573 4.801719323178 0.227272061110
N -1.094429870107 0.090475824752 2.307061655250
Si -1.225201419795 -1.005358458209 3.760796206120
C -1.637677680997 -0.041794435842 5.329135069281
P -1.265739900136 3.127101765691 2.470445576967
P -2.286337448885 1.300153669559 1.671002958974
P -3.760934140592 1.661045622379 3.367771392835
P -3.176151211626 3.902824578615 3.420739521676
N -2.746761938777 3.976173078104 5.127753328995
Si -1.332260018189 4.583530334131 6.064408530739
C 0.253515529839 4.580098435509 5.034396174045
C -3.924547470362 3.804344326253 5.934523638342
C -4.154703570958 2.712623017965 6.837668587924
C -5.298089592104 3.020603243028 7.628896221533
C -5.816813008448 4.276703458934 7.185578739051
C -4.989996963964 4.747936995166 6.125354107239
Fe -5.846077291516 2.926512886555 5.649100854765
C -6.227251259933 1.947572632609 3.818425809209
C -7.008182498832 3.144279517170 3.961940486711
C -7.828760571740 2.995845093956 5.116976221762
C -7.522839652828 1.737586845980 5.721017842357
C -6.528203909379 1.095145723442 4.931115021971
N -5.367700761348 1.629036323677 2.712098366066
Si -6.229109189252 1.482971464741 1.137465601216
C -5.053983070954 0.917012602616 -0.226724034575
C -1.629486199456 6.356117892598 6.758467700292
C -0.266476358660 6.968678282870 7.164035190911
C -1.028394813377 3.399626267307 7.503619033586
C -2.269159605459 7.263621290285 5.689118836499
C -2.524003764947 6.324461795769 8.018814410508
C -7.655385044849 0.199357732218 1.292873876128
C -8.180585197792 -0.096894251341 -0.134921071473
C -6.948027048912 3.153635742227 0.614173171665
C -7.134783160975 -1.114237267252 1.909421147700
C -8.847557753330 0.714209158501 2.130977038556
C -1.386711722016 6.937479833594 0.594694306491
C -2.253159899900 7.973775598663 -0.156976590640
C -1.522035712456 5.044858897686 -1.852035935416
C -1.633665321384 7.080265917901 2.107641826061
C 0.106004674753 7.208542192062 0.305230887308
C -2.499981811654 -2.373010013451 3.346885569298

C -2.673991762467 -3.281933252186 4.586918835420
C 0.436294600787 -1.851923339369 4.072415843634
C -3.877785866678 -1.803325204123 2.969492505122
C -1.971868688650 -3.213021940642 2.163002636254
H -3.534633684676 1.830371875961 6.905051631615
H -5.727597139392 2.392006700931 8.398154410057
H -6.706785468101 4.764938794580 7.561583768099
H -5.120703102319 5.666802212794 5.570957791241
H -6.978297238394 3.995630636041 3.297859425388
H -8.526144704813 3.729938978196 5.498887803198
H -7.949048055647 1.354963456758 6.639374527394
H -6.073383738055 0.132587422868 5.121063342942
H 0.147239137862 3.152776763230 -1.622140480493
H 1.621754793019 3.627187067522 2.450021964171
H 1.743193071291 0.112079896854 2.842316399395
H -0.900507284094 -0.001440030075 -0.612843775473
H 2.778564582912 2.632933793844 -1.643970643385
H 3.693113795029 2.890437157011 0.891277864112
H 3.265564745024 -0.335419855607 0.666246683265
H 1.620815547562 -0.369173745768 -1.487512909617
H -0.425853300686 7.946662765079 7.640255979969
H 0.273461998505 6.344268716807 7.887934764313
H 0.389264482966 7.132344561243 6.300808423686
H -2.679402372787 7.348306911815 8.389597164331
H -3.509920072644 5.892139612930 7.828416546971
H -2.059842008609 5.753924786354 8.831901291852
H -2.439604951171 8.270672082024 6.096858087396
H -1.621494845891 7.374257999352 4.812499857478
H -3.234062859131 6.879940527216 5.342265195954
H -3.406665594994 -4.071944297569 4.369475531708
H -1.742935431336 -3.781857547283 4.878441916387
H -3.046376455750 -2.725068813617 5.456207248554
H -2.690790679616 -4.005873188104 1.912240328069
H -1.832694146715 -2.602108985158 1.261703894839
H -1.017691364537 -3.702714726003 2.391693071696
H -4.581344923953 -2.622808818162 2.769209588280
H -4.311555863734 -1.192686902321 3.768822416908
H -3.839239880117 -1.189890327676 2.062006693689
H -2.012810854217 8.987992023168 0.191982131091
H -2.078043022155 7.956405933149 -1.239498331821
H -3.325650581110 7.817807505830 0.016337858767
H -1.354722864366 8.089304711185 2.442870416342
H -2.684265606628 6.926521609217 2.378829724547
H -1.032415999492 6.368275685776 2.684112712335
H 0.379323285331 8.215978000955 0.649812058571
H 0.760007567814 6.498836581086 0.827820926295
H 0.338713794937 7.160171352885 -0.765610380861
H -9.045676322659 -0.772505948656 -0.076756218530
H -8.516602269815 0.811177199451 -0.652426854620
H -7.430214456045 -0.590111486845 -0.763356051620
H -7.942195874398 -1.859680005679 1.950117473167
H -6.319508318553 -1.549586094580 1.319065707284
H -6.768057926496 -0.966850845824 2.930482066772
H -9.644897441931 -0.043228893100 2.135339108863
H -8.580693076306 0.910821046130 3.171741994143
H -9.279005354746 1.631500884378 1.713789069627
H -7.193300838362 3.128742857827 -0.455521451554
H -7.867913054356 3.398108285052 1.154155210175
H -6.235947034673 3.969709855443 0.771220564217
H -5.645679744007 0.831229681306 -1.146218613104
H -4.248982428591 1.628664003470 -0.427440642646
H -4.598127831175 -0.059378558823 -0.031269253168
H -0.141938479058 3.729251925191 8.061027361158
H -1.865586923584 3.362849280187 8.206698620545
H -0.838527638865 2.380478539567 7.147607387513
H 1.056877332241 4.941252664126 5.688202782085
H 0.515825502870 3.568803039196 4.711634744328
H 0.231351603164 5.231234254574 4.154216572595
H -4.222324271281 5.137916914778 -0.666570573516
H -3.859966080102 3.725719870217 0.321894837028
H -4.126850647021 5.293689483834 1.094553366122
H -2.187053273511 5.765935851267 -2.344109645180
H -0.500473231054 5.290014382042 -2.155989447336
H -1.785050133570 4.056018383217 -2.246636917957
H -1.087620847207 -0.488831695912 6.167579659589
H -1.336670755883 1.008595948947 5.251823071302
H -2.703289488365 -0.059788441638 5.570140018369
H 0.247739005432 -2.653316935786 4.797453548575
H 0.895140789058 -2.310975797964 3.192066401309
H 1.164977861300 -1.178942900535 4.537904701474

**5b singlet dication (*trans*)**

E(B3LYP-D3/6-31+G*) = -5671.69910151
Sum of electronic and thermal Energies= -5671.696269
Sum of electronic and thermal Enthalpies= -5671.695325
Sum of electronic and thermal Free Energies=-5672.041765
C 4.770601117959 -1.610087080136 2.449977448566
C 4.479278435095 -1.627675252629 1.057372057625
C 3.053431361209 -1.656709594910 0.918530499097
C 2.472556679676 -1.671005486535 2.234414279782
C 3.540990706541 -1.629883511255 3.171547085106
Fe 3.608298874224 0.000528875922 1.922624582250
C 2.471469082237 1.671449062417 2.233670233650
C 3.053008308205 1.657414565475 0.918065200774
C 4.478803817942 1.629140425056 1.057637389707
C 4.769446308431 1.611859098217 2.450383109789
C 3.539469636604 1.631016730474 3.171336157427
N 2.331356419073 1.883913179493 -0.298636924586
C 2.588849864063 3.195745272959 -0.996648698752
H 1.636076911504 3.733395076291 -1.090327580506
N 2.331223109525 -1.883737715025 -0.297756759430
C 2.587984811161 -3.196189847710 -0.994909151877
H 1.634987428186 -3.733557909349 -1.087927182069
P 0.959583581702 1.080932863620 -0.764082195741
P 0.959385055389 -1.080817045561 -0.763063095739
P -0.959298611518 -1.080125515726 0.764320739301
P -0.959700731449 1.081624568952 0.762835337975
N -2.331575930098 1.883993021603 0.296697390499
C -2.588779695233 3.196770554618 0.993061884127
H -1.635895053679 3.734356572687 1.085992096922
C -3.053527888766 1.656026636980 -0.919553688909
C -4.479349040713 1.626949523269 -1.058637225210
C -4.770427245099 1.608441030048 -2.451276635454
C -3.540689177476 1.627680808079 -3.172644787825
C -2.472410548677 1.669365812536 -2.235353231153
Fe -3.608295366433 -0.001876619092 -1.922633398296
C -4.769604548071 -1.613504396440 -2.449119858250
C -3.539742507465 -1.633220718025 -3.170251952775
C -2.471603658012 -1.673088329349 -2.232726016855
C -3.052923390602 -1.658095493601 -0.917047542272

C -4.478742586629 -1.629862502994 -1.056403902795
N -2.331033385255 -1.883653620728 0.299701257211
C -2.588075838317 -3.195165306635 0.998493953066
H -1.635184457308 -3.732589416273 1.092245308148
C -3.260703809082 3.099732392306 2.386166875684
C -2.332921085412 2.429642891027 3.413779873421
H -3.217917374516 3.766874969094 0.305578979829
C -4.586385592476 2.325280964266 2.314794376774
C -3.529594131754 4.555682028767 2.823352077881
C -3.259793360943 -3.095548087481 2.391511128184
C -2.331579704997 -2.424124214107 3.417872037306
H -3.217316868252 -3.766516407658 0.312144813516
C -4.585152411187 -2.320648905408 2.318983078829
C -3.529204019536 -4.550645711482 2.831191371793
C 3.260860420511 3.096771162700 -2.389578622323
C 2.332806268921 2.425971167163 -3.416489374716
H 3.218043037578 3.766601656526 -0.309844706699
C 4.586128747691 2.321705728873 -2.317174007278
C 3.530514886407 4.552073512931 -2.828435089532
C 3.259641411022 -3.098485170951 -2.388087435613
C 2.331711026188 -2.427776597195 -3.415166011021
H 3.217168624929 -3.766789241778 -0.307878455146
C 4.585397242753 -2.324174372358 -2.316544643074
C 3.528324602755 -4.554222507702 -2.826103251881
H 5.197735214682 1.606431371984 0.253836465132
H 5.758259897911 1.557575806670 2.885330492314
H 3.435071841917 1.600645180910 4.247511886578
H 1.417188217427 1.720957354576 2.465577520576
H 1.418402260474 -1.721003438380 2.466812531331
H 3.437112068571 -1.599447139254 4.247771146354
H 5.759595588593 -1.555201403589 2.884439220548
H 5.197789977350 -1.604643791293 0.253201157705
H 2.601922570277 5.129701447751 -2.906309160817
H 4.013036716434 4.565271489048 -3.810829001314
H 4.195108792241 5.065859127847 -2.124655668671
H 1.352912443333 2.916987492178 -3.464388762048
H 2.177913667730 1.358816279115 -3.204281763659
H 2.778255917004 2.479622237438 -4.415637246421
H 4.430997275693 1.292918193799 -1.968332486702
H 5.302275009527 2.814934075135 -1.650915925413
H 5.045522662906 2.268093160417 -3.309243058261
H 2.599371025636 -5.131350437389 -2.903368213125
H 4.192803016935 -5.067957608804 -2.122178639271
H 4.010585507166 -4.568307122278 -3.808612701960
H 1.351521339261 -2.918260967586 -3.462525143191
H 2.776866897744 -2.482296969750 -4.414398050974
H 2.177505010682 -1.360407326766 -3.203541042221
H 5.301303982202 -2.817214818796 -1.649889870877
H 4.430951295681 -1.294959750836 -1.968670070494
H 5.044708761771 -2.271772884351 -3.308716692706
H -1.418209817368 1.719168136393 -2.467589668359
H -5.197997314140 1.604490414736 -0.254578861560
H -5.197551934465 -1.606577999592 -0.252505159973
H -1.417364933221 -1.722792474867 -2.464776933952
H -2.600702699783 5.132922171885 2.900521315989
H -4.193955907188 5.068992151106 2.119006717068
H -4.012077773495 4.570246631663 3.805745028943
H -1.352780606992 2.920228511038 3.461082581609
H -2.778285132055 2.484651314730 4.412892274895
H -2.178594987710 1.362171837013 3.202748242980
H -5.302227896321 2.817934066656 1.647784676103
H -4.431808917578 1.295902001788 1.967467480596
H -5.045848689888 2.273344233143 3.306920461626
H -5.758481215050 -1.559460078537 -2.883952410733
H -3.435509581635 -1.603577748188 -4.246463958681
H -3.436625908261 1.596518365128 -4.248830260168
H -5.759350643668 1.553316470676 -2.885871076089
H -2.600537490001 -5.128146181412 2.909128891922
H -4.011474804960 -4.563381726783 3.813714805349
H -4.193925986318 -5.064860015259 2.127846966804
H -1.351626890813 -2.915022228354 3.465799191687
H -2.176831589891 -1.357067090520 3.205078408041
H -2.776796285221 -2.477305721617 4.417148978849
H -4.430184245428 -1.292024866184 1.969586564083
H -5.301378665267 -2.814280627208 1.653109829915
H -5.044358367566 -2.266577896580 3.311114454932

**5b singlet dication (*gauche*)**

E(B3LYP-D3/6-31+G*) = -6992.09040474
C -4.930266933793 -0.696183237789 -2.233745228590
C -5.150218842768 -2.034984554800 -1.790118027969
C -3.891119792101 -2.608109696242 -1.465003529312
C -2.879223576890 -1.627111353437 -1.727309840875
C -3.531406899136 -0.432932972631 -2.181839277043
Fe -4.260726330694 -0.915200388967 -0.291428017354
C -3.928333524548 -1.239861959486 1.733656953938
C -3.575289277068 0.110122039089 1.387159950316
C -4.743772305449 0.751589401840 0.863335356435
C -5.806653358138 -0.193215251489 0.889535606577
C -5.305855432634 -1.416279678812 1.428813512975
N -2.322210855484 0.771201719628 1.645121335440
Si -2.135457063999 1.547265507246 3.313790883661
C -2.148730515181 3.449073165919 3.154108379362
C -0.855469323029 3.982471665196 2.503133045494
N -1.449744564521 -1.801832922854 -1.641116765926
Si -0.628770561791 -2.562334768937 -3.096350780667
C -0.122468619375 -4.346135136869 -2.646134581984
C 0.999425041253 -4.338053944436 -1.593055487349
P -1.377292342874 0.753291634150 0.249034777582
P -1.023902453244 -1.632228467856 0.000288519787
P 1.101839152076 -0.789433010550 -0.126626072784
P 0.742149687709 1.473757692279 0.646124970752
N 1.076650214433 2.377746071095 -0.754988618811
Si 0.063770816148 3.294088700703 -1.988584711118
C 0.983179404508 4.843744890773 -2.635673396892
C 1.409256528347 5.772347175872 -1.479483610833
C 2.489914386245 2.283498799003 -1.025455255530
C 3.540257459257 3.022111075250 -0.395398178928
C 4.753995102368 2.708131245022 -1.066929641444
C 4.466111735017 1.756260841864 -2.092873695077
C 3.072035561091 1.473229555015 -2.057219197830
Fe 3.974751927958 0.982326158923 -0.244225469918
C 5.553808312049 -0.284176304471 0.172202583707
C 4.378618785357 -1.044985126526 -0.070719783248
C 3.402603644236 -0.667023669590 0.914671634088
C 3.976328359479 0.356748608558 1.738234698091
C 5.305955389187 0.580351088868 1.281822668371
N 2.135248370739 -1.325637656184 1.101128364013
Si 2.066262650073 -2.440137126639 2.578254095674
C 3.341896633115 -3.855648418650 2.402617889777

C 3.214997343619 -4.550490714656 1.034457205316
C -0.316194108884 2.068656924734 -3.371086010462
C -1.537856540077 3.867581592221 -1.172800103676
C 2.450488761345 -1.377825801098 4.083141809781
C 0.311137074905 -3.105477399439 2.697699666575
C -3.593845078385 0.918072025055 4.311334698905
C -0.526421108655 0.885065939066 4.022891116767
C -1.918581795992 -2.498436775200 -4.456097174975
C 0.882000140442 -1.550374303021 -3.590918420440
C -3.366073862798 3.916607206673 2.329205714982
C -2.251763712869 4.027430353982 4.587902199264
C -1.316642342547 -5.148440145910 -2.090179249114
C 0.397028383982 -5.031016347675 -3.934426797159
C 2.206249687620 4.524840164201 -3.522022964780
C -0.054223176985 5.595334614918 -3.514590890548
C 4.793037514740 -3.369792265746 2.612597110986
C 3.014011852803 -4.885576953806 3.515545727844
H 2.536219637980 0.791525990507 -2.702099471656
H 5.186634518456 1.305634977977 -2.762816605803
H 5.733251746196 3.096657715298 -0.819046774495
H 3.419970333418 3.692543458047 0.444713457667
H 3.480661148205 0.860527286865 2.554964640027
H 5.998594606715 1.308031004226 1.683966105936
H 6.465365678878 -0.324406780832 -0.409710991232
H 4.234862942111 -1.791701369260 -0.839709827999
H -3.261779645297 -1.979834181510 2.153876733342
H -4.789763045992 1.770297882800 0.504083423087
H -3.042150328517 0.489213677530 -2.460600736109
H -3.715722081076 -3.601717808382 -1.078807780296
H -5.868381324114 -2.333288410848 1.546463341857
H -6.812487086662 -0.022887095262 0.528007103384
H -5.695877333821 0.008546273712 -2.531346864838
H -6.113435417828 -2.516516968832 -1.680845884658
H 0.425355419287 6.476848568185 -3.959836346656
H -0.425202759030 4.981355386045 -4.344722767285
H -0.914098513460 5.956662335204 -2.939820198454
H 2.573110459777 5.453345163654 -3.979580771244
H 3.035828202296 4.096019472331 -2.956655876198
H 1.957810278231 3.839463826583 -4.341276788288
H 1.831061998822 6.701109252974 -1.886323115813
H 0.566150002396 6.057095365666 -0.837875229778
H 2.178646756709 5.316243399969 -0.848483133673
H 0.729624794353 -6.051791924618 -3.702950650882
H -0.380101001730 -5.111891923007 -4.703074949735
H 1.253845974759 -4.503685979828 -4.370856566507
H -1.021419212469 -6.191740056577 -1.914892443826
H -1.658494528563 -4.745237695509 -1.128739876552
H -2.169240481926 -5.164791150362 -2.779466601503
H 1.313637844105 -5.365021313560 -1.363381268924
H 1.890073606833 -3.794250388343 -1.928646037341
H 0.671247710220 -3.894130112940 -0.641884626500
H -2.215223720583 5.124168485775 4.544408094247
H -3.192004119103 3.756257049449 5.079719537159
H -1.423366105421 3.703123604372 5.230441071181
H -0.881409934353 5.080066320170 2.459325496974
H 0.041001128161 3.700711670856 3.067743573970
H -0.736468048242 3.630829026241 1.471140401603
H -3.418060633249 5.013744145905 2.325826018710
H -3.299226886918 3.592738172706 1.284252615923
H -4.312962720736 3.549073758899 2.742302755165
H 3.758463233073 -5.692254713378 3.493169053988
H 3.051397882813 -4.442835803264 4.518658746610
H 2.030836090578 -5.350018408724 3.380254347306
H 3.929079069922 -5.382182335500 0.966935477001
H 2.214742169597 -4.970692453621 0.884302864393
H 3.425447013888 -3.869047048115 0.202210416624
H 5.476212465648 -4.227456965543 2.552213824083
H 5.112144899368 -2.647302899003 1.856271797151
H 4.935617915020 -2.913462371636 3.598703697029
H 2.181077978317 -1.935107937171 4.989026324739
H 3.513881261605 -1.131224011106 4.152398530688
H 1.882755704340 -0.444043501085 4.091059701299
H 0.246455703815 -3.720452540776 3.602874796088
H -0.432375599678 -2.306779952837 2.801405895941
H 0.021531392309 -3.741164955477 1.854257128606
H -1.024926902074 2.495310442500 -4.090669420483
H 0.586570685099 1.792191607872 -3.925925920731
H -0.757482773747 1.150241067092 -2.965286450228
H -2.209560835401 4.211028428328 -1.968627038072
H -2.081463703410 3.095510551978 -0.622009801876
H -1.371815658755 4.711700659928 -0.496366932177
H -0.448655704906 1.136879391600 5.087248212078
H -0.504026461957 -0.207772506955 3.944865838517
H 0.359561661892 1.286908246169 3.521411727373
H -3.541782703848 1.339076777098 5.321679420713
H -4.559780798155 1.201748970052 3.880814748825
H -3.578490464110 -0.172882557217 4.408936878160
H 1.309324902428 -1.973543956577 -4.508166050579
H 0.605577067647 -0.512929601797 -3.804225671078
H 1.670284522923 -1.546326772440 -2.831455820386
H -1.471379689080 -2.863229618476 -5.388482958138
H -2.793907589609 -3.119940679662 -4.240780320286
H -2.270414542393 -1.476483426831 -4.636293629776

**5b triplet dication (*trans*)**

E(UB3LYP/6-31+G*) = -6992.12518641
C 0.098787937468 -0.007920398477 -0.039701185397
C 0.075861028744 -0.026032968810 1.384904129486
C 1.427293433878 -0.033315430872 1.854873253417
C 2.285453817658 0.028960604532 0.704359674739
C 1.459654184503 0.030704221644 -0.460059579054
Fe 1.042729571220 1.684063946498 0.703172290749
C 2.134952914145 3.440924028446 0.638424641385
C 1.272116498558 3.472069670866 1.786722690132
C -0.072387262804 3.327586972658 1.319004702670
C -0.044815591060 3.256253488111 -0.103837800183
C 1.315081354390 3.321257932984 -0.524033827704
N 1.646300191146 3.714249708925 3.134598389531
Si 0.906406177278 5.176690281795 4.015448243074
C 2.321581015193 6.081687266862 4.871751779531
N 1.819711259545 -0.189285701716 3.210298187784
Si 1.212455423363 -1.677654859424 4.147374665870
C 2.701879125416 -2.419596300538 5.034076068036
P 2.912511935681 2.949522805089 3.948627929405
P 3.011739328675 0.715654360361 3.991822126150
P 5.013654541015 0.782824976704 2.866657920800
P 4.914573266802 3.016703380027 2.823623763896
N 6.106553415116 3.921471352047 3.605432473065
Si 6.714000976442 5.409929178423 2.668604516004
C 5.224788449808 6.151767709651 1.781474087853

C 6.498806345711 3.765280375767 4.960871872497
C 7.850179287247 3.758138044062 5.431014087311
C 7.827081801133 3.739682960219 6.855608635685
C 6.466173887180 3.700706823425 7.275790739402
C 5.640513219401 3.702573644573 6.111270586505
Fe 6.883532451021 2.047701125717 6.112207928628
C 7.971469195990 0.475523139947 6.918691666875
C 6.611643678326 0.410177913160 7.339074137014
C 5.791625126066 0.290626216534 6.176709927652
C 6.654294012172 0.259897062086 5.028282214283
C 7.998844108708 0.404517116804 5.495825203774
N 6.279929708374 0.017922824755 3.680411820870
Si 7.019629896604 -1.444456165645 2.799316054593
C 5.604254209244 -2.349583367326 1.943470150074
C 8.046525138225 4.871710939035 1.417751450521
C 7.439663247400 3.985645503679 0.310226300994
C 7.357480650853 6.612758754379 3.957593551239
C 9.184354044966 4.097126667178 2.113190748950
C 8.629902941542 6.154774203943 0.774966790503
C 8.300562961787 -0.836221167523 1.526734432730
C 7.618140013856 -0.052170894748 0.386754332266
C 7.766291717949 -2.535475770090 4.131430110783
C 9.361759304206 0.064662441053 2.190447502010
C 8.999358117557 -2.084757373079 0.933020630330
C -0.374961922123 4.568599269934 5.287650201643
C 0.306991250430 3.784174965221 6.427658829008
C 0.160245641843 6.267758741709 2.683093140119
C -1.436289437253 3.668116957895 4.623604017263
C -1.073528067923 5.817249481615 5.881405822500
C -0.119670991428 -1.139241242576 5.398578301023
C 0.487660229851 -0.253455011560 6.506064814776
C 0.568500271154 -2.880492501500 2.858630663672
C -1.257424001881 -0.364287768915 4.703424799379
C -0.703254646573 -2.422210478117 6.041352169195
H -0.951353172373 3.271402218424 1.943725220228
H -0.905676224776 3.130446902140 -0.747412575015
H 1.671036160080 3.262160048451 -1.544478884838
H 3.211915905829 3.517206593367 0.651603121307
H 3.364937469338 0.048371090359 0.718165585729
H 1.810259133808 0.081146261967 -1.482819000724
H -0.769011464267 0.016497892320 -0.685782504646
H -0.805367832051 -0.023217075833 2.008975118705
H -0.784153037427 5.882501950173 2.286979361947
H 0.845877699288 6.411584311198 1.840202829504
H -0.043962199955 7.255065428030 3.115243322293
H 2.771599983184 5.518660026013 5.695287297268
H 1.928271012369 7.014723393001 5.295370873221
H 3.115623042464 6.356373676512 4.169281299188
H -0.405857858848 -2.596097750847 2.450015628970
H 0.452415462847 -3.865043572367 3.328111121300
H 1.265491144768 -2.994381931664 2.020494510456
H 3.098981248728 -1.787826571055 5.834637209124
H 3.518021419535 -2.648788467945 4.340674271688
H 2.392968737022 -3.367254271957 5.493662967915
H -0.369946192923 6.485987537334 6.392244993670
H -1.819232540525 5.506197231080 6.625400152290
H -1.602501498841 6.398611250918 5.116824968420
H 1.031435072249 4.395872482760 6.977890762503
H 0.827026289532 2.890059873503 6.062458828048
H -0.445790395807 3.442667780015 7.151192081534
H -0.990550714382 2.763431605101 4.193441117012
H -1.989958510331 4.193705381402 3.835342003790
H -2.174732337793 3.342807953249 5.368679505562
H 0.057310665694 -3.004739443629 6.575569536021
H -1.176944070008 -3.077728710409 5.300879766056
H -1.474658649326 -2.151432876280 6.774813417764
H 1.264015024959 -0.775716278702 7.077258794276
H -0.293494670651 0.045963369853 7.218072711714
H 0.924974772666 0.669413687350 6.105675293611
H -1.760253242253 -0.967170778263 3.936719157149
H -0.895036499384 0.560254625355 4.238618856188
H -2.023191347482 -0.079390091416 5.437390425352
H 8.331748971082 6.328430622231 4.366468167330
H 7.473612163468 7.597348025423 3.488202658046
H 6.660244242535 6.726539215082 4.795540589203
H 4.828032365028 5.519992239747 0.980745992206
H 4.408388998712 6.380816221496 2.474615592962
H 5.533738291637 7.099493562716 1.322056371899
H 4.561033631938 3.682982976629 6.097339692516
H 8.731496954396 3.755639784493 4.807068425716
H 8.710773944288 -2.150138356477 4.527267171982
H 7.080924307550 -2.679378810266 4.974522159275
H 7.970456855665 -3.522754659317 3.699198585523
H 5.153880150464 -1.786602890306 1.120096727237
H 5.997524112348 -3.282565046723 1.519691079490
H 4.810487971282 -2.624375878277 2.646215675222
H 8.877695646999 0.461006511000 4.870969763698
H 4.714673781359 0.214167011702 6.163661146476
H 7.869301876374 6.737048878789 0.240525188489
H 9.103269743101 6.810495755283 1.515467392238
H 9.401532635707 5.884118634357 0.041698406664
H 6.663194564672 4.507579032574 -0.261114625114
H 8.221028710951 3.686475127898 -0.401655419923
H 7.002645416466 3.062634902913 0.710609766218
H 9.686791935464 4.700162490421 2.880032533177
H 8.822147915178 3.172455992367 2.577881903546
H 9.950396576798 3.812484916497 1.379413409831
H 8.832401038430 0.601333364528 7.562170713528
H 6.255828913834 0.468975731448 8.359585072698
H 6.115453481954 3.649952916752 8.298495574512
H 8.694808363159 3.715265885458 7.501787783598
H 8.295851471337 -2.753772082906 0.422438093655
H 9.744815725572 -1.773613145616 0.188816904186
H 9.528654151443 -2.665850617704 1.697580660293
H 6.893847401304 -0.664213738913 -0.163290653259
H 7.097805879892 0.841777102620 0.751939927382
H 8.370675522881 0.289550926005 -0.336933018439
H 8.915832247203 0.969227796622 2.620669432673
H 9.915797738740 -0.460690530877 2.978607168611
H 10.099913134377 0.390160871813 1.445167977888

**5b triplet dication (*gauche*)**

E(UB3LYP/6-31+G*) = -6992.11813829
C 3.980024947038 2.060608798666 0.501367606970
C 3.341880451177 1.844431100262 -0.777343911943
C 4.404794281570 1.517182155870 -1.694201788375
C 5.660775775424 1.716728787279 -1.047263040420
C 5.400710037225 2.041544845425 0.313865250954
Fe 4.659454365506 0.163524790504 -0.093855396654
C 4.087218970146 -1.784852401858 -0.586172891141

C 3.630915475979 -1.552201494231 0.768250552753
C 4.800248151554 -1.188193128171 1.522667506579
C 5.948696239262 -1.300098754658 0.687467996224
C 5.510381256722 -1.658747754961 -0.616748014039
N 2.297654067305 -1.545658752365 1.219556200140
Si 1.864493038683 -2.047388219647 2.939575702214
C 0.206267114541 -1.315998138444 3.448395932467
N 1.972594378576 1.886997140057 -1.075797322287
Si 1.438701829472 2.913520273160 -2.517595608694
C -0.266967019685 2.435385908092 -3.159279659356
P 1.304243824689 -0.931704724947 -0.100003383995
P 1.044037377664 1.285256632291 0.343124861428
P -1.061352472552 0.907101236038 -0.364021019920
P -0.844587723010 -1.226188332169 0.393122647230
N -1.688803894859 -2.111404377736 -0.921023234001
Si -1.138678249706 -2.580501722343 -2.623668289849
C 0.622167775874 -1.994654612725 -2.940557758050
C -3.030676886041 -2.241862527810 -0.562555549296
C -4.175773349492 -2.336579851959 -1.432594392819
C -5.363036652802 -2.439395819643 -0.651508607224
C -4.997718346256 -2.338133877456 0.715908112158
C -3.578034226509 -2.183421799688 0.787084163783
Fe -4.409465458389 -0.601775722026 -0.266176163979
C -3.549880726117 1.340199115432 0.177025432487
C -4.783691509140 1.112495331392 0.886144013766
C -5.842524917991 0.930887147191 -0.050721637272
C -5.280128556995 0.949034938628 -1.353731650476
C -3.870824163070 1.156875664259 -1.229865715716
N -2.291181800543 1.624854154213 0.714138425524
Si -2.185213435269 2.338700926148 2.418137038332
C -0.382870754584 2.576521462884 2.890106618707
C -1.207348768409 -4.485948544915 -2.780580971210
C -0.648435782982 -4.861510884081 -4.174703681344
C -2.118053911064 -1.654517807237 -3.958595219752
C -0.318179470356 -5.118007979752 -1.684963238771
C -2.631691081298 -5.073685932167 -2.656812083258
C -3.035554390711 4.065485844684 2.484574315499
C -2.794464809889 4.629035903567 3.910104788158
C -2.833775977963 1.084459115670 3.678820999581
C -2.359266085341 5.001502206312 1.455934338833
C -4.560497790241 4.093395050659 2.232943281905
C 1.796655849866 -3.951443084659 2.915300554509
C 1.353456511539 -4.450260039451 4.310806782287
C 3.084550024967 -1.404842393203 4.227543186109
C 0.776418646063 -4.418352173295 1.855046276861
C 3.180506577645 -4.549888587738 2.576715272375
C 1.456457276791 4.732449478594 -1.941261459678
C 0.967619868563 5.629440706142 -3.104270269589
C 2.590272116750 2.675648078156 -3.989495002186
C 0.510964478137 4.909758111277 -0.737412428180
C 2.882051749826 5.167416347303 -1.534302144041
H -4.164206004924 -2.345406141895 -2.507032765456
H -6.369083165960 -2.530888852724 -1.041232825726
H -5.665861484671 -2.351473676072 1.568349380550
H -3.009461429696 -2.082429160051 1.698353373544
H -4.914962625030 1.106023329777 1.954140341799
H -6.882730786186 0.756841630076 0.194318756985
H -5.807399792936 0.804028344414 -2.288803267543
H -3.170602681418 1.220916743906 -2.049717481306
H 4.820860968010 -0.862602532974 2.547961492620
H 3.464264683634 -2.053858394910 -1.427271846512
H 4.275655741806 1.190044734918 -2.712764261984
H 3.472631872294 2.297908220585 1.426767590388
H 6.969361589861 -1.100832312064 0.988845102473
H 6.135238374143 -1.806576942462 -1.488733150886
H 6.635866773146 1.598652724345 -1.502884055747
H 6.137134562416 2.240064498039 1.082706699648
H -0.671157568750 -5.952371682796 -4.295330672197
H -1.242656599444 -4.435661740602 -4.992785220796
H 0.392533576892 -4.547219017790 -4.308335978542
H -2.598418927295 -6.158893171744 -2.818717443630
H -3.064825824335 -4.917260384317 -1.662295642800
H -3.319539923961 -4.663053292457 -3.407481361240
H -0.316731602305 -6.211060060981 -1.789644893097
H 0.726257537300 -4.789782088952 -1.752849121079
H -0.681394355644 -4.888328249963 -0.676144742868
H 0.977884033899 6.682781866785 -2.793170133972
H 1.611784033929 5.551323771588 -3.987980208028
H -0.059630335896 5.395099703429 -3.409396916845
H 2.879398527688 6.224998559086 -1.236686309909
H 3.265681133265 4.596137888086 -0.680768226139
H 3.597957290341 5.068212490167 -2.358928779636
H 0.487332587250 5.961248149452 -0.419387171805
H -0.521260748583 4.623333748380 -0.973570707054
H 0.839556247255 4.322682916010 0.129520412324
H 1.297392919728 -5.547282833101 4.316226086652
H 2.060149093727 -4.162124180184 5.098415591448
H 0.360688476832 -4.075958414926 4.591456194589
H 0.709333713582 -5.514914427910 1.847064802286
H -0.234244981003 -4.036539759284 2.052891070334
H 1.066675892514 -4.106120777126 0.844075365221
H 3.129571097451 -5.647176866610 2.597650798254
H 3.522823557876 -4.265340995215 1.574503961551
H 3.950259417046 -4.251050726432 3.298190543291
H -3.249651840614 5.625123068911 3.984410685351
H -3.253101337456 4.009733644287 4.690390401791
H -1.733420671081 4.750592447383 4.146900318698
H -2.779928592662 6.012234251341 1.539460580923
H -1.279581785747 5.089372785923 1.614616246775
H -2.524415855732 4.665940251480 0.423997438014
H -4.933786581491 5.115633031529 2.378192540724
H -4.826498853365 3.808701594995 1.209416974243
H -5.114174319745 3.455126349653 2.934042572210
H -2.632279784317 1.483854786282 4.679299833109
H -3.899523800147 0.842091700321 3.645461450416
H -2.276856772688 0.141894429840 3.589472223716
H -0.398477347334 2.982117032372 3.908652452306
H 0.184374928428 1.645675482892 2.935410781709
H 0.167695834585 3.279750589845 2.262157969386
H -1.574801369566 -1.800281692071 -4.899463369854
H -3.147285311074 -1.967416116661 -4.149630805962
H -2.124637519376 -0.574862482626 -3.757883538198
H 0.798194897900 -2.197426994827 -4.004010772608
H 0.764782799378 -0.919457490174 -2.788699855011
H 1.385749973057 -2.529685104830 -2.371078805694
H 0.151415272759 -1.405672620940 4.539888015162
H 0.121059961186 -0.251603977705 3.211484246534
H -0.658439319192 -1.835045736561 3.030875597287
H 2.621048716628 -1.587617536253 5.205231047853
H 4.051263150659 -1.913769085372 4.244038912798

H 3.249675282029 -0.322474178103 4.153908584115
H -0.384459835003 2.981638952427 -4.103856743788
H -0.354683118977 1.365537674629 -3.383554058868
H -1.096010529607 2.725970340879 -2.511120537853
H 2.133973232415 3.223182725490 -4.823839656585
H 3.595169290902 3.082885344823 -3.855392423597
H 2.666745438249 1.628230137234 -4.306022165624

**5c neutral compound (*trans*)**

E(B3LYP-D3/6-31+G*) = -5672.31316278
E (PCM-B3LYP-D3/6-31+G* (ether)) = -5672.3324593
Sum of electronic and thermal Energies= -5672.310330
Sum of electronic and thermal Enthalpies= -5672.309386
Sum of electronic and thermal Free Energies=-5672.655755
C -2.337902390450 1.861791051679 -2.187740272802
C -3.423136038235 2.777008163400 -2.296109195626
C -4.617278445989 2.101349969062 -1.896636341382
C -4.266956067764 0.768477510936 -1.527561977773
C -2.850217562770 0.610393644279 -1.698950894685
Fe -3.258608653142 2.109930899796 -0.350178204225
C -4.038172045432 2.005343838210 1.547817879582
C -2.692467044353 1.500863501309 1.559894788128
C -1.849625976805 2.564261396839 1.095342123755
C -2.662684905979 3.700563813145 0.809551798550
C -4.014350464893 3.360117100002 1.100533651280
N -2.308965032064 0.211796693651 2.003438113529
C -3.047675721964 -0.359159597846 3.159719941496
C -4.046438839171 -1.527157991621 2.904713829863
C -5.143937850033 -1.131896412967 1.904397528018
N -2.147027914230 -0.628816031165 -1.592363229622
C -2.386056740800 -1.547404644887 -2.741733974904
C -3.065940397912 -2.910328721689 -2.443565604932
C -4.404757298534 -2.708794294927 -1.717760446841
P -0.903784920888 -0.686587762467 1.537293441181
P -0.675299892650 -0.905438283493 -0.733910990821
P 0.675500604782 0.905413544089 -0.734903288805
P 0.903337832474 0.688271085926 1.536602803353
N 2.308536761921 -0.209490054212 2.003596159666
C 3.047166143206 0.362726119446 3.159347765128
C 4.045874070361 1.530559721580 2.903265126278
C 5.143762588668 1.134354317498 1.903762247367
C 2.692253312860 -1.498973540622 1.561420071286
C 1.849721530285 -2.563339649196 1.098414971708
C 2.663179208854 -3.699834302478 0.814425846951
C 4.014730644960 -3.358492211626 1.104859588540
C 4.038082411501 -2.003043637316 1.550077882467
Fe 3.258506354254 -2.110736485705 -0.347711581985
C 2.850070143868 -0.612340933746 -1.697988647444
C 4.266827067010 -0.771078155059 -1.527284743171
C 4.616127079382 -2.104563404697 -1.895180318764
C 3.421335019339 -2.779951312295 -2.293118398647
C 2.336749870609 -1.863954654060 -2.185071828382
N 2.147537567485 0.627370688127 -1.592511817766
C 2.386953297607 1.544625575986 -2.742889742140
C 3.067270123134 2.907636854831 -2.446094921733
C 4.405820759379 2.706360597694 -1.719759712134
C 4.688132283043 1.857541271939 4.267036651480
C 3.336369059425 2.792407349690 2.377969876080
C 3.319478255735 3.574386216623 -3.814296731203
C 2.166862213932 3.831978524296 -1.605790322431
C -4.689105354677 -1.852561145238 4.268648923010
C -3.336899743542 -2.789654671977 2.380988210861
C -3.317660865066 -3.578651126682 -3.811107230030
C -2.165440928297 -3.833447902108 -1.602045344075
H -2.312876547368 -0.705840531019 3.897623811166
H -1.435359350298 -1.741647027359 -3.258920230618
H 2.312274292977 0.710124593289 3.896821560075
H 1.436350424274 1.738588287434 -3.260349961312
H 3.588089331978 -0.466546040222 3.627990435117
H 3.018206592219 0.992360235181 -3.447810305715
H -3.588574924591 0.470650759426 3.627443766972
H -3.017458905104 -0.996126365237 -3.447297532838
H -4.925388374587 1.454705232718 1.812908861090
H -4.880615174810 3.995390121836 0.966096229335
H -2.306465843870 4.643965123031 0.415886611034
H -0.780615813481 2.530783493217 0.970886263997
H -1.298133480263 2.078108019018 -2.384865427527
H -3.348098784765 3.817163955876 -2.587993976991
H -5.606971865564 2.536609644738 -1.838254579924
H -4.944253222406 0.010054188546 -1.164928346591
H -3.936182404650 -2.174707433017 4.999601961547
H -5.420856067869 -2.663136634686 4.165055312056
H -5.212540000483 -0.981198275905 4.683544965279
H -2.504684849543 -3.086864526903 3.029313652932
H -2.937522944704 -2.639220450886 1.373985401193
H -4.048526930937 -3.624121960422 2.331559093465
H -4.704673537074 -0.745806372415 0.980480424723
H -5.810550995209 -0.365196391718 2.317946169241
H -5.763323158288 -2.001310711269 1.651761918474
H -2.378600765893 -3.733557835601 -4.358658525618
H -3.978738995291 -2.968231386355 -4.439823605374
H -3.791743038127 -4.558984182046 -3.679937160505
H -1.183820253418 -3.971741620943 -2.071309827858
H -2.635137316595 -4.819851425064 -1.493506932618
H -1.996273340721 -3.434462481581 -0.597708546808
H -5.091610833253 -2.092502884939 -2.311037480760
H -4.252247404140 -2.220768529435 -0.751153113665
H -4.891615189104 -3.675010802349 -1.534885401881
H 0.780707099752 -2.530378950859 0.973800984958
H 4.925149059891 -1.451769765786 1.814314840127
H 4.944867095171 -0.012778262091 -1.165780775047
H 1.296747019098 -2.079889207573 -2.381319528835
H 3.934974520574 2.180385793622 4.997438199567
H 5.211559349489 0.986693513418 4.683017348035
H 5.419818753711 2.668082937540 4.162744067952
H 2.504118763721 3.090417460065 3.025883802294
H 4.048010024795 3.626808997587 2.327577163177
H 2.937054628227 2.640774656283 1.371121706590
H 5.810291349515 0.368176279322 2.318406870863
H 4.704965434391 0.747252608252 0.980043790333
H 5.763139283136 2.003586692321 1.650476470294
H 5.605633132538 -2.540275630933 -1.837035959776
H 3.345508468976 -3.820331345608 -2.583991388603
H 2.307310014456 -4.643919274290 0.422078825866
H 4.881257208024 -3.993628684105 0.971480034979
H 2.380563479075 3.729121169096 -4.362147181129
H 3.793957453982 4.554660903416 -3.684119441105
H 3.980377828029 2.963008351916 -4.442268760408
H 1.185338569907 3.969901604880 -2.075362015141
H 1.997425061901 3.434240850204 -0.601011591573

H 2.636766379653 4.818401540186 -1.498338776544
H 4.252807700256 2.219320052727 -0.752747364681
H 5.092613793296 2.089227715309 -2.312243647867
H 4.893001529959 3.672568243726 -1.537705084569

**5c neutral compound (*gauche*)**

E(B3LYP-D3/6-31+G*) = -5672.32795710
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5672.33502775
Sum of electronic and zero-point Energies= -5671.387043
Sum of electronic and thermal Energies= -5671.335000
Sum of electronic and thermal Enthalpies= -5671.334056
Sum of electronic and thermal Free Energies=-5671.468490
C -0.128958368275 0.052022321633 0.071579065697
C -0.043804418992 0.054473775222 1.499144437371
C 1.340224456182 0.009705183567 1.872250033564
C 2.102909192508 0.033510248270 0.657261562975
C 1.195955552216 0.028537053606 -0.448224789861
Fe 0.907023093212 1.719100817338 0.672610781853
C 1.946571162638 3.439425413540 1.236514325456
C 0.620759567891 3.520992771251 1.777189947807
C -0.289588962422 3.404296109201 0.674422794375
C 0.469955256652 3.316338366118 -0.533897503485
C 1.850150942811 3.327532837673 -0.185937784266
N 0.287574619531 3.688741402281 3.148212724156
C -1.140774113193 3.715114703388 3.507152862611
N 1.845278111453 -0.049754287525 3.198993732451
C 3.307707591475 -0.054600897426 3.375002634645
P 1.498646393097 2.946513475399 4.180695041158
P 0.771017384713 0.778763165116 4.313990063518
P 1.750319954190 0.907352996780 6.308307273549
P 0.780591369699 2.982451288104 6.286962110267
N 1.895674774444 3.930407046653 7.257413219827
C 3.313157946832 4.092494098145 6.891062192366
C 1.578606472609 3.825697838644 8.638500353574
C 0.268535656369 3.634642759042 9.189824015887
C 0.371907729588 3.637773229377 10.616184532298
C 1.743327860114 3.807453059915 10.957606747200
C 2.492389146575 3.892549941970 9.742570881646
Fe 1.493407550908 2.087844943928 9.872109619044
C 1.392012526523 0.461432522703 11.113990653774
C 2.708162455517 0.596513136538 10.588958113203
C 2.629766775192 0.485547643515 9.165320136791
C 1.261341058007 0.257800882616 8.801592702672
C 0.495338381590 0.283600925363 10.014441902869
N 0.772188820642 0.045256746303 7.484607105488
C -0.679470918857 -0.138320878170 7.315093796062
H -1.215728042266 0.381468691633 8.119000830266
H 3.949693586625 3.635398224584 7.659116982359
H -1.717882501185 3.134635330762 2.776387702230
H 3.784585206286 0.462970576214 2.533134043296
H -1.367263195495 3.400240093178 0.729403809220
H 0.057084577704 3.220011900026 -1.530028125628
H 2.686044361008 3.244811679094 -0.868785188022
H 2.866338130489 3.461856208053 1.802883649424
H 3.178829629885 0.036530549982 0.574759240276
H 1.478769560760 0.042974385840 -1.493129239621
H -1.045056045179 0.084135245811 -0.504247021128
H -0.884287655344 0.081879095044 2.177442295982
C -1.745774398478 5.135261613506 3.660324795225
H -1.265687149981 3.198721165717 4.463690887478
C 3.934604936918 -1.461015361462 3.562887356757
H 3.550123876650 0.535678905527 4.263836899961
C 3.753826836309 5.557288021040 6.633117675000
H 3.499325152743 3.525967267022 5.973676212108
C -1.141767159611 -1.616719666186 7.232228727906
H -0.983433277614 0.354554962395 6.386711862289
H 3.563822725330 4.006114691923 9.683029954042
H -0.645870511134 3.512153836368 8.627573356240
H -0.574405763483 0.171117069763 10.100534190678
H 3.464827462899 0.558324419388 8.483673595092
H 2.160880101144 3.830704195168 11.956170423717
H -0.451727164579 3.511057132898 11.307134853450
H 1.104592696587 0.519798961821 12.156104851840
H 3.612120370087 0.773702741372 11.157559476774
C -3.205455384313 4.958474813908 4.119926069627
C -0.961148989807 5.925024512620 4.721417002705
C -1.717407665576 5.910162672808 2.331424648699
H -3.692903550759 5.933752649202 4.239674384218
H -3.787767645760 4.381898022244 3.388844186957
H -3.259886887377 4.436395794588 5.084124909318
H -2.120206780934 6.920938496854 2.474356042045
H -0.697001493731 6.003370840094 1.945915109142
H -2.325553278069 5.415973270493 1.564126996838
H -1.409839682408 6.914540829989 4.874353469417
H -0.956071093387 5.404501858743 5.686901677729
H 0.076837098563 6.068135324744 4.406354162550
C -2.659571671054 -1.602463494227 6.968999844687
C -0.421938696145 -2.324283122660 6.071872749297
C -0.855820900814 -2.374531259358 8.540365619523
H -3.049841863978 -2.625661492808 6.906846287610
H -3.200186375683 -1.087442718738 7.774290473021
H -2.896069082091 -1.096004241162 6.024130973295
H -1.162139054452 -3.423944251720 8.444209456623
H 0.210352937782 -2.354037273986 8.788135293967
H -1.408008410847 -1.943583736974 9.384268308559
H -0.776958705300 -3.357639071403 5.971841588113
H -0.599751417182 -1.813147786457 5.117802159431
H 0.657693695152 -2.351922430389 6.247274835905
C 5.225858928376 5.514318962888 6.180950824042
C 2.888735135758 6.174373947149 5.521350415070
C 3.632853394495 6.417886092868 7.902766710126
H 5.600063803982 6.527339724723 5.988927699458
H 5.867021080328 5.061767517402 6.949138330252
H 5.342728552153 4.933499407371 5.256721441345
H 3.223079890751 7.194656517746 5.295288887645
H 2.946172697416 5.588245442107 4.595986414240
H 1.840076164751 6.221506418750 5.829956242961
H 3.918954574781 7.454839490075 7.685460825595
H 2.607038379969 6.422399840016 8.285150944361
H 4.290268927000 6.052520826257 8.700964935956
C 5.439808574847 -1.255346490823 3.818388607300
C 3.294822281409 -2.159954958700 4.774243070928
C 3.742277955023 -2.339136204742 2.314212644657
H 5.943579990674 -2.220374157230 3.952717273967
H 5.921826854664 -0.741695569629 2.975877001233
H 5.613156435251 -0.658403578860 4.723274010619
H 3.764723985284 -3.136175291917 4.947595891646
H 3.409008367156 -1.564094814575 5.688053236586
H 2.226151516313 -2.322983143035 4.605412412285
H 4.165164619102 -3.337299960551 2.485036915841

H 2.681778901114 -2.457695007554 2.069629841653
H 4.245847713905 -1.910642369367 1.439216977062

**5c radical cation (*trans*)**

E(UB3LYP/6-31+G*) = -5672.10233017
E(PCM-UB3LYP/6-31+G* (ether) = -5672.16035755
C 0.112917048617 -0.014652319190 -0.000028146088
C 0.155326712052 -0.031412021481 1.422289740344
C 1.521413975118 0.049525874777 1.828884838460
C 2.331288277106 0.130287614940 0.658208364414
C 1.460532158523 0.101582178029 -0.481440935430
Fe 1.022431421541 1.704377820616 0.702286017946
C 2.119902841152 3.392840511809 1.093375285326
C 1.569467332114 3.456298339280 -0.231383917914
C 0.137616841487 3.386465646804 -0.101046266423
C -0.177511531645 3.282787452519 1.283426431171
C 1.042207369603 3.296923878390 2.019094826200
N 2.313048950216 3.678457632592 -1.421971891350
C 3.400278710494 4.704909555347 -1.368493651944
C 4.872761252624 4.207450372705 -1.428440238681
C 5.201483236186 3.252154075683 -0.269915683898
N 1.893680510221 0.016989411365 -1.843199015551
C 2.477024702620 -1.309602139874 -2.234061177032
C 3.961288446182 -1.320664850413 -2.677729092963
C 4.862548336957 -0.703377362542 -1.597081192215
P 1.924053822839 3.143993566551 -2.987073009004
P 1.336522175522 0.987196335210 -3.112081845357
P -0.843773784985 1.573868258334 -3.042621527385
P -0.295102199834 3.686255058415 -3.541654459977
N -0.437343488362 4.080659068056 -5.188070263645
C -0.877375074858 5.485631201806 -5.454483332808
C -2.399336704668 5.797027572807 -5.377726290417
C -3.206649342693 4.954580091870 -6.378421385999
C 0.047398481660 3.330431227904 -6.293496440480
C 1.250827470132 2.542614479159 -6.348426425746
C 1.413664347102 2.073344269945 -7.682607725880
C 0.329635454232 2.568108429240 -8.463105169897
C -0.519102286356 3.332686348934 -7.612990005335
Fe -0.382990816454 1.411894253535 -6.905496008775
C -1.503571962194 0.451309191960 -5.497047269124
C -2.295352557898 0.721615282734 -6.662289671640
C -1.683444099580 0.062682377529 -7.768733566065
C -0.519490643177 -0.615826410330 -7.296546056767
C -0.412036872787 -0.392056123906 -5.895298170637
N -1.861872969206 0.813689473052 -4.159347961286
C -3.006151943535 0.031612191797 -3.583285385856
C -4.281584585740 0.826730517044 -3.207669218306
C -4.807356828117 1.623197936908 -4.411968414708
C -2.539565355312 7.292261330199 -5.734552879769
C -2.967917834356 5.568907006136 -3.965249950615
C -5.331143602830 -0.221623363616 -2.781959816113
C -4.034637940104 1.786814875684 -2.029094869532
C 5.747761802675 5.473925042060 -1.313646794347
C 5.193452795769 3.502155203706 -2.758921018237
C 4.337543962404 -2.803565763413 -2.880911512652
C 4.170016978413 -0.570513444311 -4.006438635509
H 3.240221706625 5.405864730815 -2.197959740268
H 1.863091605473 -1.755811791227 -3.028287158955
H -0.356219284207 6.140314371729 -4.744016200963
H -2.658316675789 -0.523659191388 -2.701525131474
H -0.503650149751 5.737211454037 -6.451009069534
H -3.261437603670 -0.713645263033 -4.342502679949
H 3.242653221543 5.266439552279 -0.443366925941
H 2.363478519188 -1.948872490539 -1.353473846186
H 3.166393953841 3.399313055310 1.349173808515
H 1.141848502341 3.203152033248 3.092531890192
H -1.173170497005 3.185210526117 1.695815219848
H -0.584893126027 3.422115695182 -0.899634174987
H -0.777457119681 -0.043905586713 -0.611750504524
H -0.702711400906 -0.059588218534 2.081481941552
H 1.878662631343 0.091514572129 2.849611025584
H 3.406625708998 0.224647673344 0.628302384292
H 5.572579568640 6.161437315840 -2.150510781391
H 6.809646560101 5.203779812527 -1.321973754972
H 5.550154324325 6.016492301238 -0.380741112324
H 4.914049486743 4.113195090095 -3.625309491124
H 4.685132408248 2.535253196198 -2.844086109408
H 6.269783298942 3.302355269361 -2.821884137839
H 4.522677030362 2.392545737951 -0.257212213594
H 5.142379067805 3.760424832126 0.699622336689
H 6.223354356490 2.870234913352 -0.374417968720
H 3.711783118827 -3.275144807651 -3.649472651168
H 4.224366424385 -3.377170069136 -1.952768365012
H 5.381437565624 -2.892588731192 -3.202248146885
H 3.506787860598 -0.950948935603 -4.793297085748
H 5.204108346517 -0.694452229907 -4.349509594042
H 3.991286626409 0.505773585639 -3.905248684046
H 4.779935416023 -1.248982644749 -0.649476899367
H 4.600263171230 0.344412640878 -1.417889871831
H 5.912417241244 -0.736653384810 -1.910366476444
H 1.930343132308 2.346124163994 -5.535606007339
H -1.435849377473 3.813311314717 -7.911683211504
H -3.181071220448 1.338543503167 -6.693967270060
H 0.373327218461 -0.758126285784 -5.249502680722
H -2.011577117902 7.929252543941 -5.014013234642
H -2.140955742722 7.506697029040 -6.733983222803
H -3.594947194532 7.586834693972 -5.727873079820
H -2.385830083859 6.093875312390 -3.198667170726
H -3.998734191285 5.939629839112 -3.916840551411
H -2.999714479237 4.505749018881 -3.702157635467
H -2.946561683326 5.201841956273 -7.414311962072
H -3.041724327460 3.883087910281 -6.221666181042
H -4.278263435574 5.149558237304 -6.257436827646
H -2.017610875443 0.109779813722 -8.797027552356
H 0.182647799067 -1.170825610897 -7.905259708431
H 2.212481947683 1.431358455691 -8.029970862461
H 0.150538374995 2.362688387565 -9.510347855256
H -4.986517053184 -0.808399059472 -1.920814740029
H -6.267833239634 0.269677160177 -2.495364312312
H -5.556497920239 -0.918475505334 -3.598597491356
H -3.611199597339 1.262651634350 -1.163240178844
H -3.353276117584 2.602098086892 -2.296742309849
H -4.979194428248 2.246571418359 -1.714704494030
H -4.070582418895 2.360198356787 -4.747790009273
H -5.045959557953 0.962243972870 -5.253794405590
H -5.722277927927 2.163476707971 -4.142712305831

**5c radical cation (*gauche*)**

E(UB3LYP/6-31+G*) = -5672.12804026
E(PCM-UB3LYP/6-31+G* (ether) = -5672.17762121

C -0.033147813249 0.014223617973 -0.031681890827
C -0.049730704164 -0.008423950338 1.396485799955
C 1.296831654538 -0.047406922525 1.853237237403
C 2.152082262295 -0.070357949579 0.708807491921
C 1.330849413111 -0.060120757124 -0.466391568817
Fe 0.967049222071 1.650993171477 0.740142331957
C 1.949386004708 3.286681043777 1.536796850701
C 1.922738005668 3.442096882645 0.111972743869
C 0.547578494285 3.418752104654 -0.293012522125
C -0.262200067742 3.294865044249 0.877718456960
C 0.601496430390 3.226613614704 2.005877293689
N 3.047014308385 3.608930718943 -0.754606928748
C 4.388718487581 3.617870850707 -0.139477340173
C 4.964237859727 5.031394959713 0.130706784077
C 5.031677052026 5.825815894134 -1.184569004869
N 1.799551831400 -0.130384995088 -1.814787556499
C 0.789432922446 -0.119249869598 -2.890969871079
C 0.408360403004 -1.521006017982 -3.431459687037
C 1.665005683213 -2.235172037424 -3.957212925376
P 2.721818834329 2.870441869647 -2.294788973066
P 3.331116728785 0.681245115929 -1.952031981124
P 3.879021644958 0.805246233982 -4.109517977811
P 4.594914836860 2.893192505594 -3.503640740139
N 4.260489857738 3.781995795121 -5.012568530317
C 2.891443385406 4.016337177228 -5.524987163034
C 2.468968195512 5.506895976085 -5.590668487128
C 2.587161974755 6.147993163224 -4.197953350220
C 5.312859339689 3.760644495155 -5.905723880369
C 5.224144363167 3.672620102140 -7.338465825996
C 6.538885829951 3.697109445261 -7.889219277971
C 7.463499732833 3.703193557490 -6.810597117991
C 6.720759139842 3.688696600717 -5.586602837506
Fe 6.334221282677 1.976331260180 -6.722725644801
C 5.960150043759 0.107439803314 -5.599443516710
C 7.341397833618 0.273793215103 -5.963931903105
C 7.444408521038 0.335241039256 -7.384525963196
C 6.128377716636 0.305445680930 -7.918892373466
C 5.205830478933 0.219013220351 -6.827347403512
N 5.451110624398 -0.008546006701 -4.321518620602
C 6.382727788551 -0.269436113167 -3.200893197595
C 6.641200207207 -1.769950534676 -2.907305240585
C 5.311200823763 -2.484563418581 -2.615651178299
C 3.332247409532 6.296984570995 -6.590169467851
C 0.999172674192 5.527430404628 -6.053021022217
C 7.345129233833 -2.464899705187 -4.086296964174
C 7.548374253780 -1.824682335528 -1.662904039756
C 4.105079930809 5.805893922469 1.145401066471
C 6.384084012073 4.840620394389 0.696893536257
C -0.246315330516 -2.387233872158 -2.341205778920
C -0.588589194199 -1.304642921535 -4.585671309854
H 7.330929335581 0.251953700289 -3.377652448223
H 2.777864814932 3.545543512814 -6.508670854288
H 4.372108307343 3.029931516546 0.785628853661
H -0.105469972450 0.413434724382 -2.548675944438
H 2.825144585135 3.242656399413 2.165554759887
H 0.301671577828 3.110021124619 3.039217454726
H -1.343078583025 3.243499479435 0.892276011375
H 0.176435011073 3.492245625114 -1.305601804175
H -0.909706397004 0.058202058571 -0.659327159252
H -0.937292182919 0.036189537958 2.014162840649
H 1.625779081592 -0.041625873801 2.884211955303
H 3.232287713050 -0.100869403022 0.735471877156
H 5.081597521824 3.097860755024 -0.809116140396
H 1.180946086737 0.466476552109 -3.729152883434
H 2.198999216150 3.497000611921 -4.858713180482
H 5.951330055836 0.181729759642 -2.304535317597
H 4.314203233010 3.637891646543 -7.917305470441
H 7.141988135115 3.697039480546 -4.591738623707
H 8.178353533128 0.304088258516 -5.283608308619
H 4.129804654649 0.170995457754 -6.911734129150
H 6.780219935843 3.679729734069 -8.943988357143
H 8.543024644751 3.706069846237 -6.889194908568
H 8.365387934462 0.423063510573 -7.945922606811
H 5.858488517457 0.351650370181 -8.966071848508
H 6.844708377567 5.811071032896 0.914866520583
H 6.368816005070 4.263127338187 1.630116388380
H 7.033442871357 4.315201126615 -0.016128799144
H 4.517512806610 6.810087311665 1.300582668128
H 3.073148441817 5.914718165465 0.796539540296
H 4.082834268925 5.303336649739 2.119298052388
H 5.484583416359 6.810157084206 -1.017283556848
H 5.636928165876 5.303601378265 -1.937691827741
H 4.029343502257 5.980336254385 -1.595379500995
H 7.773095391537 -2.864472468719 -1.400114119548
H 8.503606324074 -1.312516335125 -1.837267562061
H 7.065682647877 -1.358584046305 -0.794790366239
H 7.534305406416 -3.516935198816 -3.844158123932
H 6.732775582163 -2.443660204366 -4.994772667610
H 8.313183176271 -2.000220216545 -4.311131601749
H 5.490540290999 -3.535251146890 -2.360518486483
H 4.781938863381 -2.022864372207 -1.773733061671
H 4.651499763894 -2.461139557294 -3.488849705051
H 0.635719848547 6.558794100220 -6.123118542233
H 0.880968032318 5.065907438683 -7.042065469474
H 0.350252289046 4.992775033913 -5.348105457283
H 2.244820203343 7.188749976696 -4.226703470937
H 1.977815909786 5.617109846310 -3.457027627637
H 3.625288790759 6.147677243072 -3.850794028803
H 2.998896528746 7.340190703339 -6.632542484205
H 4.388530579026 6.303035194604 -6.298652600912
H 3.256072685697 5.886182862878 -7.604589555326
H -0.901860463810 -2.266178674467 -5.008485031363
H -1.491178452543 -0.782788705298 -4.242688626740
H -0.142333366855 -0.712828284438 -5.396068890508
H 1.402763703744 -3.207982898809 -4.389537273549
H 2.163426509619 -1.646087583938 -4.738741294997
H 2.380148256490 -2.407048933942 -3.147061179805
H -0.483343301745 -3.380823806469 -2.740183672473
H 0.417708920587 -2.518294925819 -1.480784224479
H -1.182108164736 -1.942757262314 -1.983062851050

**5c triplet dication (*trans*)**

E(UB3LYP/6-31+G*) = -5671.81818191
E(PCM-UB3LYP/6-31+G* (ether) = -5671.9857993
C 0.463296270370 -0.558624595262 -0.286557111066
C 0.612704204570 -0.677591856812 1.123672415724
C 1.946563062521 -0.293632104650 1.460735342127
C 2.614450777490 0.071975505176 0.251434360822
C 1.703498139275 -0.109776021586 -0.842105590303
Fe 0.965214822963 1.320478999055 0.595495372484

C 1.572531542673 3.293435440340 1.067473625842
C 0.945961572933 3.341832564069 -0.226986676677
C -0.366893166854 2.780678837664 -0.054700711704
C -0.565376849065 2.482624244288 1.328482305295
C 0.635958911841 2.802960770267 2.021502454487
N 1.551557537349 3.764442396316 -1.396863668387
C 2.553699743550 4.885396383134 -1.300840612102
C 4.066919273714 4.573375620467 -1.449262116706
C 4.557092264258 3.577776722410 -0.385502500048
N 2.027732514580 0.055775985559 -2.209585871174
C 2.925740544389 -1.030651923762 -2.747970186966
C 4.336715522074 -0.639424584106 -3.248704110337
C 5.135063816886 0.076922214329 -2.149073498337
P 1.187931539606 3.271251095551 -3.038152695899
P 1.174244948273 0.982944345220 -3.387737170703
P -1.055266244286 0.983086050326 -3.033803380957
P -1.057956746906 3.282527083191 -3.293468742808
N -1.416998891999 3.841542388602 -4.914793430590
C -2.411964426636 4.971664898431 -4.967887627224
C -3.927274335040 4.663816782995 -4.832434732652
C -4.422957988066 3.713170795355 -5.934102719613
C -0.813422407049 3.460418057989 -6.099802285461
C 0.495817302843 2.897588461815 -6.292882315251
C 0.693527606104 2.651753838600 -7.686400401557
C -0.505092654773 3.006499501647 -8.367244713741
C -1.439214510518 3.466051147779 -7.395563074629
Fe -0.845198924097 1.472408701074 -6.999626593606
C -1.592527454361 -0.007723639936 -5.618871907296
C -2.502461053783 0.222481391559 -6.704154570644
C -1.837184055087 -0.100276725589 -7.926998360739
C -0.505928499549 -0.506056762778 -7.605666886440
C -0.355502291691 -0.443079170745 -6.191949399669
N -1.915320397522 0.107104348735 -4.245821878675
C -2.819761474179 -0.993565980817 -3.748983096851
C -4.228291215121 -0.613090880623 -3.233302679574
C -5.022524540869 0.149023442057 -4.304798686596
C -4.643006730467 6.024935760031 -4.974153827692
C -4.274432932690 4.064180263556 -3.457933424506
C -4.937132703195 -1.949660929715 -2.921942829823
C -4.165795735557 0.223534437355 -1.942150129800
C 4.791479209346 5.923375528339 -1.255612917109
C 4.409458634032 4.025029668499 -2.846153175784
C 5.037644683936 -1.967552294141 -3.610143893925
C 4.279824348493 0.245679359412 -4.507392780711
H 2.273439268550 5.614229293157 -2.069144246476
H 2.387300607747 -1.543221875923 -3.555556341525
H -2.127681590764 5.668416642685 -4.171789926694
H -2.284435992221 -1.539768324397 -2.961614303716
H -2.227762398017 5.492410728740 -5.912769264558
H -2.928887910691 -1.689870321626 -4.587226173991
H 2.373304329934 5.370318970537 -0.336360401837
H 3.030370889693 -1.758956288286 -1.936791980598
H 2.588833897614 3.578523217519 1.284693551465
H 0.821877043814 2.677043265971 3.080452891843
H -1.473035634620 2.079860251570 1.759342738549
H -1.111171504888 2.638530905384 -0.819994413670
H -0.445428758507 -0.734445529497 -0.843931109032
H -0.160573303218 -0.983264800935 1.817008582573
H 2.375097932048 -0.274520438807 2.454564006845
H 3.634213009031 0.416124449552 0.165850264175
H 4.495743210655 6.652624151032 -2.019308678375
H 5.875402147262 5.785459178607 -1.332153217042
H 4.581527094373 6.358312517619 -0.270775865480
H 4.042158927902 4.682882327293 -3.641849456232
H 3.990853131067 3.026811381439 -3.008585789108
H 5.496505306959 3.938934399894 -2.955739128857
H 3.968411490301 2.654441381569 -0.405700880040
H 4.509175542052 4.006398786949 0.622942845396
H 5.603278558018 3.310200060466 -0.568371275557
H 4.494804588926 -2.509932948068 -4.394507192172
H 5.125713828906 -2.628413889455 -2.739361573080
H 6.049299757957 -1.773532344955 -3.982320342646
H 3.696411121686 -0.232002747224 -5.304452658814
H 5.292456775703 0.417118841262 -4.889907506320
H 3.837249310590 1.226790805016 -4.306413894482
H 5.249555916746 -0.557885049700 -1.261572193568
H 4.651460476517 1.013102237476 -1.854062922572
H 6.140811406264 0.323953094067 -2.506027551222
H 1.238593137159 2.721384479523 -5.533263894184
H -2.453431990048 3.766011444542 -7.602259284705
H -3.519881067272 0.569792866493 -6.604767517097
H 0.552133298594 -0.646552140343 -5.642228182874
H -4.343452380146 6.722068815226 -4.182460540390
H -4.429207672464 6.496437444681 -5.941172105703
H -5.727866185421 5.891097936125 -4.903940630784
H -3.903314642967 4.688342415716 -2.637259568529
H -5.362110490573 3.981192435876 -3.352255029880
H -3.862563343625 3.057680122571 -3.333983153794
H -4.371447669840 4.180014947341 -6.925252353068
H -3.840274337184 2.785951839140 -5.949208065217
H -5.471004954224 3.445544070980 -5.762294034354
H -2.265688104815 -0.039548438758 -8.919168828118
H 0.265219200881 -0.789613741951 -8.310672281329
H 1.598863766748 2.259851285178 -8.131915862306
H -0.691008910734 2.922613691249 -9.430351036198
H -4.397379545948 -2.524509048321 -2.158861119760
H -5.947515357681 -1.763769132162 -2.542247610557
H -5.029375464229 -2.576644991719 -3.817004529075
H -3.585293514296 -0.287486370917 -1.163865354776
H -3.717176121475 1.208780329663 -2.106148037844
H -5.177301777006 0.386727545193 -1.553099565669
H -4.533668676177 1.093043716540 -4.564043854206
H -5.140479171458 -0.450905301431 -5.215795125712
H -6.026898570340 0.387947221251 -3.938577954373

**5c triplet dication (*gauche*)**

E(UB3LYP/6-31+G*) = -5671.85002527
E(PCM-UB3LYP/6-31+G* (ether) = -5672.00897851
Sum of electronic and zero-point Energies= -5670.908186
Sum of electronic and thermal Energies= -5670.855442
Sum of electronic and thermal Enthalpies= -5670.854498
Sum of electronic and thermal Free Energies=-5670.993138
C -0.165877485749 0.107162786126 -0.176882481079
C -0.268888341443 -0.002654222104 1.240247781602
C 1.041280597258 -0.170391224545 1.762694811897
C 1.960976209754 -0.174538773029 0.664683824021
C 1.205232321781 -0.081381787529 -0.561005687280
Fe 0.936002501379 1.649048835487 0.783428555014
C 2.133183052408 3.196747318047 1.611174402013
C 2.051579317154 3.463455441922 0.202185665906

C 0.646067425621 3.517183535494 -0.119982631256
C -0.099913295859 3.412055298400 1.098190599478
C 0.819746666232 3.220671134756 2.163661421612
N 3.115587028637 3.541644625030 -0.689837788098
C 4.495645818838 3.612885214954 -0.148485999298
C 5.019087647420 5.049842900471 0.103161098603
C 4.977624087810 5.858409539734 -1.204306244755
N 1.713539206790 -0.064224883486 -1.855330522067
C 0.763547511182 -0.109297060033 -2.994712560579
C 0.417507504613 -1.535447744779 -3.493234981859
C 1.702037056151 -2.268727467046 -3.914247019107
P 2.726336733936 2.873411816342 -2.275506081608
P 3.311515236974 0.677276972307 -1.950388555243
P 3.888866712120 0.796477556565 -4.103972443557
P 4.586150240245 2.901915136144 -3.510724267291
N 4.237129390018 3.781010396259 -4.999926814397
C 2.864366792275 3.990438406196 -5.523675444852
C 2.417095899397 5.472746093641 -5.593389711745
C 2.496720285181 6.109689076603 -4.195908996547
C 5.298525171305 3.759126699957 -5.898255937380
C 5.207555954297 3.673692111205 -7.329158878260
C 6.522170211248 3.697816957644 -7.878820829055
C 7.447207737961 3.707792313495 -6.800913572904
C 6.703904104442 3.699642999626 -5.576604406328
Fe 6.320419783991 1.975446622646 -6.703631193583
C 5.957541102663 0.107829214007 -5.583485353468
C 7.337865454563 0.271421918820 -5.945418842490
C 7.439852408975 0.333160695957 -7.365527439196
C 6.124518090308 0.299525285696 -7.900731562588
C 5.202126573615 0.206705837210 -6.808907889046
N 5.446539015993 -0.009357055319 -4.295393465713
C 6.389123016678 -0.244819234408 -3.173455726318
C 6.659056549348 -1.737856800434 -2.857003148032
C 5.336794113253 -2.450125468293 -2.526426364440
C 3.287735400866 6.280638554367 -6.572188194613
C 0.956603929653 5.468904825502 -6.085419688229
C 7.341331778552 -2.451721271702 -4.037532512203
C 7.590817573567 -1.765947388182 -1.629740240895
C 4.188163576498 5.774321892146 1.177138226713
C 6.475656549454 4.909087001279 0.586621346741
C -0.304475407873 -2.354079027890 -2.408192858347
C -0.510708245557 -1.362533997807 -4.711288535971
H 7.330207819147 0.280840024283 -3.369851789310
H 2.771686576225 3.516199866280 -6.507054722171
H 4.560211280618 3.016168396697 0.768190495143
H -0.149593631567 0.436005983122 -2.731363317720
H 3.036316297744 3.040456322935 2.180636486093
H 0.574831447761 3.083481435676 3.208900731304
H -1.177818051899 3.465955652192 1.181012661847
H 0.225636188490 3.682097108465 -1.101796489237
H -0.999692419843 0.267684370848 -0.842726356184
H -1.186055320937 0.064091394878 1.810931114355
H 1.309040211607 -0.273426898543 2.806405413976
H 3.031543592442 -0.300054022804 0.742456922115
H 5.159374756588 3.127523433299 -0.868727371346
H 1.213697299324 0.443618065734 -3.823271632323
H 2.174064012766 3.454634226680 -4.866973262182
H 5.965501703797 0.223518664682 -2.281231033763
H 4.299302277113 3.636222860331 -7.910555577115
H 7.129216762395 3.719582000740 -4.583314250141
H 8.176595872563 0.304680058630 -5.267349779474
H 4.126766979052 0.147361236403 -6.898313955399
H 6.762882590809 3.678748397362 -8.933821010709
H 8.526708214829 3.715666782459 -6.880046069098
H 8.361172171820 0.422667327509 -7.926321373612
H 5.855338197768 0.340766947407 -8.948341488221
H 6.908494772883 5.895927733385 0.782510549493
H 6.538569511457 4.330585287791 1.516850158111
H 7.103681771864 4.414094502946 -0.165342089829
H 4.589887806841 6.779044922693 1.347923828219
H 3.141162318034 5.889039607435 0.874776931127
H 4.216565519711 5.244387283788 2.136783258281
H 5.392833868742 6.859892601993 -1.047552635619
H 5.568639256778 5.375750185630 -1.993486843332
H 3.950287969406 5.977793995614 -1.563519854726
H 7.821185481021 -2.799674194110 -1.350615840604
H 8.542502836909 -1.259148925789 -1.833210226294
H 7.126674253918 -1.282564904666 -0.760376617999
H 7.536657842504 -3.498593042637 -3.780794480662
H 6.712868781521 -2.448127547681 -4.935206927748
H 8.305212791978 -1.991778210947 -4.286427604050
H 5.523340497281 -3.494131844454 -2.252226452115
H 4.824584885841 -1.973094696788 -1.680765233406
H 4.660568981918 -2.449114485970 -3.387486042488
H 0.576220815712 6.493563183188 -6.155805996948
H 0.866439184897 5.014364339032 -7.080011769198
H 0.301500660844 4.917709293883 -5.398467204979
H 2.134622627742 7.143094008596 -4.225816953389
H 1.879090272524 5.564267043086 -3.470576215818
H 3.527817820352 6.130052452526 -3.828307818489
H 2.939354355741 7.318305730978 -6.615605521170
H 4.338409719938 6.302343521688 -6.261683010433
H 3.234580467673 5.876037693003 -7.590046277144
H -0.793585987409 -2.340238657789 -5.115825521437
H -1.435416887527 -0.836234244863 -4.443202932687
H -0.019449266946 -0.799675485889 -5.515488224716
H 1.462427559978 -3.259514497643 -4.315329978930
H 2.240862387744 -1.717566493674 -4.695882217359
H 2.374792904175 -2.409717123888 -3.062057961080
H -0.552944179699 -3.349457244373 -2.792255431672
H 0.320543207127 -2.494497352929 -1.519133277439
H -1.244016009842 -1.879327126094 -2.100898967373

**5d neutral compound (*trans*)**

E(B3LYP-D3/6-31+G*) = -5043.21346981
E(PCM-B3LYP-D3/6-31+G* (ether)) = -5043.21965252
Sum of electronic and zero-point Energies= -5042.728821
Sum of electronic and thermal Energies= -5042.696219
Sum of electronic and thermal Enthalpies= -5042.695275
Sum of electronic and thermal Free Energies=-5042.789987
H 0.537718602898 0.780513967195 -0.378903726149
C 0.431777756078 0.396148031767 0.627721600913
C 1.507658803564 0.224284330728 1.562128673743
C 0.945027157230 -0.283610783392 2.781701809433
H 1.497151981342 -0.484181233023 3.688910875877
C -0.462729216065 -0.410047261302 2.599651492103
H -1.173717465098 -0.722637387300 3.354247374970
H -1.772818040226 0.047595704423 0.835770338976
C -0.780791698949 -0.000381874384 1.266975279441
Fe 0.108975053499 1.546122854360 2.292723089994

C 0.726168962696 2.999348804284 3.630988164134
C 0.893066030365 3.484927803646 2.293532052283
C -0.651886004909 2.682366841861 3.827687683485
C -0.398561175859 3.439546174913 1.664702728519
C -1.348401518181 2.957890359925 2.616284102699
H -1.077547162822 2.274683629048 4.735525431627
H -0.619087413836 3.701551911811 0.639892024238
H -2.402448648223 2.796328167096 2.429773949716
H 1.495201526042 2.885584554575 4.377093382798
N 2.060481922708 3.983791133868 1.681766690351
C 1.842223582085 4.673084380017 0.401314142023
H 2.778334371643 5.132567841394 0.078207542461
H 1.503423954573 3.984209744605 -0.386815093759
H 1.091270780255 5.461545308917 0.529225706862
P 3.711829344757 3.528054814414 1.948149950836
P 4.039994384575 3.604887136719 4.172504884164
N 5.651124037848 4.200373094391 4.408088316489
C 5.813153110385 4.977730163155 5.645745641248
H 6.201581504010 4.363802602752 6.472005266233
H 6.502154732979 5.812319331126 5.470535721778
H 4.843992448130 5.382609446239 5.943448406227
H 6.305067351906 2.995232876821 1.779318480966
C 7.061359188883 3.210022124629 2.516156861709
H 8.917855998762 2.563180029323 1.451463883359
C 8.460102838448 2.988649482599 2.335206872191
C 9.130622323038 3.385939363370 3.527307008189
C 8.144451133293 3.847441887829 4.451524729884
H 8.341855397733 4.184128193497 5.459093781604
C 6.854652207850 3.757667325780 3.823744972278
Fe 7.784855203984 1.887694151973 3.934606558338
C 8.504590177832 -0.033699701597 3.739667225924
H 9.238738312966 -0.334311388197 3.002586557675
H 9.772591862751 0.623536187815 5.470916523500
C 8.787938002956 0.475266224640 5.045677182525
H 10.193499438709 3.316540327906 3.720646954089
C 7.091654326847 -0.025647164282 3.554139513014
H 6.558237182980 -0.319779546778 2.661370253376
C 7.547443614910 0.814478138522 5.663994334325
H 7.410554480267 1.247206466877 6.646981851067
C 6.489581624496 0.507446172813 4.743745215967
P 3.817548535738 1.305819122656 4.242393664364
P 4.110078149014 1.252194948223 2.009937426115
N 2.883624830035 0.344758290807 1.219091860600
C 3.338641227374 -0.731781034592 0.320240892133
N 5.107734986824 0.542416507685 5.082427700421
C 4.734256716966 -0.511119307592 6.043856448673
H 5.328694988930 -0.413432007791 6.959979818596
H 3.676510952728 -0.409675531145 6.301317434956
H 4.905427784883 -1.514071003044 5.625449563155
H 4.385901434246 -0.564718094056 0.054275580693
H 3.244326674504 -1.718532720054 0.797407241054
H 2.739985240631 -0.734116776303 -0.598333670751

**5d neutral compound (*gauche*)**

E(B3LYP-D3/6-31+G*) = -5043.22308323
E(PCM-B3LYP-D3/6-31+G*(ether)) = -5043.22972513
Sum of electronic and zero-point Energies= -5042.736557
Sum of electronic and thermal Energies= -5042.705237
Sum of electronic and thermal Enthalpies= -5042.704293
Sum of electronic and thermal Free Energies=-5042.795062

C -0.079507677563 0.046675593752 0.031015758078
C -0.052757379737 0.053393055049 1.460669236698
C 1.315215510438 0.002983252295 1.884826206686
C 2.128841492617 0.025660057706 0.704130768506
C 1.265749385756 0.023047258149 -0.436459705761
Fe 0.931111039649 1.716116130879 0.668860024802
C 1.994922454894 3.443106165984 1.164294257125
C 0.689529899554 3.543690909789 1.747074518459
C -0.263546690527 3.409038445206 0.684033496413
C 0.452018994607 3.293267774969 -0.549029535732
C 1.844837323782 3.307875583309 -0.251282480663
N 0.385604248013 3.761067504515 3.116486930966
C -1.042628477923 3.768527927104 3.437077327850
N 1.787293445539 -0.079427624828 3.220964331620
C 3.244207369744 -0.063876162682 3.361834724455
P 1.554634877997 2.968246126154 4.158492505125
P 0.751063592898 0.819987563465 4.315610598784
P 1.766849568951 0.954950570398 6.297630867879
P 0.792288617612 3.036725624978 6.254341324491
N 1.889677950840 4.015921567965 7.212411197565
C 3.313890606731 4.108093615289 6.887139569035
C 1.599019411276 3.904995890599 8.597371912697
C 0.303757877226 3.755034389199 9.192021094655
C 0.458846966060 3.766550726834 10.613458330045
C 1.847168832495 3.892364685377 10.905935640954
C 2.555782581483 3.948502359593 9.664727664762
Fe 1.501336706713 2.173854489320 9.844183510511
C 1.299926149432 0.571246504375 11.105640412996
C 2.640683474304 0.658906486285 10.632886600311
C 2.618927731906 0.528476382055 9.209094020018
C 1.261083137773 0.328257463703 8.796819772441
C 0.443779396477 0.396675390514 9.973200426111
N 0.802264662854 0.082352095803 7.476244255136
C -0.650624668377 -0.032846035782 7.340142825683
H -1.010263986415 -0.834227233435 7.993741002105
H 3.746570161203 4.968095403308 7.408607048274
H -1.541188525648 4.537823756994 2.838443069902
H 3.669732328939 -0.891804977446 2.785463695328
H -1.339021118777 3.393751065098 0.788426531487
H 0.005080337111 3.176063411718 -1.528087875899
H 2.654058463396 3.207857698435 -0.963387474234
H 2.934145886951 3.477526488429 1.697971419069
H 3.208860716944 0.044533629580 0.672847394981
H 1.587607047711 0.039826406284 -1.469983923978
H -0.971088871806 0.080624183905 -0.582063807250
H -0.918638587426 0.077887510505 2.107033108371
H -1.178630456227 4.017796302108 4.490536896188
H -1.516470781744 2.793707213289 3.239344150550
H 3.510822896979 -0.208286655235 4.409913778529
H 3.683987038131 0.883589134678 3.011401281912
H 3.433426500226 4.266966030846 5.814350005532
H 3.863935862804 3.197629226696 7.174202306841
H -0.900780742085 -0.296562002080 6.311414488980
H -1.166603034167 0.904963271999 7.601256460068
H 3.629384108119 4.010124261425 9.558136332267
H -0.633142717308 3.663153136743 8.661067480296
H -0.634364569904 0.331381603755 10.006684599589
H 3.482480049188 0.561504677025 8.559999750207
H 2.298358600691 3.904482629515 11.889971780553
H -0.342397832622 3.669327011181 11.334908460018

H 0.973826810402 0.659526723529 12.134188895557
H 3.524292406307 0.822258784861 11.236614382348

**5d radical cation (*trans*)**

E(UB3LYP/6-31+G*) = -5042.98805906
H -4.670442463963 -1.601127814591 -1.970231234037
C -4.390157266046 -1.661109786200 -0.926838891044
C -3.046754568781 -1.683254362599 -0.423554332642
C -3.109073291366 -1.746377945395 1.009831840777
H -2.265116534004 -1.770241162282 1.683339176672
C -4.484537674625 -1.746818354621 1.381300685114
H -4.864902617359 -1.744378946267 2.394440351549
H -6.353061101748 -1.660345215841 0.148178171687
C -5.272659558717 -1.703331151777 0.191630619161
Fe -4.040917811631 -0.052515461839 0.289249794434
C -3.181341141271 1.630686380036 1.113679168094
C -3.127726597256 1.668287735130 -0.321861581649
C -4.553510651156 1.546040214947 1.489651706239
C -4.471705716888 1.613604957235 -0.819207506468
C -5.347209293302 1.542859517223 0.302669305728
H -4.926709793313 1.462373842484 2.502052510755
H -4.755565119756 1.609940221390 -1.863276644135
H -6.424717550094 1.453049935709 0.260390656777
H -2.335480379313 1.655476173271 1.785594580129
N -1.994499073225 1.925790226946 -1.149077600860
C -2.074094855789 3.215798808268 -1.880640996300
H -1.141704808233 3.392324412441 -2.422784201369
H -2.894169433873 3.176340371390 -2.603259578123
H -2.251598740802 4.038484760525 -1.179505977979
P -0.471841316836 1.214712940682 -1.074123029758
P 0.473676791288 1.230826037964 1.071050828385
N 1.996917773622 1.942826380183 1.128412698326
C 2.080494187499 3.238700316129 1.848592585066
H 2.899709437109 3.203332927299 2.572376618433
H 2.261284265021 4.053841512794 1.139604114804
H 1.148160282597 3.423622738093 2.388073543340
H 2.345717798425 1.625587684032 -1.802705249718
C 3.189080369865 1.611188645630 -1.127549072656
H 4.938853641209 1.420083191340 -2.507353317089
C 4.562495455410 1.520238411573 -1.497584971193
C 5.352542055256 1.536212845342 -0.308304086385
C 4.473615255545 1.624873869983 0.809346301211
H 4.754063091920 1.637883878194 1.854219230425
C 3.131106637430 1.671339131527 0.307334821206
Fe 4.046194013705 -0.059034023139 -0.273654663523
C 4.506736541424 -1.768419917404 -1.336189550347
H 4.897511809857 -1.779272968564 -2.345328414826
H 6.362924130163 -1.654966748073 -0.087021558982
C 5.283142702904 -1.703809109757 -0.139368535089
H 6.429864549565 1.446541929979 -0.261153947977
C 3.127955270497 -1.767054186264 -0.978043154207
H 2.291220484715 -1.802395072355 -1.660078651893
C 4.389777861537 -1.647530484932 0.969440771816
H 4.655054644595 -1.570546369955 2.015882080258
C 3.051507723691 -1.680859721572 0.453570302737
P 0.417796916579 -0.996005937241 1.076502213889
P -0.417165904198 -1.016278736013 -1.085641128563
N -1.893654047202 -1.809049503652 -1.254642517529
C -1.878311069665 -3.049117122938 -2.071574325552
N 1.893716905092 -1.794088223303 1.283844469936
C 1.790357615770 -3.111242134732 1.967397785833
H 2.739982403641 -3.317004891366 2.467426475491
H 0.999628204404 -3.072886587848 2.719938641935
H 1.586681205800 -3.918089642218 1.251605226755
H -0.939343005232 -3.115064894405 -2.626897631770
H -1.985587882388 -3.930777448221 -1.429890525836
H -2.704185935166 -3.024105278610 -2.788073794084

**5d radical cation (*gauche*)**

E(UB3LYP/6-31+G*) = -5042.91197357
Sum of electronic and zero-point Energies= -5042.425046
Sum of electronic and thermal Energies= -5042.392909
Sum of electronic and thermal Enthalpies= -5042.391965
Sum of electronic and thermal Free Energies=-5042.485480
C 0.137427208960 -0.041916961200 -0.046842617142
C 0.082731073951 -0.056333970258 1.380721815741
C 1.430954281183 -0.004880411888 1.878776661389
C 2.296752978727 0.138141449200 0.744300928689
C 1.498768036380 0.078018531429 -0.439569811943
Fe 0.930052427264 1.724124603396 0.680184515443
C 1.843804624260 3.555466168177 1.115978332779
C 0.562760231005 3.555816302877 1.769689186848
C -0.428084727248 3.316719794065 0.760651256093
C 0.226823531054 3.266729726269 -0.508418962422
C 1.623907025249 3.414011991930 -0.288576344399
N 0.315283507557 3.734788713961 3.143418490716
C -1.089832908755 3.872949334250 3.539316032339
N 1.837088908176 -0.061806560029 3.224968550038
C 3.279351537465 -0.171387940573 3.465894603065
P 1.521169363008 2.973565527328 4.164157339658
P 0.753834295572 0.793742980425 4.306680845086
P 1.754612699197 0.930461284814 6.302858896533
P 0.759444625628 3.020697210849 6.267138730096
N 1.873116818331 3.987897691725 7.215819616999
C 3.257374735697 4.241212269376 6.803676747814
C 1.639927182809 3.898532947497 8.600705251625
C 0.363257488609 3.816529269621 9.257846658634
C 0.590695320869 3.816484529392 10.668318387683
C 1.994530723362 3.837063935032 10.893466775563
C 2.646056389025 3.850613798377 9.621741653561
Fe 1.464244475334 2.135097844757 9.840301971433
C 1.068688735810 0.536642860732 11.095496768768
C 2.436807776539 0.529882186817 10.708106755292
C 2.499119562357 0.402804768731 9.286443682942
C 1.155303250085 0.268993739606 8.791773806102
C 0.274145323790 0.412979602443 9.914242608779
N 0.763540432345 0.057591943359 7.456823241808
C -0.657838362516 -0.224296118350 7.232275133973
H -0.982388935548 -1.000734284281 7.930568933604
H 3.656701193040 5.075137598419 7.387551960218
H -1.572895254725 4.608358561014 2.889995173276
H 3.687642705442 -0.964286414236 2.833119919083
H -1.491902040003 3.213809596916 0.923225793238
H -0.260016253720 3.119898319930 -1.463756080067
H 2.396606171695 3.399967948672 -1.046462631081
H 2.802796735201 3.693426074685 1.596035819654
H 3.371685297494 0.249739114647 0.772506579823
H 1.870682896986 0.136522332953 -1.454211639925
H -0.718050229356 -0.091637989226 -0.708158552392
H -0.813338919320 -0.146017382139 1.979194901246

H -1.142041678942 4.239635433136 4.565464451185
H -1.634855776451 2.919382646472 3.478508469667
H 3.452180075484 -0.445336812511 4.507647129643
H 3.808658078435 0.770110255558 3.257441233725
H 3.274890458931 4.524883499676 5.750407702867
H 3.900316571998 3.359288583713 6.941028554666
H -0.795926532821 -0.600693403122 6.217677924735
H -1.285099108487 0.669686781677 7.364061003001
H 3.715497395586 3.847985124886 9.463572570495
H -0.602814368844 3.811559115422 8.772223036033
H -0.806421537243 0.406914938942 9.881591986163
H 3.402308811070 0.359503614099 8.693549585004
H 2.489952800236 3.822628609358 11.855543716329
H -0.179508108369 3.783594877840 11.428159422480
H 0.688115250417 0.639400236699 12.103389760611
H 3.289753591707 0.626538643646 11.367496311405

**5d triplet dication (*trans*)**

E(UB3LYP/6-31+G*) = -5042.71141600
Sum of electronic and zero-point Energies= -5042.224294
Sum of electronic and thermal Energies= -5042.191646
Sum of electronic and thermal Enthalpies= -5042.190702
Sum of electronic and thermal Free Energies=-5042.286418
C 0.069115465639 0.159227010529 0.522685195301
C 0.237658446265 -0.077563892312 1.917773760618
C 1.637955589449 -0.138586841929 2.192781957836
C 2.350302048288 0.101100128976 0.973326068057
C 1.368117966822 0.239820592743 -0.066651873546
Fe 1.060437118767 -1.641295645471 0.838417872492
C 1.668791559439 -3.483725851516 1.600224740977
C 2.193397861533 -3.413586483824 0.265148047418
C 1.073622740646 -3.189826698732 -0.607954540351
C -0.124143468075 -3.219567322838 0.166024853193
C 0.240948130118 -3.400366335284 1.529509787050
N 3.514941198038 -3.475543764762 -0.151522455731
C 3.715767009711 -3.699778868148 -1.605920838854
N 3.730940278314 0.180287376561 0.782729650703
C 4.159184124121 1.010869896114 -0.371464431909
P 4.979665396859 -3.011095338529 0.675238523385
P 4.844488209286 -3.722965680407 2.799506863899
N 6.396661294871 -4.375798717513 3.257035242496
C 6.296651096149 -5.443413043596 4.284787240086
P 5.010085098863 -0.805592510545 1.436767758016
P 4.471428955143 -1.525619129865 3.489476751450
N 5.628242421721 -0.952064359470 4.659457619450
C 5.141405415220 -1.037482877144 6.059834409514
C 6.996044525859 -0.708628938915 4.523460218047
C 7.995981007293 -1.076680942951 5.487850170087
C 9.264912711894 -0.609877738307 5.026116336353
C 9.067096411947 0.004522677498 3.755661361823
C 7.677981518174 -0.077234827950 3.433342367032
Fe 8.521999344842 -1.990657371359 3.660053567250
C 8.142996418336 -3.086741532475 1.928147783446
C 9.546894594308 -2.862801633117 2.100452851039
C 9.945582792746 -3.475695577184 3.321287969303
C 8.792432773191 -4.077923245969 3.906165440983
C 7.675891235658 -3.895088007094 3.019490610725
H 4.760996066933 -3.953833531515 -1.786256150741
H 8.771972656344 -4.593208937980 4.855932275643
H 10.940445861408 -3.473194280532 3.747610307910
H 10.183181636026 -2.317406057498 1.415520678932
H 7.562301916284 -2.756656383196 1.080921562139
H 7.818714668568 -1.604437160188 6.414764718497
H 10.206469565953 -0.715785364984 5.549283795778
H 9.830406650346 0.450599121393 3.131136265464
H 7.220981768885 0.285067980104 2.525470079343
H 1.121972412464 -3.033390308133 -1.676222220136
H -1.128212336492 -3.104424324679 -0.221398509867
H -0.433001643731 -3.462244945543 2.374144881982
H 2.236153225497 -3.642202810872 2.504076604222
H 1.574584280624 0.394546243937 -1.116676478797
H -0.871605715085 0.253028308113 -0.004281584910
H -0.550810182059 -0.200130097181 2.649180215287
H 2.081224200006 -0.324652804121 3.158825456706
H 5.306659598567 -5.897945047914 4.231169565210
H 7.043908342296 -6.215833464015 4.081612912075
H 6.445395295063 -5.043829358022 5.295540409535
H 5.573267981702 -0.220377531694 6.644444847272
H 4.054764892212 -0.932486190419 6.065087671973
H 5.401378367289 -1.996135622033 6.525376959815
H 5.218972966662 1.249644917620 -0.263391504345
H 4.014726852912 0.490073599511 -1.326048785197
H 3.590353863338 1.944855069987 -0.377056985321
H 3.094013197013 -4.537428407210 -1.934682699965
H 3.466212041551 -2.804769657806 -2.189113195287

**5d triplet dication (*gauche*)**

E(UB3LYP/6-31+G*) = -5042.63240421
Sum of electronic and zero-point Energies= -5042.146252
Sum of electronic and thermal Energies= -5042.113698
Sum of electronic and thermal Enthalpies= -5042.112754
Sum of electronic and thermal Free Energies=-5042.207751
C 0.148531143031 -0.073510302432 -0.046794051220
C 0.092907851909 -0.059958155573 1.384971724421
C 1.443621122216 -0.038147163943 1.885967887088
C 2.305764602341 0.088284649203 0.745146131877
C 1.511974714118 0.016202067583 -0.438498759676
Fe 0.927927092335 1.722447484199 0.642433460085
C 1.834169859360 3.559633113901 1.121039440416
C 0.550828817371 3.589656841362 1.775281817635
C -0.437170773778 3.366412277190 0.758045721528
C 0.213559697850 3.328439261563 -0.511372107080
C 1.612753785688 3.445646384528 -0.290064097678
N 0.298216115285 3.728565800487 3.138446580683
C -1.109272195313 3.875226180867 3.541125961541
N 1.853387382421 -0.056159992193 3.217544205127
C 3.298831116494 -0.173620484595 3.465695745556
P 1.519884518137 2.974812880580 4.162081556352
P 0.754810457783 0.792284611526 4.304610893910
P 1.753708746351 0.929098781442 6.305138279494
P 0.760529537943 3.022272553720 6.269153786057
N 1.890670734040 3.983979143747 7.221178802936
C 3.276398405818 4.245323293112 6.801489852105
C 1.648187265389 3.932817109557 8.592275192078
C 0.372401633011 3.821134192417 9.252424390149
C 0.598402316825 3.849005279818 10.667124873796
C 2.001133623589 3.899891014275 10.891211985106
C 2.649781954423 3.901118410087 9.620162040015
Fe 1.466530861663 2.136782543282 9.878072539443
C 1.062247418054 0.473929000971 11.099660293880

C 2.429229289318 0.497311852296 10.710722016342
C 2.489444193785 0.397645342244 9.282551184115
C 1.146289946141 0.234137710441 8.787474849112
C 0.270545867195 0.362652764091 9.917653504526
N 0.746658555766 0.062083970081 7.463838585255
C -0.677021007859 -0.228454707896 7.232745414935
H -1.000234878164 -1.009389161574 7.925718289732
H 3.673750432869 5.083291323269 7.379813330502
H -1.590820764948 4.615270029578 2.896934989985
H 3.706243503909 -0.970695726746 2.838621577638
H -1.502665637308 3.269612991162 0.916457303344
H -0.279038060883 3.212197114452 -1.468429998383
H 2.384874363075 3.452781393783 -1.049001155667
H 2.796054651112 3.687278756326 1.598645293915
H 3.381923598719 0.193294844694 0.769605447168
H 1.889606737708 0.044006950153 -1.452769687993
H -0.706372559322 -0.144333000275 -0.707347141800
H -0.806397848151 -0.139469386716 1.980413098783
H -1.153575951932 4.246618633761 4.565171943504
H -1.656721256743 2.924020004596 3.483842760155
H 3.463565795250 -0.452368864734 4.506717965815
H 3.830979711293 0.765816945288 3.260634111720
H 3.285564114219 4.532918426246 5.749934246215
H 3.921517482706 3.365713372809 6.935215572423
H -0.806615540477 -0.608693006331 6.219242484260
H -1.306839711035 0.662925404100 7.361371498399
H 3.720224602550 3.905214223807 9.465627965736
H -0.595469350797 3.805740041977 8.770125657073
H -0.810560677399 0.350353987666 9.889325145805
H 3.394738208693 0.364898590869 8.691794347785
H 2.499035664577 3.916591410023 11.852429549363
H -0.173472197690 3.837146689652 11.426253130938
H 0.679306399827 0.545667900284 12.109776269818
H 3.283882380616 0.572851070926 11.371076848132

**6c neutral compound** *(cis-cis)*

E(B3LYP-D3/6-31+G*) = -2786.62235660
Sum of electronic and zero-point Energies= -2785.955911
Sum of electronic and thermal Energies= -2785.922680
Sum of electronic and thermal Enthalpies= -2785.921735
Sum of electronic and thermal Free Energies=-2786.015996
C -0.252588082208 0.003186010019 0.360194013950
C -0.505820919747 0.199885294240 1.761888197052
C 0.738368713058 0.193515573819 2.459504073160
C 1.779043515991 -0.009641696570 1.504487563356
C 1.176473459666 -0.102745662256 0.211691731128
Fe 0.741049289064 1.696001752863 1.028390871988
C -0.085407695425 3.111747280753 -0.243536171280
C -0.268779892739 3.509313068771 1.125390414291
C 1.011342334533 3.621018209893 1.744955555006
C 2.003238861899 3.294837183277 0.770305819585
C 1.330505444506 2.956209393835 -0.445427300684
N -1.130767716631 2.816130661450 -1.162649051196
P -2.175487007839 1.565161376909 -0.426111918868
N -3.555034886039 1.466601097696 -1.531214175181
C -4.488918040181 2.650843337656 -1.432364728310
C -3.906432949875 3.974169570250 -1.916068107268
N -1.232204979282 0.053833583691 -0.676179190794
C -0.798613009271 -0.398805072212 -2.012151995656
C -0.809472187796 2.836859805078 -2.601320538960
C -4.404992577738 0.217114815173 -1.533324789784
C -4.296414421014 -0.503490064137 -2.881794809501
C -4.281173780189 -0.713936243909 -0.315005401272
C -5.134504129073 2.831523898330 -0.042102773277
H 0.144097708281 0.090216155853 -2.301159993936
C -0.387919483680 4.199619316644 -3.274431742246
H -1.712252114715 2.467002435723 -3.093333349706
H -0.018557752550 2.108810941160 -2.834164632010
H -1.550019940418 -0.020806431812 -2.706100097802
C -0.620656382782 -1.939163102983 -2.268266780620
H -1.477977021227 0.372291865761 2.202060898195
H 0.864189957967 0.327983126485 3.526043869928
H 2.840609154558 -0.060180293403 1.710211642927
H 1.715706004133 -0.207870772897 -0.716457268737
H -1.226275746770 3.657181504792 1.606107359960
H 1.193339422340 3.898435013239 2.775215197864
H 3.074585599471 3.277952204536 0.924819730809
H 1.805109938852 2.609432201867 -1.350940963064
H -5.286526358536 2.402459466527 -2.143134066003
H -5.437065691681 0.580037220177 -1.488968657412
H -5.918278045545 3.597369958167 -0.091500418258
H -5.593130983797 1.906114272311 0.321306577833
H -4.394734266602 3.153453519875 0.698637896708
H -4.711559601921 4.717337009674 -1.970379771322
H -3.134168860650 4.353419809495 -1.246329314462
H -3.477296580697 3.866317022259 -2.914402792612
H -5.013244333675 -1.525289396439 -0.412068564629
H -3.292056995535 -1.154011674486 -0.213437833857
H -4.504766756274 -0.169003517406 0.609194789834
H -5.022370919272 -1.325433096663 -2.936576775600
H -4.507284113938 0.199237371027 -3.695997217114
H -3.306125024614 -0.921209712673 -3.051537833869
C -0.729113604113 -2.129378962059 -3.798005945779
C 0.766153628835 -2.463999604231 -1.838420524205
C -1.680659833613 -2.795156546950 -1.557533036516
H -1.497859661083 -3.857164680238 -1.765017062481
H -1.633813886926 -2.650655040837 -0.473118649184
H -2.695746869976 -2.565082001936 -1.887569584246
H -0.548824979072 -3.176370660234 -4.070955224411
H -1.720383046388 -1.853550691909 -4.176251801661
H 0.013326591435 -1.515612337491 -4.325704930644
H 0.887780147369 -3.500728932047 -2.177011899840
H 1.577127248791 -1.875704195655 -2.286710858296
H 0.891594399328 -2.453861803733 -0.752927127670
C -0.930759603365 4.148060059886 -4.719883123192
C -0.926703397846 5.455403009766 -2.565351075097
C 1.149685147195 4.341797455763 -3.364955686650
H -0.464667907371 6.347605992832 -3.006945773209
H -2.007282964370 5.563894438355 -2.671493826731
H -0.685461026637 5.445757618805 -1.497649948348
H -0.628603926005 5.040413067491 -5.282071490452
H -0.545451563838 3.269828215269 -5.255713202862
H -2.026311949047 4.096382359467 -4.736529034634
H 1.409191597746 5.159848133123 -4.048727355390
H 1.594259641542 4.574799697863 -2.394390767400
H 1.619476869252 3.427848385203 -3.752209026503

**6c neutral compound** *(trans-trans)*

E(B3LYP-D3/6-31+G*) = -2786.63782190
Sum of electronic and zero-point Energies= -2785.971228

Sum of electronic and thermal Energies= -2785.938192
Sum of electronic and thermal Enthalpies= -2785.937248
Sum of electronic and thermal Free Energies=-2786.031090
C -0.035879748041 -0.060723339913 0.258394669452
C -0.121570232516 -0.095242315494 1.690503500082
C 1.198144558987 -0.166114146768 2.228769177783
C 2.119727637044 -0.190283243861 1.138799148050
C 1.367934446786 -0.113197980226 -0.072204669268
Fe 0.971492257481 1.521906559777 1.059925831637
C 0.008605363273 3.014814939911 0.053569046658
C -0.249022725249 3.107635092097 1.465861715540
C 0.992653148119 3.272836044640 2.149251441591
C 2.035194076928 3.286898689265 1.176879687708
C 1.437532908093 3.123324247628 -0.109525480885
N -0.943507708980 2.790012556122 -0.980067402012
C -0.456400798665 2.996243629910 -2.361842872540
N -1.116620789055 0.017344838440 -0.663965473102
C -0.873112900104 -0.666731970927 -1.960655237968
P -2.112038161788 1.461305334960 -0.936230413030
N -2.960137657987 1.840802319595 0.574844006151
C -3.783077046547 0.819875756652 1.309926553206
C -3.604889345406 1.031591156369 2.823163982080
C -3.815497184291 3.089646356294 0.458218143378
C -3.088838690397 4.422892147520 0.681580941119
C -4.696262137212 3.126810809228 -0.809273775567
C -3.602952303227 -0.652142999308 0.938089786613
H -1.029356842891 -0.018302933804 2.265452233808
H -1.212541977324 2.970981037084 1.925341026150
H 1.115357434569 3.344771913707 3.222417313756
H 3.095662203007 3.384690832920 1.370505401028
H 1.984120001348 3.074352588659 -1.039566287698
H 1.450535992317 -0.179164173278 3.281440830002
H 3.198873521141 -0.232362756273 1.212335899159
H 1.788035033284 -0.087304342444 -1.067886559710
H -1.060727808449 2.356481726530 -3.015735124655
C -0.550290554443 4.439183587652 -2.927055394654
H 0.573157899974 2.628219221285 -2.460017627639
C -0.935743702102 -2.219229935595 -2.011217486127
H -1.634835176847 -0.294600788733 -2.654107435951
H 0.094558690340 -0.348372117882 -2.376484220265
H -4.509638967196 3.007334363688 1.299597672573
H -4.837825046549 1.030871189516 1.073506198994
H -5.452019908115 3.915323650625 -0.707369750918
H -4.119715077460 3.333198992249 -1.714523629607
H -5.217020734601 2.172971108171 -0.955304122222
H -4.321437737515 -1.238188775116 1.524482649005
H -3.818576032808 -0.823434725417 -0.119091529149
H -2.603496312837 -1.034264791362 1.142954740228
H -4.306207106425 0.401838461652 3.385603901415
H -2.588038416750 0.780320251427 3.138385977390
H -3.786536166358 2.074200690068 3.106567622174
H -3.806791002416 5.241553901592 0.546448274999
H -2.695160749586 4.493903169357 1.699360924753
H -2.262726997642 4.569660376836 -0.012321551440
C -0.668883662693 -2.598889207462 -3.484582436095
C 0.124511915914 -2.901545355278 -1.127690157843
C -2.327514810540 -2.733359897686 -1.608763794762
H -2.410906727797 -3.807551123685 -1.817708302100
H -2.508162045975 -2.587261120724 -0.542018613256
H -3.122356774099 -2.219860068108 -2.165170242326
H -0.690887850076 -3.688221446233 -3.609933398474
H -1.426768420637 -2.170626775779 -4.153713782192
H 0.315410884763 -2.244941889943 -3.818146487641
H 0.068790934933 -3.990548326881 -1.255250654291
H 1.138141134246 -2.582508565164 -1.395321589769
H -0.024777905814 -2.677601022948 -0.067540368480
C 0.119317400129 4.416701051775 -4.315853844535
C -2.026067931713 4.845005090708 -3.088206985483
C 0.164217184917 5.471712910852 -2.037518610810
H 0.056703758394 6.475207461321 -2.469029060207
H -0.254940484836 5.491973467210 -1.026868748337
H 1.235111628730 5.258256396975 -1.948695114248
H -2.104422089857 5.833487227200 -3.558122683985
H -2.570460141520 4.128742673841 -3.717314838044
H -2.529836948325 4.894287108257 -2.120230207347
H 0.058823077285 5.404193671311 -4.789669113769
H 1.180806498805 4.145581044232 -4.243755452784
H -0.369131989415 3.695347964579 -4.984386081264

**6c radical cation** *(trans-trans)*

E(UB3LYP/6-31+G*) = -2786.43159984
Sum of electronic and zero-point Energies= -2785.764027
Sum of electronic and thermal Energies= -2785.730673
Sum of electronic and thermal Enthalpies= -2785.729729
Sum of electronic and thermal Free Energies=-2785.825104
C -0.155271785689 -0.037456925832 -0.058571475414
C -0.092664088891 0.026929670377 1.382032590094
C 1.308197507392 0.091980332036 1.709131526786
C 2.070067044994 0.151348552625 0.502690180342
C 1.156314803534 0.073149930330 -0.593234564681
Fe 1.058249373573 -1.639554112677 0.615452865632
C -0.005958499894 -3.454986131462 0.397335713889
C 0.053256490333 -3.136360453126 1.804315976153
C 1.448795762414 -3.006788176704 2.118335675269
C 2.223124332663 -3.309545180075 0.957260162314
C 1.314081300127 -3.594024050631 -0.108354784311
N -1.015859003503 -2.849686418592 2.638626148660
P -1.252433979868 -1.333998032919 3.588967810952
N 0.222501426639 -1.015423868161 4.487067565379
C 0.133685673835 0.322187174815 5.237330564759
C -1.209911371286 0.542809860846 5.960217415532
N -1.156382846228 -0.110854847861 2.264381063262
C -2.514287100421 0.150112669124 1.706903431890
C -2.966152342317 1.632951349271 1.636183249867
C -1.995722456672 2.514066014979 0.830061044131
C -2.350593908878 -3.342409438978 2.181217912655
C -2.696980481271 -4.834213510736 2.437046257863
C -2.752829179909 -5.126544574677 3.946480647412
C 0.694125213520 -2.034147475022 5.516356331350
C 0.193287555111 -3.472824210882 5.377931868130
C 2.227885558695 -1.991985378974 5.610718429210
C 0.558281916578 1.563170247698 4.445612254683
C -4.343536503323 1.627068782338 0.941353400588
C -3.116346810283 2.211305151658 3.053946175996
C -4.099947755384 -5.043564258083 1.827427969964
C -1.709709124850 -5.810854875592 1.774349919041
H 1.839200183842 -2.688782056984 3.069186028925
H 1.706127262117 0.049151637668 2.707987691484
H 3.146315928136 0.247478226457 0.443366475561
H 1.406783418061 0.086460406172 -1.646022826481

H -1.050472158058 -0.152291028374 -0.650944270528
H 3.304076934079 -3.328971614547 0.909571027041
H 1.573588703783 -3.859206722063 -1.125004794904
H -0.904400708799 -3.570569142194 -0.189336161377
H -3.224195578748 -0.376320005460 2.351509120716
H -2.605647594420 -0.316188321338 0.718318497386
H -3.098173139315 -2.746657237241 2.712468627296
H -2.481838410007 -3.107918006188 1.116710022424
H 0.887664602732 0.215514862107 6.020053618353
H 0.298981644659 -1.697599820771 6.483916554232
H -1.107848513742 1.375177288020 6.665185081996
H -2.022380406230 0.794345869222 5.273477957863
H -1.512459848468 -0.342377608727 6.530603919806
H 0.589241571209 -4.045753754733 6.223699210332
H -0.896267133084 -3.525206420346 5.432630399622
H 0.516686135989 -3.970545622286 4.461915951387
H 2.558829067210 -2.531122564231 6.505743407415
H 2.706945117515 -2.468040465909 4.748670524155
H 2.608002400487 -0.967782229688 5.678749514226
H 0.447615055012 2.439670865668 5.093884352062
H 1.611765950123 1.512346554128 4.155132772195
H -0.045737181727 1.731581681633 3.554083913710
H -3.171825466080 -6.123782474052 4.121949590922
H -1.755266848057 -5.107218168192 4.390722021980
H -3.383265043131 -4.401403344841 4.476396784600
H -4.426297887981 -6.079000533287 1.973588307223
H -4.845769344685 -4.391538479637 2.299258056710
H -4.106740627462 -4.843509867277 0.748248118667
H -2.016305039214 -6.842589559170 1.981333541785
H -1.682869804695 -5.691037820241 0.685149518531
H -0.691822992187 -5.689060363283 2.160647314329
H -2.372434712804 3.542466221245 0.792165839045
H -0.999977984814 2.547408524129 1.285877991672
H -1.888730238779 2.165749961459 -0.203840729701
H -3.527426225508 3.226155724362 3.009113102453
H -3.795649100198 1.603785206595 3.665134009487
H -2.152659026575 2.268520607891 3.566469450677
H -4.745260899940 2.644668073751 0.883987153726
H -4.277033214496 1.237846031254 -0.082736751321
H -5.069547726869 1.014969392851 1.491300990113

**6c singlet dication** *(trans-trans)*

E(B3LYP-D3/6-31+G*) = -2786.03314996
Sum of electronic and zero-point Energies= -2785.366916
Sum of electronic and thermal Energies= -2785.333135
Sum of electronic and thermal Enthalpies= -2785.332191
Sum of electronic and thermal Free Energies=-2785.428027
C -0.217046184560 -0.136782580402 -0.076890639396
C -0.083229949494 0.094107474875 1.347821641761
C 1.338098390110 0.121870839940 1.647031002065
C 2.036608574056 0.036182101974 0.414824339067
C 1.086524850761 -0.127152770206 -0.638719018083
Fe 0.866176244899 -1.651447409206 0.754181500320
C -0.174656088369 -3.355509232276 0.329075539752
C 0.026454680146 -3.242768209179 1.757442191695
C 1.450490468860 -3.168506366971 1.993008358012
C 2.100463804751 -3.326940916092 0.739426920804
C 1.106304771682 -3.441217777245 -0.278210527254
N -0.960188289843 -3.007813346050 2.721589549384
P -1.154698998183 -1.377933833896 3.372811432180
N -0.226913810899 -1.082658560947 4.711299112418
C -0.348516712358 0.295283359739 5.392328865336
C -1.818684015155 0.634409413510 5.653127824030
N -1.098539492509 0.087959821032 2.302892504280
C -2.478701372174 0.474821608723 1.829807949942
C -2.728002769859 1.991793792877 1.584030112889
C -1.718782545432 2.632073489577 0.614273346329
C -2.331066789076 -3.613819784911 2.488317823120
C -2.480250433137 -5.158022106483 2.560026431913
C -2.037825526049 -5.718291228029 3.919942586415
C 0.465197718017 -2.074920188530 5.640214938346
C 0.162383142548 -3.550512476669 5.442836337697
C 1.972755167901 -1.768060526604 5.618913655964
C 0.453495256906 1.406253406430 4.714182373989
C -4.140610986635 2.056021222492 0.957371204794
C -2.731443054235 2.778516497475 2.906064395154
C -4.001340717670 -5.393504679313 2.383412313709
C -1.736060023452 -5.901200684922 1.434977210966
H 1.933096504838 -3.065165782003 2.951858488900
H 1.779417724838 0.245423866096 2.623258559386
H 3.112925663357 0.052512643591 0.299610379340
H 1.321158715299 -0.257078177519 -1.687363499626
H -1.140511456228 -0.248244701723 -0.625346222657
H 3.171411601311 -3.331575826949 0.581618299138
H 1.296131646829 -3.537790863134 -1.339425140917
H -1.125379072917 -3.397310605311 -0.181263798341
H -3.173387656475 0.127830731007 2.602962188685
H -2.718272752404 -0.091354453142 0.922609750268
H -2.968717900378 -3.170307703966 3.264789360127
H -2.714268544968 -3.253218397542 1.525645364656
H 0.117468132731 0.117586477904 6.362267222573
H 0.066593714733 -1.806179726954 6.623930455397
H -1.880440029534 1.549527225746 6.249894227414
H -2.364447565135 0.816246663832 4.724310835720
H -2.313093239135 -0.167768130460 6.210860771612
H 0.590933535151 -4.083993803989 6.297396255218
H -0.911969034194 -3.742077000284 5.443351862023
H 0.597013866626 -3.972883603859 4.537489090374
H 2.472599835340 -2.428885768626 6.334370166475
H 2.402485553938 -1.947830321218 4.629277607189
H 2.195739552691 -0.738293131447 5.908732188313
H 0.388192928448 2.296364866920 5.348723087586
H 1.511249353135 1.139051714224 4.637553926657
H 0.071503934766 1.668535542938 3.729272922325
H -2.298884064560 -6.779563096429 3.982831007040
H -0.955620029543 -5.643363675806 4.058424329494
H -2.540515466769 -5.211068050705 4.752533702672
H -4.211827329026 -6.467188136667 2.411948977314
H -4.583341212883 -4.922763738364 3.184815250043
H -4.365416408133 -5.012717153528 1.421411849957
H -1.982154521673 -6.966872210454 1.481137180945
H -2.033392266276 -5.544524671335 0.442168410288
H -0.647926708068 -5.819753328908 1.527802155072
H -1.995849821757 3.676974312081 0.441611437216
H -0.698505132781 2.632177105819 1.015064512117
H -1.710438874469 2.135285120416 -0.361656480460
H -2.973644690916 3.828159747661 2.710947838963
H -3.488663744712 2.397119939188 3.601448376619
H -1.756756645750 2.758824931056 3.402291701790
H -4.427278871541 3.100254713389 0.796906883532

H -4.177538350240 1.550121487796 -0.014945086057
H -4.897288345498 1.604226338608 1.610356581210

**6c triplet dication** *(trans-trans)*
E(UB3LYP/6-31+G*) = -2786.07225826
Sum of electronic and zero-point Energies= -2785.405402
Sum of electronic and thermal Energies= -2785.371579
Sum of electronic and thermal Enthalpies= -2785.370635
Sum of electronic and thermal Free Energies=-2785.467653
C 0.136440555061 0.090648699893 0.026783899650
C 0.085589193457 0.032710760045 1.470875810441
C 1.450516957861 -0.031303703078 1.921477399761
C 2.307905916611 0.049342639895 0.790175239686
C 1.505390183242 0.127846834093 -0.374203272356
Fe 1.003137823459 -1.661759428243 0.684892573213
C -0.367817019417 -3.159146930563 0.267931759848
C -0.116865935189 -3.081557600330 1.687291337647
C 1.285675624798 -3.352296601351 1.872897546311
C 1.858309400363 -3.644107328074 0.602937324723
C 0.844581663484 -3.526564015900 -0.381668310748
N -1.075518318805 -2.814163785782 2.692874662981
P -1.242249612340 -1.277609323974 3.457438792861
N -0.049341309660 -0.942172462270 4.645388129187
C -0.137110538489 0.418913710759 5.359105150674
C -1.539661176940 0.615600761280 5.957888979975
N -1.077706716177 -0.049082226273 2.259874789342
C -2.397771200347 0.233989251696 1.583819984778
C -2.837443588971 1.717425663179 1.511415432743
C -1.776785623413 2.616925500585 0.851918417304
C -2.445460574763 -3.450917336073 2.489460564948
C -2.576353766332 -4.991097001972 2.597096116367
C -2.178936126862 -5.502610427984 3.990439942480
C 0.619301500118 -1.951753534385 5.553626916117
C 0.173768739912 -3.401801805617 5.437173023825
C 2.140847055012 -1.782730545658 5.381630102335
C 0.368289120562 1.618754810068 4.556363959784
C -4.123479399574 1.728700539331 0.656383396259
C -3.160666640750 2.250767521918 2.917937610961
C -4.083029794027 -5.263072358992 2.367439145280
C -1.770684455544 -5.748054677773 1.524693614139
H 1.811299875043 -3.359759209728 2.815567588832
H 1.776493779008 -0.146571364986 2.942947622872
H 3.389636069208 0.003171918882 0.818515286499
H 1.862056740874 0.176001395832 -1.395374920852
H -0.705552832467 0.139869200646 -0.646708852493
H 2.900135702568 -3.875536281852 0.418539346522
H 0.976639767813 -3.651984131007 -1.449148354285
H -1.317237821935 -2.989469303032 -0.220809741010
H -3.161283862993 -0.315595016775 2.146898153296
H -2.380758784726 -0.212707713353 0.583953786920
H -3.088647929920 -3.004208646459 3.255587557332
H -2.834420320926 -3.119075638042 1.518585639796
H 0.553608635167 0.291909787332 6.194502713864
H 0.349296334885 -1.622267117853 6.562682737736
H -1.522558681807 1.486188866574 6.620623109282
H -2.291645210024 0.795459954513 5.185385342658
H -1.842636719529 -0.254122673160 6.550200250348
H 0.645730080440 -3.955146992979 6.255371000232
H -0.907733661250 -3.502408556647 5.553895717459
H 0.467703080929 -3.874557988491 4.501335453450
H 2.651410313718 -2.407251616868 6.121481070344
H 2.464676518568 -2.100177689959 4.386129282270
H 2.465524068913 -0.749384866742 5.537489017965
H 0.265824165303 2.504320993999 5.191877078461
H 1.429832696200 1.521329674878 4.313407691646
H -0.195411744545 1.795532208717 3.642305845769
H -2.445806198508 -6.559880285630 4.088181582356
H -1.101614364507 -5.425284230721 4.158655930187
H -2.701924991632 -4.958979897630 4.787119082524
H -4.278040395667 -6.338525629007 2.425634510903
H -4.705855396084 -4.774602572301 3.126585744520
H -4.413790357259 -4.921870098367 1.378823830092
H -2.002345345044 -6.816686964053 1.581021487743
H -2.023917352506 -5.414452816610 0.511199980357
H -0.689083651568 -5.648245525261 1.666710348172
H -2.131669878694 3.652510989225 0.837079131782
H -0.826874776950 2.609311336467 1.399263534641
H -1.582066964498 2.329923121193 -0.187598565349
H -3.581867968464 3.259074172947 2.850941786971
H -3.900813178129 1.621417298837 3.428613227123
H -2.266585638696 2.316541821313 3.543648983257
H -4.513541513139 2.748749982928 0.581036603428
H -3.936698844954 1.371018970676 -0.363869591248
H -4.911567538939 1.107277252768 1.099247180300

**6d** *(cis-cis)*
E(B3LYP-D3/6-31+G*) = -2472.09134455
Sum of electronic and zero-point Energies= -2471.652761
Sum of electronic and thermal Energies= -2471.629921
Sum of electronic and thermal Enthalpies= -2471.628977
Sum of electronic and thermal Free Energies=-2471.701577
C -0.033942290080 -0.020453203320 -0.014800186076
C -0.033359910653 -0.016799643478 1.412964923220
C 1.322096363787 0.010754679121 1.855244017259
C 2.162543466569 0.016915576117 0.699043096561
C 1.327637875734 0.004354906142 -0.473665155547
Fe 0.989413029484 -1.669678641353 0.699463025650
C 0.043174617636 -3.287599481030 -0.176112735946
C 0.126582962974 -3.468534590557 1.237709197775
C 1.506136350685 -3.453296641700 1.605448674012
C 2.275539412267 -3.244067687607 0.419011108670
C 1.373845814727 -3.155121403615 -0.699735181781
N 1.718980254609 -2.857867923499 -2.044714244829
C 3.053672095217 -3.266115798479 -2.479151479417
N 1.765023415472 -0.120028395549 -1.821907256373
C 3.227474022774 -0.093179783666 -1.962095886851
P 0.857301573531 -1.432151953699 -2.614464653937
N 1.419472314896 -1.283645916036 -4.277176595239
C 0.994696236679 -2.369882111972 -5.237150113132
C 0.465030789544 -3.687945804685 -4.649970144595
C 1.128757839883 0.046700740145 -4.931640904219
C -0.281576052130 0.597359000366 -4.640843229972
C 2.190370423306 1.129168240867 -4.710796120516
C 2.155191801688 -2.656445223339 -6.203216625339
H 3.852976323634 -2.903091260885 -1.819622485491
H 3.600894831171 0.916551753783 -1.754479323234
H 3.498146749263 -0.367288520281 -2.980060675438
H 3.722526383433 -0.795170245066 -1.278592571120
H 3.240536691754 -2.866813204912 -3.476365732375
H 3.112213597114 -4.361817523143 -2.516590579399

H -0.865723798434 -3.214446455290 -0.757995635884
H -0.713815685226 -3.588819513055 1.909271612187
H 1.904983544761 -3.564528111177 2.605487669419
H 3.352318261648 -3.153125903014 0.376907937477
H -0.909304387379 -0.081085170724 -0.646404688269
H -0.913556171285 -0.044807404029 2.042350529709
H 1.663289438431 0.016998034185 2.882390187527
H 3.242874814803 0.011283619910 0.716740217851
H 1.163941825059 -0.177288238865 -6.002620514125
H 0.155316106467 -1.965196162617 -5.823949009407
H -0.497120576704 1.438302260898 -5.311296566737
H -1.051107287751 -0.167594956510 -4.796854102644
H -0.365211490950 0.963162217710 -3.611640101601
H 1.993812632522 1.958969984023 -5.401649254773
H 2.164725101460 1.527309967525 -3.694601202329
H 3.193574298277 0.745030316048 -4.922991505151
H 0.102871131629 -4.297776901003 -5.486486798899
H 1.230458973279 -4.260042767216 -4.123050527592
H -0.375372333108 -3.533846583351 -3.966195312063
H 1.825202811641 -3.313903404013 -7.017859105398
H 2.548230064269 -1.736343118441 -6.648813734124
H 2.978900883697 -3.151640375909 -5.677140704567

**6d** *(trans-trans)*
E(B3LYP-D3/6-31+G*) = -2472.09414372
Sum of electronic and zero-point Energies= -2471.656197
Sum of electronic and thermal Energies= -2471.633032
Sum of electronic and thermal Enthalpies= -2471.632088
Sum of electronic and thermal Free Energies=-2471.705892
C -0.088088926900 -0.096066339864 -0.131950772769
C -0.172745444747 -0.079027266544 1.293693453201
C 1.150815967617 0.019910418878 1.818415455312
C 2.057868365791 0.062936597739 0.715107661741
C 1.296953499634 -0.006600839975 -0.505907903005
Fe 0.960648567938 -1.665735151882 0.635882859198
C 0.045889038200 -3.259302362870 -0.258716906592
C 0.129464851968 -3.489298933026 1.147114386459
C 1.508117774997 -3.456993411370 1.524774625712
C 2.279049315931 -3.194422774843 0.353295910649
C 1.376351731950 -3.054419853711 -0.762189640645
N 1.780435830479 -2.760138771472 -2.088801076503
P 1.580952853210 -1.293213547988 -2.983317442339
N -0.169659178551 -1.069893687520 -3.217294519361
C -0.509513123539 0.243633497401 -3.890581643781
C 0.452939430635 0.649111343149 -5.027153579013
N 1.847839255795 -0.017871705958 -1.813612278170
C 3.202601397499 0.543384825828 -1.903534197206
C 2.660945445440 -3.772450362575 -2.681906067685
C -0.973630321592 -2.147038109893 -3.885128527516
C -0.395185813768 -3.568209229798 -3.919993547855
C -2.376116637082 -2.175529853290 -3.252233258031
C -0.748236170415 1.421492723448 -2.938761577109
H -0.862515840332 -3.172828289114 -0.835695483626
H -0.904674725342 -0.242527623254 -0.818744928911
H -1.085158105063 -0.159296835975 1.870869730313
H 1.426978696501 0.042986931332 2.864713533209
H 3.135790200966 0.105734090520 0.788864002031
H -0.710345060860 -3.635419851977 1.814614707932
H 1.897155206041 -3.581193059466 2.527229402106
H 3.354207490456 -3.076907467247 0.305193939165
H 3.479626875870 0.646977832483 -2.955925135140
H 3.215635032316 1.535380281469 -1.438954733780
H 3.964334944630 -0.081682159485 -1.411168595034
H 2.131706809719 -4.728304175251 -2.799929519017
H 2.995504135765 -3.435673511267 -3.667310008134
H 3.547690666073 -3.945128235562 -2.058269681262
H -1.475475679320 0.058369514898 -4.371050026469
H -1.088434866912 -1.864514998180 -4.945183878335
H 0.007837137217 1.467541150163 -5.606360363425
H 1.416556656191 1.003194546830 -4.644627345011
H 0.644627728823 -0.186916068078 -5.709616280216
H -1.101374523054 -4.199748458074 -4.472800577908
H 0.562644575733 -3.613256328758 -4.446858236383
H -0.261203706265 -4.000477309151 -2.926832296000
H -3.041534833556 -2.846796596908 -3.810528171187
H -2.320325850962 -2.527843047828 -2.216745311623
H -2.834928770304 -1.181133754862 -3.237787200551
H -1.049044784458 2.297886751644 -3.527410071267
H -1.555670142978 1.204059469503 -2.233558105780
H 0.147967122040 1.678024729565 -2.371602578413

**6d radical cation** *(trans-trans)*
E(UB3LYP/6-31+G*) = -2314.62286231
Sum of electronic and zero-point Energies= -2314.297655
Sum of electronic and thermal Energies= -2314.279257
Sum of electronic and thermal Enthalpies= -2314.278313
Sum of electronic and thermal Free Energies=-2314.342136
C 0.068891333870 -0.031334451752 -0.060430278402
C 0.053900201990 -0.110082963480 1.366508398128
C 1.400035953821 -0.107686778731 1.818579741409
C 2.278893340545 -0.059015925750 0.678106556662
C 1.433104925318 0.016554944659 -0.483645457463
Fe 0.990573162830 1.660763173628 0.692470866297
C 0.357658749733 3.452132218811 -0.126045139319
C 0.360289518176 3.585598383294 1.296896105701
C 1.689072567588 3.378558870549 1.752884096050
C 2.544365577380 3.143254897577 0.617744120470
C 1.694053212918 3.164536284733 -0.542967422421
N 3.896942372821 2.825742399224 0.677454676514
C 4.604947418685 3.321924936817 1.878790941557
N 3.665459473709 0.033533061168 0.730108384956
C 4.285831611468 -0.527067204653 1.951392691416
P 4.644036727131 1.345509999960 0.035660743121
N 4.021530178455 1.366526991063 -1.586742498819
C 4.292840433299 0.113197744204 -2.323070934000
C 4.493235892437 2.529593198712 -2.368664613810
H 1.775945459067 0.122317646907 -1.500755630363
H 2.011623522746 2.965787354452 -1.554346540281
H -0.495526272451 3.563324484863 -0.782393759539
H -0.496441169524 3.794025325093 1.924674246580
H 2.002290831203 3.373377234632 2.787831817415
H -0.792975100657 -0.025041137211 -0.714822034854
H -0.823518066323 -0.151003803238 1.998961859397
H 1.713019308353 -0.115414536628 2.853583081190
H 5.678948273642 3.190337086396 1.734057529735
H 4.399353845248 4.388430062901 2.004913974133
H 4.311898259097 2.789447406490 2.794070659337
H 3.907897057909 -1.539708348490 2.116718028254
H 5.366393857523 -0.579552051653 1.805202113709
H 4.087231723052 0.080280483351 2.845168604659

H 3.927126614603 2.568782944636 -3.306165643817
H 4.322959341121 3.459297557426 -1.821165627638
H 5.563379450141 2.464344126774 -2.619766858101
H 3.725071062038 0.132657768993 -3.260185491920
H 5.358330823908 -0.008097773834 -2.573137557978
H 3.973523263200 -0.754603389542 -1.741642006762

**6d triplet dication** *(trans-trans)*
E(UB3LYP/6-31+G*) = -2314.23874993
Sum of electronic and zero-point Energies= -2313.914722
Sum of electronic and thermal Energies= -2313.895584
Sum of electronic and thermal Enthalpies= -2313.894640
Sum of electronic and thermal Free Energies=-2313.961391
C -0.013630893279 -0.093876106113 0.002171953935
C -0.018603056212 -0.125368195439 1.421676271213
C 1.325867964358 -0.057713620834 1.878754265987
C 2.188075467462 -0.015943098753 0.723253464889
C 1.339645595591 -0.018948287751 -0.441203485664
Fe 0.991473006862 1.661159774371 0.716277613706
C 0.286780569874 3.529749816625 -0.066094105924
C 0.291481681584 3.614718465740 1.351215682501
C 1.607889186429 3.343807661640 1.814656570725
C 2.447855498320 3.117464552462 0.664197905552
C 1.607870772992 3.216526517910 -0.502172080063
N 3.834917016320 2.849545028788 0.695073303834
C 4.636508025648 3.656922193760 1.665582887653
N 3.600404306010 0.020952301636 0.748404650121
C 4.261140743615 -0.870453929344 1.750959525421
P 4.512073913096 1.359975352620 0.222712530171
N 4.338202027512 1.342073013208 -1.491138826529
C 4.479687215385 0.074201019894 -2.228516651553
C 4.684456629379 2.540729950095 -2.275092341886
H 1.668767027946 0.016793745824 -1.470563433012
H 1.923407500149 3.088603269951 -1.528451880629
H -0.577413466767 3.653856059251 -0.707090301765
H -0.572335789398 3.799885892917 1.978235107734
H 1.923789502071 3.318255171130 2.849586162731
H -0.888441230499 -0.097919117664 -0.636420533880
H -0.899176503384 -0.142214188549 2.052491267463
H 1.644860431845 -0.045810116822 2.912982151845
H 5.699706160779 3.493457124007 1.475214683846
H 4.411841155393 4.712929050769 1.501102514781
H 4.415482734983 3.387374201840 2.702892469140
H 3.865201834775 -1.880479913189 1.625423315238
H 5.336152030428 -0.891476531934 1.557931935942
H 4.090696657562 -0.529556301650 2.776755496295
H 4.047428351775 2.556593927880 -3.166340802797
H 4.528292663063 3.445113258027 -1.687498607158
H 5.729550646561 2.489448766658 -2.605425804819
H 3.845969236785 0.130146634153 -3.120509999383
H 5.517901430971 -0.059906634894 -2.557298312289
H 4.178418690087 -0.769388485867 -1.607902822168

**7a (with 1 dimethylamine substituent)**
E(B3LYP-D3/6-31+G*) = -4775.68592501
E(PCM-B3LYP/6-31+G*(ether) = -4775.69188255
Sum of electronic and zero-point Energies= -4775.208397
Sum of electronic and thermal Energies= -4775.170347
Sum of electronic and thermal Enthalpies= -4775.169403
Sum of electronic and thermal Free Energies=-4775.278503
C 0.000000000000 0.000000000000 0.000000000000
C 0.000000000000 0.000000000000 1.428030000000
C 1.353932592089 0.000000000000 1.872552032663
C 2.190243882399 0.024094636440 0.715729318321
C 1.357547165965 -0.034794416636 -0.458131572823
Fe 0.967472604196 1.678168252822 0.768123583463
C 1.550894568353 3.498253439126 -0.072353763011
C 0.124504285423 3.394536586503 -0.007099506601
C -0.240720672510 3.237725088282 1.361404288480
C 0.955999872568 3.211683361423 2.142228076344
C 2.062977027485 3.378607601509 1.260971362479
N 2.318730174747 3.789722886991 -1.250231029213
P 3.519741402628 2.641474734581 -1.503774592002
Cl 3.777937723521 2.728517020401 -3.626074217247
N 1.862785599119 -0.235003988816 -1.775735091487
P 1.100961188256 0.060374457040 -3.307404806871
Cl -0.415941656691 1.565693018534 -2.848155909584
Si 3.267229154617 -1.387074026024 -1.941854018202
C 4.849511268977 -0.834938234217 -1.067638309577
C 3.714894838352 -1.578065234458 -3.765604199788
C 2.709502842367 -3.039026539717 -1.226276874055
Si 2.007268927114 5.387970324067 -2.066442168039
C 0.850120391867 5.079632784275 -3.514028186262
C 3.623364109915 6.164801506934 -2.629847216604
C 1.210543196222 6.499062746517 -0.770801552981
Cl 5.349438266749 3.665140321761 -0.917786912291
N 0.162119193482 -1.342799491256 -3.564701046180
C -0.454049885983 -1.405498047318 -4.893288353338
C -0.609677700212 -2.044523162025 -2.543115960869
H -1.584171037946 -1.561813969859 -2.368289486115
H -0.878031111453 0.036288083938 -0.624510981232
H -0.881442127764 0.034311657336 2.055866026881
H 1.694834207888 0.032580549978 2.899385982465
H 3.266207321943 0.084313026115 0.725875023578
H -0.543364585099 3.417889384461 -0.854644882224
H -1.248148854428 3.111112893927 1.736815185423
H 1.015033969527 3.059435262010 3.212503897122
H 3.110474234851 3.404965031318 1.532833031234
H -0.056134798659 -2.077060075352 -1.605399014538
H -0.789005866173 -3.074941838421 -2.874647910858
H -0.548902296393 -2.453285759641 -5.203876781559
H -1.453489858828 -0.943265834925 -4.901757656830
H 0.173559217331 -0.883853573934 -5.623479240815
H 3.393236719291 7.113570718396 -3.133999460764
H 4.280088367339 6.379974615845 -1.780569671457
H 4.177592958214 5.536097576923 -3.331759453516
H 1.125550416279 7.516859515524 -1.174032429287
H 0.209227124837 6.163909170103 -0.482440081111
H 1.822054674134 6.547177720426 0.138079115591
H 0.574501123070 6.025516883473 -3.998869249946
H 1.327983720032 4.435446842205 -4.259825080416
H -0.068353401458 4.577532372058 -3.190851412459
H 5.688701186514 -1.346578633976 -1.557745990194
H 5.035802252628 0.240359682760 -1.141420505284
H 4.872439335841 -1.117749337598 -0.009932975395
H 4.584111609643 -2.249864266479 -3.803602432750
H 2.922301868636 -2.027415814636 -4.371635919647
H 4.010560051204 -0.628633229803 -4.225657801743
H 3.555904504002 -3.735347652270 -1.164414647370
H 2.302499216836 -2.915949938198 -0.215540997518

H 1.937474904955 -3.499982464408 -1.852862751149

**7a' (with 2 dimethylamine substituents on the same phosphorus atom)**

E(B3LYP-D3/6-31+G*) = -4450.04462518
E(PCM-B3LYP-D3/6-31+G* (ether)) = -4450.04933195
Sum of electronic and zero-point Energies= -4449.485397
Sum of electronic and thermal Energies= -4449.444221
Sum of electronic and thermal Enthalpies= -4449.443276
Sum of electronic and thermal Free Energies=-4449.558249
C -0.454795439139 0.305447710026 -0.272668534542
C -0.558331041209 0.065638058770 1.126582894820
C 0.759014076062 -0.125694946399 1.646171113432
C 1.681707680731 -0.017663481900 0.567521676109
C 0.934745679631 0.261683482745 -0.621190516165
Fe 0.324522574438 -1.555754433827 0.219857760261
C -1.146185026805 -2.964316376942 0.335560087640
C -0.143243132360 -3.210074930419 1.322067269522
C 1.085874130455 -3.462461820855 0.641761280462
C 0.844282193636 -3.427281329666 -0.769499467238
C -0.529021949598 -3.049287434067 -0.947799011214
N 1.711883133027 -3.882963158372 -1.794739563286
Si 3.486778874665 -3.636136694111 -1.809598775124
N 1.490420876836 0.584616768367 -1.906560473829
Si 2.195164465169 2.250644458038 -2.104919238328
P 1.055013815607 -0.580410737111 -3.041246079258
Cl -0.742558708906 0.239480616369 -3.967637190769
Cl 2.446254693891 -0.161854118156 -4.616409345071
P 1.300295658967 -5.408799457422 -2.612838608382
N -0.198241863031 -4.952004612393 -3.408993661045
C -0.921979911421 -6.068464370560 -4.027282263233
N 0.652486640760 -6.500642828422 -1.468834229684
C -0.574982930501 -6.326063384365 -0.696532586193
C 1.568152056391 -7.475918346771 -0.890444355640
C -0.038674669701 -3.852970741988 -4.365814177749
H -1.232990396259 -5.613695350001 -1.194099611419
H -1.015118887065 -2.919306528604 -1.901944932644
C 1.733266506828 3.211592446654 -0.553266983580
C 4.377560511228 -5.035336660233 -0.893287749495
C 3.953882164637 -2.033110770104 -0.943693007810
C 1.455394241556 3.101887041697 -3.608312406550
C 4.063972470978 2.067369808694 -2.228486992400
C 4.078158853337 -3.566192198479 -3.596235233730
H -2.180992235649 -2.708969070464 0.526184995543
H -0.279283405725 -3.174786153482 2.396015362240
H 2.036699434748 -3.686383052193 1.107533663259
H -1.265597382054 0.475987955848 -0.968391307821
H -1.479657455884 -0.005746684609 1.690855201865
H 1.009787392677 -0.355137126360 2.673951112963
H 2.755642709022 -0.105653278170 0.627630564847
H -0.371806465888 -5.954930720555 0.318270428657
H -1.094838148317 -7.292277124574 -0.615773703089
H 1.938774156336 -7.161029153102 0.099172910910
H 1.059003030097 -8.442971801186 -0.770223139604
H 2.429547428830 -7.622385512786 -1.548849604627
H -1.902515692332 -5.707232761150 -4.361827796822
H -0.396486562397 -6.484477377394 -4.906670267776
H -1.079549969415 -6.875417090950 -3.309163925447
H -1.027400938821 -3.462120267937 -4.636376763897
H 0.533828441574 -3.045250678096 -3.910622131490
H 0.473355244184 -4.163893795777 -5.294269603685
H 1.853388730047 4.123748715634 -3.672441313575
H 1.689096249175 2.587404466130 -4.544234674488
H 0.364933075398 3.165649618617 -3.524218421846
H 4.549227234094 3.051478011382 -2.269443409767
H 4.459099518072 1.533839137266 -1.355053580554
H 4.351341815386 1.506764448000 -3.123770416946
H 2.074857987777 4.249421528002 -0.663250292031
H 0.648547591656 3.228007857913 -0.397086907426
H 2.193785543048 2.797908779999 0.349987314486
H 5.153780874249 -3.343707188127 -3.617492920535
H 3.919354613789 -4.514851796450 -4.119336938256
H 3.564057553292 -2.776333528029 -4.154497357806
H 5.439924022367 -4.790288868009 -0.759523696697
H 3.945289669924 -5.201001799737 0.101916246375
H 4.320480282252 -5.982015195754 -1.442074671903
H 3.717561007583 -2.063616106907 0.123984086377
H 5.039312540833 -1.900063315266 -1.046442097676
H 3.467951985133 -1.155432060538 -1.376393820526

**7c (with 1 dimethylamine substituent)**

E(B3LYP-D3/6-31+G*) = -4351.41653201
E(PCM-B3LYP/6-31+G* (ether)) = -4351.42181634
Sum of electronic and zero-point Energies= -4350.858425
Sum of electronic and thermal Energies= -4350.822660
Sum of electronic and thermal Enthalpies= -4350.821716
Sum of electronic and thermal Free Energies=-4350.924806
C 0.388934462159 0.061198347165 -0.271447226216
C 0.223398414306 0.153287803906 1.146607495702
C 1.530039537932 0.059600002533 1.741081201998
C 2.487654326095 -0.051835312874 0.689528765311
C 1.781795838908 -0.064851433889 -0.549164238941
Fe 1.166189827524 -1.635018841744 0.630363279624
C -0.006524061401 -3.274117586891 0.192211885177
C 0.317611532866 -3.300706987541 1.592590658685
C 1.745772527800 -3.317611322620 1.696143834288
C 2.293614238132 -3.331145470910 0.378377787237
C 1.212319939933 -3.318982850418 -0.550926058731
N -0.600651311359 -3.388144199006 2.679649949328
C -0.425279033680 -2.425415211065 3.800492828410
N -1.002136221259 0.351880739638 1.856104360895
C -2.176693310016 -0.462306249150 1.447471065734
P -0.831071710636 1.477212114803 3.106455977421
Cl -2.363271533977 0.857699307074 4.416109513512
Cl -1.686581834294 3.337946569428 2.373210105986
P -1.964182566719 -4.384602033244 2.338570710190
Cl -3.551911116238 -3.345471143353 3.337023382285
N -1.758934109612 -5.679943616050 3.499262838289
C -2.921077779614 -6.534931574035 3.760904711700
C -0.558662139636 -6.481429412385 3.220422961390
C 0.059169157291 -2.887530606143 5.201231179248
C -3.352033770249 0.173988352797 0.652005583817
H -2.588049796960 -0.923128191675 2.347208748547
H -1.740186645292 -1.267555503490 0.854677043620
H -1.373599722201 -1.899996191639 3.939830773805
H 0.284145268579 -1.691340673692 3.413843557384
H 2.308663134950 -3.304705828267 2.616381310916
H 3.347897381057 -3.318124778840 0.132499204896
H 1.295413046368 -3.298117914538 -1.629930284872
H -1.002188621665 -3.242974573137 -0.227491732498

H 1.750525966933 0.072637580321 2.799803972426
H 3.557047635206 -0.157248096970 0.817916959507
H 2.219824765243 -0.184661331627 -1.531842487849
H -0.404715131696 0.066608637100 -1.001112605528
H -0.283014993938 -7.032052319625 4.128451862562
H -0.715132854079 -7.211376644222 2.407185568640
H 0.281561522222 -5.838927109769 2.948611220493
H -2.670896588013 -7.214155674773 4.584747803662
H -3.777372455296 -5.932805632506 4.070019185122
H -3.210738330136 -7.149468859833 2.889748148209
C -4.118209170136 -1.021673859441 0.041733660168
C -4.319582542265 0.935904082027 1.579169683844
C -2.874457568085 1.103935787042 -0.474109260461
H -5.203704420281 1.253498579656 1.012102226770
H -4.657636744371 0.298344888127 2.404000017524
H -3.865970141761 1.831131203882 2.007310775454
H -5.000055373363 -0.669169558800 -0.506657046898
H -3.489147531433 -1.583595356530 -0.661597551104
H -4.458448740741 -1.716385242565 0.819237684176
H -3.734187515958 1.601528429213 -0.939031517288
H -2.200229875828 1.879270070569 -0.097494914355
H -2.359842488376 0.545574923246 -1.264557868335
C 0.372583206422 -1.584711404914 5.971851120272
C -1.039745700904 -3.650269023722 5.962685548618
C 1.333786281049 -3.740551228849 5.126885092473
H -0.702014621221 -3.879005287009 6.981871386650
H -1.953138103922 -3.047933875690 6.035546965281
H -1.297534058227 -4.584286493553 5.457837139401
H 1.626414055962 -4.074042170840 6.130206156077
H 1.186152949569 -4.629882712455 4.507872072867
H 2.174372213574 -3.167702056889 4.716145743497
H 0.694134506772 -1.814281712995 6.994927244474
H 1.177797665346 -1.013950310299 5.489508746943
H -0.508743825549 -0.935749855745 6.034367395598

**7c' (with 2 dimethylamine substituents on the same phosphorus atom)**

E(B3LYP-D3/6-31+G*) = -4025.77943080
E(PCM-B3LYP/6-31+G* (ether)) = -4025.78443399
Sum of electronic and zero-point Energies= -4025.139586
Sum of electronic and thermal Energies= -4025.100847
Sum of electronic and thermal Enthalpies= -4025.099903
Sum of electronic and thermal Free Energies=-4025.209582
C -0.033337306298 -0.029629453551 -0.202870895682
C -0.301144350016 0.039214721230 1.195073707301
C 0.944672302308 0.175288622834 1.882195822861
C 1.983137376281 0.220988488830 0.909196633512
C 1.380092531357 0.111940937732 -0.385254856137
Fe 0.915956403573 -1.568102426753 0.787572828274
C -0.040487672991 -3.075701930557 1.762067743744
C 1.315508020759 -2.992924769282 2.186546650052
C 2.142769976064 -3.230679083656 1.045613711048
C 1.304349660635 -3.554294596987 -0.077496505645
C -0.048509371733 -3.360236430067 0.360462437817
N 1.748307761305 -4.015899082666 -1.330197652539
C 3.210641658177 -4.173920499863 -1.506108100276
N 2.044900889294 0.312275487942 -1.634595900526
C 1.530748199388 1.352272859045 -2.551188675020
P 3.286201546565 -0.766665766792 -1.970292994153
Cl 2.822521117001 -1.431019038760 -3.968774605353
Cl 4.916633663300 0.508663547172 -2.508159190575
P 0.829551560895 -4.685188916449 -2.667420188316
N -0.642801458181 -3.715719775684 -2.554120454665
C -1.740784964866 -4.267967825375 -3.351117791701
N 0.259075824199 -6.217199740361 -2.141431315271
C -0.502443403479 -6.488963026484 -0.929015060039
C 0.191207823266 -7.287947188698 -3.128531828491
C -0.438427112174 -2.297493649044 -2.859333996511
H -0.280650273006 -5.751933855989 -0.158695554217
H -0.915937406310 -3.456907773948 -0.272079820692
H 0.501927036478 1.083919766262 -2.828098516975
C 3.882025274224 -5.538533144595 -1.131501940748
H 3.689113156108 -3.376486803678 -0.936835357455
H 2.131109880313 1.280117708074 -3.461684588495
C 1.559670407302 2.826540427041 -2.058974124115
H 3.435986621071 -3.962790709189 -2.556357620626
H -0.917526063729 -2.909241320869 2.374855766847
H 1.668391877611 -2.759096428981 3.182951023983
H 3.221854351785 -3.227838450098 1.059947318094
H -0.767698233093 -0.129776669850 -0.988348828868
H -1.276582464863 -0.046489027584 1.656213814064
H 1.079198599291 0.203263096315 2.956055380594
H 3.044066978386 0.326529667273 1.095230925899
H -0.228477246924 -7.479571390736 -0.539231014959
H -1.591285049135 -6.487117350949 -1.109355961184
H 0.594983728823 -8.221280382083 -2.708897683245
H -0.844796239206 -7.483748358168 -3.453812390124
H 0.780139592463 -7.024608572567 -4.012369886824
H -2.650963940893 -3.690048056219 -3.147085828375
H -1.553053171190 -4.227087530150 -4.440654262782
H -1.934700334889 -5.306902275506 -3.074600416573
H -1.363567008354 -1.750845363427 -2.634705289672
H 0.355831854685 -1.892433043963 -2.233026050128
H -0.176408277223 -2.115553794711 -3.915233286112
C 1.201351698978 3.683539946066 -3.292220258454
C 0.519806796391 3.105759649000 -0.954721696511
C 2.957686817787 3.213326951136 -1.552621866309
H 1.188693634931 4.747511604073 -3.026948119068
H 1.930318534853 3.548416651343 -4.101086937012
H 0.208056298364 3.426161621728 -3.683390238857
H 0.460421098852 4.185856100411 -0.769983688488
H -0.479542851024 2.760946688689 -1.248084780439
H 0.777623259875 2.622096955535 -0.009624376481
H 2.957440579043 4.254505637397 -1.206521452751
H 3.263823903353 2.576619331889 -0.715818265161
H 3.712297541745 3.114473789304 -2.339181284620
C 5.360131121360 -5.223496493496 -0.824086857759
C 3.232218216592 -6.212368149132 0.088725009690
C 3.830043257572 -6.517251193887 -2.321883479689
H 4.382929094646 -7.435484536227 -2.084734908171
H 2.802184674394 -6.799743128033 -2.560901651866
H 4.279063675886 -6.075493899186 -3.220234069550
H 3.722052371533 -7.174521583878 0.286494005819
H 3.315838019421 -5.603770006382 0.993882913615
H 2.170831896619 -6.405339619358 -0.092083989659
H 5.922164185160 -6.144750124351 -0.627096419176
H 5.841763383401 -4.711992735673 -1.667980522992
H 5.454523836976 -4.577782699095 0.058912337973

**7d (with 1 dimethylamine substituent)**

E(B3LYP-D3/6-31+G*) = -4036.88152601
E(PCM-B3LYP/6-31+G* (ether) = -4036.88414513
Sum of electronic and zero-point Energies= -4036.551582
Sum of electronic and thermal Energies= -4036.525722
Sum of electronic and thermal Enthalpies= -4036.524777
Sum of electronic and thermal Free Energies=-4036.608001
C 0.315271272092 0.178955668614 0.139049231701
C 0.018257263844 -0.018456601757 1.528783391364
C 1.261390259919 -0.086448303540 2.239312223870
C 2.315769568548 0.053087615402 1.290570662821
C 1.733560537193 0.233290419459 -0.001528372401
Fe 1.149396168320 -1.578080412374 0.799909908758
C 0.672039854884 -3.080079273437 -0.534585051294
C 2.076421701744 -3.063062395232 -0.278882856698
C 2.273099955353 -3.276184040169 1.118495136136
C 0.992582974333 -3.406161803651 1.735170120888
C -0.005268723368 -3.314563724675 0.708740488186
N -1.407194124624 -3.444793735302 0.874925221232
P -2.270018736961 -4.803630799797 1.498430491249
Cl -1.381946307732 -4.989365606163 3.491205684099
N -1.301418114265 -0.061616578948 2.074364467695
P -1.555242052906 -1.260841247427 3.248570737904
Cl -1.548096480986 -0.099084948127 5.072409587006
C -2.034314648876 1.215101435300 2.025396747692
C -2.224357521369 -2.662729271779 -0.072421339620
Cl -3.659000951196 -1.521918717668 3.064267209242
N -1.642136714181 -6.187900119586 0.721888488915
C -2.455804474384 -7.387030124603 0.977023919926
C -0.215326561113 -6.511928001421 0.613753590396
H 0.349497295997 -5.660182995773 0.240530088256
H 0.797320760975 -3.551684507145 2.785687254104
H -1.581359841265 1.949325017752 2.703289634228
H -2.171972267314 -3.059885688907 -1.095746573624
H -1.869403214957 -1.629674090653 -0.064225282465
H -3.073662543711 1.051937195292 2.315072119184
H -2.008387691149 1.602164370592 1.002754688329
H -3.266058976399 -2.671339193973 0.256716334921
H 3.224481592020 -3.286905914376 1.634454694575
H 2.850927372961 -2.883888753160 -1.013879302565
H 0.199500109740 -2.927983675459 -1.495216590073
H 1.369185332518 -0.244186928911 3.304800116253
H 3.374663918416 0.004669052122 1.510005220129
H 2.273630451118 0.347986714345 -0.932437595793
H -0.413888747833 0.262001549810 -0.656324962456
H -0.097806767675 -7.340133888540 -0.094645834240
H 0.199361699712 -6.816471752391 1.586664847340
H -2.350579607779 -8.078393363341 0.132479948685
H -2.144248401709 -7.904237270323 1.898069512895
H -3.512207035581 -7.116103139979 1.069721696774
C 1.632173600593 -0.124727830731 1.822557411687
C 2.565653477013 0.233838624400 0.793108649848
C 1.872026671570 0.269401836348 -0.455998064990
Fe 1.105736630072 1.690739959732 0.788495188070
C 1.342027005254 3.421254658873 -0.294010048423
C -0.039785049327 3.223752457275 0.015448174388
C -0.179083420777 3.203987384947 1.432961617403
C 1.124629510279 3.376393904234 2.004767366728
C 2.066687737805 3.498762620372 0.931672414679
N 1.458340356837 3.570936959999 3.382615601763
P 0.721117147820 2.504438714348 4.458858909448
Cl -0.890553816876 3.700588393072 5.274262669808
N 1.891569872027 -0.360715980878 3.185218382556
P 3.396842175177 -0.970769572567 3.899678497344
N 3.815340654167 -2.452624172501 3.138700524163
C 3.382502525571 -3.670015821646 3.819014889815
C 0.730389058624 -0.849758181221 3.944616355716
C 1.858760946159 4.947005379468 3.726619928988
N 4.560444511412 0.070090846007 3.094788549451
C 4.343544300281 1.506225713088 3.308297848335
C 5.952323168525 -0.296351952972 3.386198956326
C 4.008002279766 -2.631352953379 1.701798015309
Cl 2.050659911547 2.621123346476 6.112293481717
H 4.457771684908 -1.736455791281 1.270591009362
H 3.618566857245 0.406916388319 0.942977149852
H 2.666625662326 5.258492120187 3.059157526880
H 0.385826931957 -1.829741400282 3.580375058078
H -0.099310610268 -0.141253107023 3.876419350665
H 2.218548784315 4.980068039002 4.756239769330
H 1.010642225338 5.634173282332 3.616141832523
H 1.005778711378 -0.941338660704 4.998195350595
H 2.317476109471 0.501534417819 -1.415167479758
H -0.303697120725 0.000118845606 -0.936918352382
H -0.597555592953 -0.413355624351 1.694864821565
H 3.136051865951 3.618860572266 1.045559229259
H 1.772673091708 3.456182795310 -1.286489327671
H -0.838619826740 3.085944579801 -0.701940479866
H -1.098418406992 3.078759168293 1.990329351792
H 3.060340225793 -2.833034058870 1.177831735539
H 4.684613679223 -3.479947523040 1.528780648089
H 2.424495547149 -4.049996726147 3.424987095094
H 4.136394618937 -4.459424701046 3.691065757455
H 3.263975903239 -3.479130053646 4.890149470527
H 6.612150648243 0.284623060819 2.729985240076
H 6.241421234998 -0.086091698442 4.432067796423
H 6.117148753274 -1.357645445124 3.188928643797
H 5.050600613738 2.061410519435 2.678210278690
H 3.335617419333 1.790581304379 3.009236699560
H 4.498472630748 1.817732671394 4.354643450051

**7d' (with 2 dimethylamine substituents on the same phosphorus atom)**

E(B3LYP-D3/6-31+G*) = -3711.23423702
E(PCM-B3LYP/6-31+G*) = -3711.23944059
Sum of electronic and zero-point Energies= -3710.822062
Sum of electronic and thermal Energies= -3710.793438
Sum of electronic and thermal Enthalpies= -3710.792494
Sum of electronic and thermal Free Energies=-3710.881701
C 0.494025424532 0.008964534039 -0.205179036046
C 0.339031883470 -0.205870542226 1.198809201939

**7d" (with 1 dimethylamine substituent on both phosphorus atoms)**

E(B3LYP-D3/6-31+G*) = -3711.24525268
E(PCM-B3LYP/6-31+G*(ether)) = -3711.25228423
Sum of electronic and zero-point Energies= -3710.833093
Sum of electronic and thermal Energies= -3710.804098
Sum of electronic and thermal Enthalpies= -3710.803154
Sum of electronic and thermal Free Energies=-3710.892256
C 0.219370549137 0.182325456034 0.307923535019
C 0.462932991969 0.037635825698 1.706966279923

C 1.864328512483 -0.167412914747 1.894587509717
C 2.493528209988 -0.121759282535 0.616710552400
C 1.476339645900 0.081080375582 -0.370113153066
Fe 1.063133440026 -1.650443163704 0.696372417511
C -0.462701996376 -3.011645112829 0.520139905842
C 0.244673843695 -3.215501003322 1.743420332918
C 1.602182917918 -3.518852940190 1.423762548373
C 1.727528239848 -3.528712756836 -0.004894882817
C 0.455778964903 -3.176071610203 -0.559305880974
N 2.888101638083 -3.905950865683 -0.723314190100
C 4.158228141853 -3.338312344843 -0.240391193764
N 1.657853695322 0.265184851614 -1.770702446927
C 1.504740242471 1.662327660347 -2.214567450088
P 2.660652283683 -0.858949697161 -2.562028650053
Cl 4.619792546397 0.194639087412 -2.588402205166
N 2.193936859700 -0.517548206157 -4.197289631338
C 0.765803283488 -0.684246623937 -4.508957778730
C 3.045424833669 -1.107123761990 -5.239736403949
P 3.045878869331 -5.010471370142 -2.000689830921
N 2.195569267365 -6.413132827719 -1.548226568975
C 0.927240881554 -6.448927831533 -0.813859948815
Cl 1.622119764194 -4.219563735498 -3.579286812514
C 2.259498198875 -7.448839370505 -2.590661373209
H 0.994499344083 -5.867137736549 0.103933410713
H 0.241452948991 -3.073573887707 -1.611577590928
H 2.181447050311 2.318462932829 -1.652602200310
H 4.416479281917 -3.738356901672 0.748508508202
H 4.071512243130 -2.252093512832 -0.181102761680
H 0.471657059285 1.990668210768 -2.054952386288
H 1.745803942075 1.728067769027 -3.276679977463
H 4.964247239760 -3.591151008103 -0.934191359236
H -1.503174141815 -2.727763582846 0.426369892373
H -0.163412826021 -3.114846329936 2.741295767510
H 2.397394640782 -3.713063806816 2.130724566765
H -0.741503414722 0.317255138333 -0.171810427825
H -0.290099655109 0.032515197363 2.484732996894
H 2.359139072236 -0.346883392366 2.840653322834
H 3.550796361197 -0.212221306756 0.410612618928
H 0.714480846095 -7.489907683288 -0.545417596712
H 0.096060210507 -6.063874608959 -1.423261884885
H 2.176185843895 -8.435348858410 -2.120301823331
H 1.451880729648 -7.331321217998 -3.328792291216
H 3.218371142338 -7.398477653929 -3.116943887090
H 2.884813985042 -2.190736372115 -5.348877259852
H 2.810454248837 -0.620049632089 -6.193963531666
H 4.098431739483 -0.919706051941 -5.019501390937
H 0.480517657861 -1.743177221379 -4.607033676883
H 0.146357144289 -0.225319488343 -3.735856887409
H 0.559353709657 -0.179048804371 -5.460934628927

**TS(7a/2a)**

E(B3LYP-D3/6-31+G*) = -4775.61778887
E(PCM-B3LYP/6-31+G*) = -4775.63110349
Sum of electronic and zero-point Energies= -4775.139703
Sum of electronic and thermal Energies= -4775.102805
Sum of electronic and thermal Enthalpies= -4775.101861
Sum of electronic and thermal Free Energies=-4775.204259
C 0.084150652314 0.006886813030 -0.024602275629
C 0.052268008481 -0.001926473453 1.397998853695
C 1.409363256377 -0.000383410621 1.871848027108
C 2.268128893222 0.060679597089 0.719252884572
C 1.448440185362 0.048278191285 -0.444797105805
Fe 1.117156555901 -1.627682949673 0.729813035271
C 0.298185880713 -3.250346970109 1.663762430292
C 1.700448899539 -3.118780280704 1.981959166996
C 2.415943808039 -3.193920424977 0.734667328356
C 1.473589817414 -3.372239882403 -0.319131695620
C 0.168892928830 -3.405901330958 0.254039584691
N 2.243699720259 -2.988206593314 3.321158113322
Si 1.665360877603 -4.442984355542 4.380481633187
C -0.144462083757 -4.480459740918 4.876285191936
N 1.883103104432 0.031358984095 3.226424891083
Si 2.445554119154 1.724545808323 3.720823110142
C 4.276280572866 1.911814216774 3.362515673319
P 1.648608033676 -1.143439871562 4.396231890961
Cl -0.664595162273 -1.316199824071 4.264735728394
P 4.272411594717 -3.064328454627 3.614266398300
N 4.955382409113 -4.392050640736 2.807898637546
C 5.251477919230 -4.665321953809 1.400580702507
Cl 4.839703374100 -1.529355497405 2.313872474728
C 1.950261658260 2.068875662395 5.499830642873
C 1.452707755977 2.897376396204 2.624173581108
C 2.626968835887 -4.397157696702 6.005780894258
C 1.961666281190 -5.965991089692 3.305212091147
C 5.396228107122 -5.474665217554 3.703426357371
Cl 3.987468927824 -0.759249498921 5.695115717836
H 5.339070388710 -3.737026122468 0.835898722981
H 3.471621269279 -3.063557330903 0.594813521393
H 1.714072836928 -3.432240847789 -1.372657114327
H -0.766073942648 -3.492437852453 -0.284089953326
H -0.515616092170 -3.163525319487 2.364581064306
H 3.346673185366 0.065595080356 0.744333488616
H 1.803252851024 0.034972771080 -1.467395551203
H -0.781229376093 -0.041809545478 -0.673149443880
H -0.827153485353 -0.058829817545 2.018599218691
H 4.482728114977 -5.301043278173 0.941954428768
H 6.215931493277 -5.182317769415 1.338557219068
H 4.853093097473 -6.406585760592 3.503065942115
H 6.469428294758 -5.651905010061 3.560429215266
H 5.237045644329 -5.195776850007 4.747108449626
H 2.131616425659 3.131901121923 5.710362807555
H 0.878597928123 1.882588596050 5.645686102236
H 2.515879762415 1.472616420211 6.219249759579
H 1.680520529234 3.927380819693 2.930867920998
H 1.693518158059 2.801141367539 1.560566345795
H 0.373812420247 2.743710209069 2.741546595159
H 4.600157582432 2.930586103072 3.615108296764
H 4.859219504598 1.199461514733 3.951894145435
H 4.487501365688 1.748643259679 2.298867863459
H -0.265663830619 -5.465247949867 5.353503807618
H -0.404007621698 -3.714032700179 5.608944891170
H -0.856835290947 -4.422280990767 4.051638277173
H 1.970321303604 -4.817465250536 6.779046269750
H 3.546340975000 -4.989474335638 6.002822927153
H 2.891128051989 -3.377026444896 6.309378522086
H 2.072351378911 -6.857538161220 3.935569341838
H 1.095747171527 -6.121057670336 2.651678840019
H 2.842473360549 -5.880942806326 2.665779251072

**TS(7a'/2a)**

E(B3LYP-D3/6-31+G*) = -4449.97522177
E (PCM-B3LYP-D3/6-31+G* (ether)) = -4449.9907514
Sum of electronic and zero-point Energies= -4449.415641
Sum of electronic and thermal Energies= -4449.375139
Sum of electronic and thermal Enthalpies= -4449.374195
Sum of electronic and thermal Free Energies=-4449.485004
C -0.048039854555 0.023859409969 0.046839639768
C -0.101275366246 -0.009066211576 1.484802880556
C 1.235130244404 0.010865595000 1.978457091763
C 2.116806247086 0.073873960167 0.856082449810
C 1.334696298171 0.098125199171 -0.333758982952
Fe 0.914547432506 -1.605824016672 0.724342226443
C -0.168371100841 -3.264094193905 1.171550055640
C -0.075778853703 -3.098354067506 -0.260135465277
C 1.333974515391 -3.111444668414 -0.577628343255
C 2.075219212192 -3.306329676670 0.624888674119
C 1.149245736082 -3.400873933896 1.705185372908
N -1.150927680453 -2.959737418263 -1.197772625927
Si -0.884949036481 -3.977830119610 -2.720029930686
C 0.490943659209 -3.375964682740 -3.858369389377
N -1.216979612396 0.074350820275 -0.782348095705
Si -1.944213584216 1.775435941778 -0.774298100935
C -3.289060373389 1.792965272784 0.545022455458
P -3.236068047638 -3.747929769601 -0.468697769897
N -3.320482028025 -3.143063495747 1.103970759022
C -3.210079743183 -1.703191668409 1.361724447725
N -3.057575855446 -5.404272569249 -0.172897221352
C -3.831626039372 -6.314847559384 -1.021795346292
P -1.495051599610 -0.955306132724 -2.094517515905
Cl 0.331310504329 0.185634477270 -3.518099229828
C -2.586079748525 2.301403414295 -2.458714377565
C -0.542963725231 2.945033204561 -0.309755276876
C -2.495364639099 -3.986511681572 -3.710724977930
C -0.382162579180 -5.726298782534 -2.202771523496
C -2.188121834233 -6.092050745916 0.783276108425
C -3.723699685189 -3.899334718945 2.289380438207
Cl -3.900543304906 -0.825809970161 -1.923757319465
H -1.574973975446 -5.379025822861 1.329747624151
H -1.074046690983 -3.243201426949 1.751811702822
H 1.397041928474 -3.517674518810 2.752668237673
H 3.154546631384 -3.331685641302 0.702737215560
H 1.761053146018 -2.934932481544 -1.552968703947
H -1.002206017525 -0.067770386795 2.076939203840
H 1.528247305899 -0.046421198425 3.018927744635
H 3.198630199887 0.068734719705 0.897168790063
H 1.692802842533 0.123466632870 -1.351924305032
H -1.515058242407 -6.772171481043 0.247805598577
H -2.779708610590 -6.683435994921 1.496203981251
H -3.176618157948 -7.004212458739 -1.569679304831
H -4.517701453469 -6.908401984016 -0.401644582896
H -4.429981033874 -5.750558669898 -1.742052925820
H -2.881761645920 -4.048296330687 2.982766560291
H -4.499984350604 -3.330908005776 2.815814042293
H -4.137937511573 -4.870577328404 2.019956039534
H -2.646554249280 -1.554684891550 2.290818623621
H -2.682643668302 -1.193124776313 0.560844830942
H -4.203338910017 -1.252012879938 1.474034564993
H -2.770264025772 3.384110531536 -2.417753097460
H -1.833467705701 2.117505198545 -3.233497532770
H -3.515176631141 1.803343358936 -2.743842462581
H -3.700228735566 2.805931464851 0.648934656925
H -4.104243625442 1.116409551362 0.270355219158
H -2.896787703836 1.492754946279 1.524284298740
H -0.926361695153 3.973857929104 -0.343364390084
H -0.136644226219 2.764690859064 0.690338754416
H 0.277002010942 2.865978507656 -1.032439972869
H 0.130053172512 -6.201549853614 -3.049273338937
H 0.320195575124 -5.707644872661 -1.361985107627
H -1.228846178367 -6.359567258783 -1.932632562207
H -2.244768693476 -4.181619652380 -4.761210576995
H -3.188506311933 -4.771111376607 -3.390746781953
H -3.033256167123 -3.033880840039 -3.668940776858
H 1.482929565694 -3.675262890709 -3.503222112278
H 0.330685133815 -3.884073008816 -4.820138937601
H 0.502138008305 -2.299798687217 -4.048006573883

**TS(7c/2c)**

E(B3LYP-D3/6-31+G*) = -4351.35600439
E(PCM-B3LYP/6-31+G*(ether)) = -4351.37345815
Sum of electronic and zero-point Energies= -4350.798249
Sum of electronic and thermal Energies= -4350.763155
Sum of electronic and thermal Enthalpies= -4350.762211
Sum of electronic and thermal Free Energies=-4350.861832
C 2.113327060370 3.399759207091 -0.636124631673
C 2.165579899158 2.340320766121 0.313797382082
C 1.969251642272 1.104969411562 -0.391384409905
C 1.832625869592 1.420232890832 -1.789029709204
C 1.914814977168 2.834726809620 -1.931930978997
Fe 0.362040388638 2.289474461998 -0.674644855278
C -1.086883922484 2.307221878938 0.773376972051
C -1.162645921809 1.105245291340 -0.017531205819
C -1.386835467798 1.509543011902 -1.378249899368
C -1.455193293425 2.932089501830 -1.418482897007
C -1.272198887405 3.422993962532 -0.091440457392
N -1.084815089284 -0.240320494346 0.491119783501
C -1.940708675176 -0.481174834903 1.713608469834
C -3.455720944919 -0.037279869112 1.797184562969
C -3.595898239467 1.013463704578 2.921717609647
N 1.919315165577 -0.222769043012 0.132055187708
C 2.873994109696 -1.201680808414 -0.486149947877
C 4.244441397270 -1.315892314048 0.219749547451
C 4.985369343528 0.032225788882 0.235407810908
P 0.850147739286 -0.837100357615 1.272400844038
Cl 0.966001019047 0.733858513637 2.864784292081
P -1.515106446983 -1.935909340523 -0.756197659714
N -2.890815837984 -1.769969954293 -1.732040450847
C -3.173460378950 -1.009482126917 -2.951026058581
Cl -0.071467464626 -1.481278686355 -2.205001428771
C 4.070548035455 -1.836629203948 1.657473055657
C 5.053062305525 -2.343958226078 -0.598572835815
C -4.065895599880 0.562227707989 0.514829943121
C -4.266506300663 -1.284265989636 2.214931134114
C -4.041839581077 -2.571076358695 -1.282354736342
Cl 0.670131995602 -3.678773202426 0.421623037148
H -2.251634739874 -0.659325359348 -3.412509505353
H -1.450880677316 0.861874337444 -2.233660436895
H -1.425902661427 -0.010519071409 2.551799968130
H 3.016884901181 -0.882568939764 -1.522406357105
H 2.387373984444 -2.178589928302 -0.502609016780
H -1.870877633925 -1.561662433966 1.883885793781

H -1.589005865552 3.530345057280 -2.310361533903
H -1.241482351095 4.462489641551 0.208001627930
H -0.883124205548 2.351098761649 1.831075095142
H 1.647990647726 0.708597207356 -2.580410582603
H 1.806085315635 3.383651577968 -2.858455510216
H 2.187480225989 4.454671591651 -0.405205557189
H 2.282108641905 2.445197844569 1.380113496196
H -3.822722946569 -0.151019876771 -2.732481714157
H -3.683937222178 -1.661634258659 -3.669681110596
H -4.890205420546 -1.931922682531 -1.009019813316
H -4.348299391887 -3.246314402814 -2.090423835842
H -3.765061131013 -3.181218309474 -0.418192735244
H -5.154928428698 0.622801784291 0.632636598356
H -3.698213370971 1.572007184919 0.320593943701
H -3.854337746450 -0.040540673441 -0.367754202165
H -4.648779252437 1.292476466207 3.053179633915
H -3.230505432040 0.625341686716 3.880559023282
H -3.035521637324 1.923943344390 2.687014037896
H -5.318517481725 -1.023710093340 2.383601758660
H -4.231204473225 -2.064433395236 1.448751773423
H -3.876561945480 -1.715154598090 3.145272970297
H 6.044985255362 -2.489924935142 -0.153977388531
H 4.546269655923 -3.316166946711 -0.623765921361
H 5.197534751048 -2.006239791416 -1.633499311199
H 5.989754717392 -0.090071522264 0.660093227043
H 5.093502799474 0.441669115518 -0.777298071153
H 4.454751216442 0.773283584197 0.841779659892
H 5.050375823675 -2.035300982260 2.109794896710
H 3.567308374135 -1.098912270769 2.294462150786
H 3.487172006855 -2.764719520353 1.676364709092

**TS(7c'/2c)**

E(B3LYP-D3/6-31+G*) = -4025.71524926
E(PCM-B3LYP/6-31+G* (ether)) = -4025.727973
Sum of electronic and zero-point Energies= -4025.074650
Sum of electronic and thermal Energies= -4025.036688
Sum of electronic and thermal Enthalpies= -4025.035743
Sum of electronic and thermal Free Energies=-4025.141134
C 0.179540268704 0.003578363767 0.073493974586
C 0.235683807957 -0.085285990389 1.513087129098
C 1.602715384379 -0.146100236864 1.901471115518
C 2.398586834570 -0.075687582120 0.719470599257
C 1.533094139620 0.037283397740 -0.404287313749
Fe 1.112461420488 -1.697779061556 0.614711320121
C 0.069054762086 -3.385505899048 1.152025279338
C -0.021312801889 -3.193210936091 -0.269568082703
C 1.324915232206 -3.168803852567 -0.778281917272
C 2.219332909106 -3.402077488369 0.306926993105
C 1.444970679210 -3.528751801723 1.499948636042
N -1.220232407650 -3.083877556488 -1.043556405457
C -1.171234333600 -3.769659525927 -2.393647161372
C -0.604370602421 -5.229509347938 -2.645539866857
C -0.243582210658 -6.056648047858 -1.399406054759
N -1.051428220109 0.074204610574 -0.658832150854
C -1.941463535509 1.207454164402 -0.246395384678
C -1.780600486961 2.505056995758 -1.075283831989
C -0.335849330516 3.030550947533 -1.020083186497
P -3.129166820829 -3.792795450126 -0.272803174235
N -3.169368319009 -3.063214971533 1.287570998389
C -2.773724090415 -1.683635479599 1.543491820903
N -3.044423076032 -5.398983928972 0.293160449423
C -3.723180794271 -6.431445414119 -0.490519042337
P -1.581910466869 -0.978142749054 -1.880213146171
C -2.195788137276 2.274707413663 -2.538754835151
C -2.732848015081 3.534495233631 -0.431890377793
C -1.682242685959 -5.978070351441 -3.463104601643
C 0.651694197228 -5.139148220236 -3.543446973744
C -2.472088811531 -5.911270829907 1.537349213867
C -4.340592359661 -3.416768412446 2.109217121116
Cl 0.356669661439 -0.925662888375 -3.208754309857
Cl -4.191969843897 -0.951511397874 -1.343225306809
H -2.013847508391 -5.102388672034 2.102981805948
H -0.763225118107 -3.403439506012 1.836488824517
H -0.612211267366 -3.117104463005 -3.060743626895
H -1.709588907705 1.419502428275 0.800923539760
H -2.974907123269 0.866131825228 -0.302144070458
H -2.211207146096 -3.735373762175 -2.734331524980
H 1.830081261134 -3.675128684616 2.500913221591
H 3.299206565413 -3.430503099704 0.238719647295
H 1.600176271732 -2.968660460422 -1.801397540664
H -0.610764899463 -0.129041929123 2.182192925665
H 1.967715939560 -0.264082612799 2.913536536850
H 3.478750689975 -0.130871029108 0.674008553141
H 1.835551031456 0.080632212436 -1.436960527069
H -1.713658513198 -6.676477995293 1.324696281438
H -3.256623700037 -6.370123926978 2.156378736688
H -3.027027724975 -7.220852652096 -0.802852056699
H -4.518850083909 -6.890615439906 0.113532194854
H -4.183346052018 -5.990271268092 -1.378340996811
H -4.067320738623 -3.340088592498 3.169819438159
H -5.177631918198 -2.730482797438 1.913314223802
H -4.678750270378 -4.435903659108 1.916718413651
H -2.462319485971 -1.605090504592 2.595235071366
H -1.933063735396 -1.414079000330 0.919375149035
H -3.588853378472 -0.977047665143 1.350506323468
H -0.263794681117 3.998054470286 -1.532825543491
H 0.001845352642 3.169411466775 0.015020051841
H 0.357246820050 2.340203885059 -1.510422182330
H -2.184804855150 3.223984370400 -3.089116195166
H -1.501504534825 1.599553953537 -3.053323990165
H -3.203642664911 1.848964588761 -2.606424260464
H -2.684382458680 4.488140333375 -0.971181267757
H -3.772543078798 3.185217524123 -0.458158187167
H -2.463476646428 3.729468347683 0.614721023304
H 0.981714215559 -6.145678612169 -3.829980689212
H 0.446411077588 -4.579484939679 -4.463980439592
H 1.486845282096 -4.653181094903 -3.033096972349
H -1.327380337115 -6.976311843979 -3.747996311403
H -2.610123766983 -6.098003883964 -2.899031775825
H -1.922415927299 -5.434974657351 -4.385893083227
H -0.039623377117 -7.091899057699 -1.701728829900
H 0.649770172389 -5.678660399465 -0.897133661260
H -1.053922374396 -6.066998178015 -0.674463706387

**TS(7d/2d)**

E(B3LYP-D3/6-31+G*) = -4036.81948869
E(PCM-B3LYP/6-31+G* (ether)) = -4036.83595181
Sum of electronic and zero-point Energies= -4036.489117
Sum of electronic and thermal Energies= -4036.464499
Sum of electronic and thermal Enthalpies= -4036.463555

Sum of electronic and thermal Free Energies=-4036.541157
Fe 0.000892329297 -0.017549944432 0.028100653231
C 0.023329269319 0.016780870586 2.065898007582
C 1.932764281898 0.063196164124 0.743295235925
C 1.456860817817 -1.278374049315 0.798430250111
C 0.286113642235 -1.310390937357 1.617583257069
C 1.029591059646 0.878389003819 1.505524838114
P 0.988524121828 3.534700956933 0.625541597701
N 1.091683725774 2.281143172097 1.745922410202
P -2.356671289529 3.921583963098 0.404763031044
Cl -0.362786980858 5.292495813009 2.203516018368
Cl -2.584845044240 2.692237493661 2.075182558535
N -0.689502664912 2.972238512545 -0.482558372822
Cl 2.515121878038 2.810268324673 -0.947362919875
C -0.842997615010 1.579273336178 -0.873073690961
C -4.024161517144 4.360472319145 -1.613878388740
H -4.507886368074 1.768484821168 0.497629536014
C -4.608523683720 2.295672310526 -0.449982168302
C -1.627331608761 -0.595617626025 -1.100664288570
C -1.853320509480 0.646677012429 -0.439598908243
H -2.602786544983 0.811350914953 0.311089245424
C -0.009067920005 0.884328569747 -1.822826808508
C -0.490436803305 -0.448268613796 -1.948269452623
C 1.191792175059 2.626394268193 3.187698992374
C -0.577822562754 3.828380672490 -1.707548711715
N -3.706706320550 3.448740573465 -0.502304591861
H 1.924844946582 1.953173682059 3.642177596787
H -1.442921008548 3.658559069881 -2.354170929384
H 0.329483565524 3.581659292248 -2.259855088660
H 0.218566524345 2.515009719607 3.675018473520
H 1.513830806859 3.658958099392 3.312253236121
H -0.529845201918 4.880463450085 -1.409123905678
H -2.202900475956 -1.499539437646 -0.948348403119
H -0.043196389848 -1.220946150366 -2.559813746965
H 0.868106459580 1.285860696213 -2.304511286961
H -0.813633652895 0.344901323413 2.667123331214
H -0.320143466443 -2.181710035406 1.829590805541
H 1.896859790030 -2.123584301063 0.284884535602
H 2.779836535293 0.423777934356 0.181406020456
H -4.411119379812 1.601904349415 -1.276695545860
H -5.641198179801 2.656792334778 -0.528185625772
H -3.889836295786 3.858014411413 -2.581159270740
H -5.065727471663 4.695007258196 -1.531732167525
H -3.377593593317 5.242774590913 -1.585319255531

**TS(7d'/2d)**

E(B3LYP-D3/6-31+G*) = -3711.18802008
E(PCM-B3LYP/6-31+G* (ether)) = -3711.20076595
Sum of electronic and zero-point Energies= -3710.774838
Sum of electronic and thermal Energies= -3710.747476
Sum of electronic and thermal Enthalpies= -3710.746531
Sum of electronic and thermal Free Energies=-3710.829059
C -0.060118308434 0.033179350952 0.026591090879
C -0.128831911661 -0.090279558899 1.443336892004
C 1.200159049734 0.073301869207 1.961303265046
C 2.072232932965 0.348275657406 0.846870535858
C 1.291144816275 0.308481364791 -0.342612416195
Fe 1.189692004270 -1.484150380824 0.686345841247
C 0.546077097093 -3.322194840946 1.344521739767
C 1.875970368740 -3.047622084293 1.829669859861
C 2.711306398246 -2.836595353552 0.674812645700
C 1.909701168533 -3.009316004637 -0.491443924810
C 0.576409018686 -3.304420305345 -0.078734110994
N 2.252963261054 -3.030606339078 3.224738623412
C 1.511821837096 -4.103465966393 3.964196531225
N 1.661940189719 0.059684330085 3.315271999549
C 2.379869496231 1.314355730552 3.670978363496
P 1.560761482548 -1.203240044471 4.442541020728
Cl -0.742083941539 -1.708696346962 4.138057253375
P 4.120101747032 -3.513513446247 3.779881012667
N 5.052567200311 -2.668085654772 2.587110362735
C 6.471597232369 -3.053319930667 2.538179650838
N 4.301779606815 -5.090645554186 3.176022262678
C 4.327365534600 -5.527536667391 1.782025318334
C 4.185936466528 -6.191362742866 4.131706983799
C 4.900190646381 -1.214118528648 2.469928714816
Cl 3.787243191719 -0.728813958651 5.547298728285
H 4.554414692551 -4.688489303962 1.126745598874
H 3.758834668000 -2.594316412040 0.689875674886
H 1.843989598050 2.137974456556 3.191347096407
H 1.682638051965 -5.070719436595 3.483507717775
H 0.445377831186 -3.892179458118 3.982683119542
H 3.416594356085 1.289391013950 3.322698958707
H 2.385785867946 1.463618981366 4.748747781246
H 1.872397171632 -4.136650130896 4.996832863767
H 2.255751353747 -2.898768521815 -1.511208101352
H -0.277882748205 -3.450558457600 -0.727006948434
H -0.333312362209 -3.456034249364 1.956317018512
H 3.138501847456 0.515047050327 0.904055554425
H 1.667444119334 0.426097542447 -1.350631241734
H -0.892793502131 -0.091171327100 -0.653760111681
H -1.005332425898 -0.326235373216 2.023516680622
H 3.359013459099 -5.954000482579 1.481898258569
H 5.101139493175 -6.296589634500 1.651453640457
H 3.276330989018 -6.784689964368 3.953723816595
H 5.053053410768 -6.860369137217 4.043217869989
H 4.152470261216 -5.802601225498 5.153448959958
H 6.895205869300 -2.694644765486 1.591631012277
H 7.053823575169 -2.610990663033 3.362948055606
H 6.584401436709 -4.138575582073 2.573211252685
H 5.274193102705 -0.906531023701 1.483031864485
H 3.850311239464 -0.940811836715 2.535172683986
H 5.444128466233 -0.667336721880 3.249578099453

**TS(7d"/2d)**

E(B3LYP-D3/6-31+G*) = -3711.16437882
E(PCM-B3LYP/6-31+G* (ether)) = -3711.18823856
Sum of electronic and zero-point Energies= -3710.751086
Sum of electronic and thermal Energies= -3710.724055
Sum of electronic and thermal Enthalpies= -3710.723111
Sum of electronic and thermal Free Energies=-3710.805555
C 0.024322494847 0.142380095324 0.232373939130
C 0.037879523305 -0.043419576565 1.643612463746
C 1.397598304687 0.096175849939 2.091609382011
C 2.205352861634 0.420678080260 0.943719000298
C 1.357569000431 0.423544491036 -0.201572723501
Fe 1.288452483304 -1.407055293715 0.777614854564
C 0.477701562015 -3.166799955923 1.414271320296
C 1.784519606395 -2.948630651939 1.972020547256
C 2.718971124176 -2.863336358926 0.881578980349

C 1.986356414175 -3.005483287697 -0.336228203303
C 0.608463570191 -3.195765351217 -0.005708666510
N 2.083524824742 -2.902130189640 3.374329664563
C 1.293975452226 -3.919869809809 4.121435275045
N 1.823874785537 -0.008918928887 3.449828715240
C 1.206899286867 1.034881495642 4.309810840843
P 2.245950149735 -1.411540237359 4.334044583787
P 4.593233191212 -3.715406440891 4.114845065632
N 4.076758311996 -5.246868935858 3.654924040700
C 3.878817124034 -5.836288492844 2.328656009054
Cl 5.971900841864 -3.408525352711 2.562081586208
C 3.659813632633 -6.126871944156 4.759325593712
N 4.143304846884 -1.405258621183 4.080454768695
C 4.672032320083 -0.598510646323 2.972813364896
C 4.800289636755 -1.011357000356 5.340457505543
Cl -0.955181509302 -1.597268963475 4.535205787968
H 4.167832526018 -5.139263526473 1.544901286903
H 3.783610885592 -2.701957034108 0.965779123631
H 0.120487555336 0.912727803638 4.351760328058
H 1.415166169285 -4.874001362827 3.605193980176
H 0.238673246659 -3.638658511487 4.182428613305
H 1.477377629529 2.015527768410 3.902858377924
H 1.599983542239 0.958715681970 5.327722069387
H 1.677498505776 -4.002115075879 5.142421188261
H 2.403344905809 -2.952632104292 -1.333751388853
H -0.206155925465 -3.298829770391 -0.710933230650
H -0.438126134539 -3.198078064484 1.990914903829
H 3.269910727297 0.599885449837 0.936438084284
H 1.675948272323 0.587087534925 -1.223385823461
H -0.842454294426 0.043092194783 -0.408583107011
H -0.781372302842 -0.337776472119 2.288553891358
H 2.823626943948 -6.097967384709 2.187961524275
H 4.486827708652 -6.745923964325 2.243541763001
H 2.621410737802 -6.449587485848 4.635528929090
H 4.312417014897 -7.009302462536 4.773238233396
H 3.754987883404 -5.611463156356 5.719457070702
H 5.877709586624 -1.214299762321 5.277554997942
H 4.664657352899 0.061103434506 5.539791258400
H 4.379396460896 -1.571035631560 6.180275687777
H 5.765640592961 -0.633718354285 2.969454895362
H 4.299760751476 -0.982761910498 2.025076726331
H 4.344019920292 0.443071789328 3.077328721082

**8a**

E(B3LYP-D3/6-31+G*) = -1030.21467102
Sum of electronic and zero-point Energies= -1030.095515
Sum of electronic and thermal Energies= -1030.086941
Sum of electronic and thermal Enthalpies= -1030.085997
Sum of electronic and thermal Free Energies=-1030.129026
C 0.006830943631 0.015447661145 0.009887196993
N -0.020484471986 -0.029360007334 1.459495993938
C 1.216284257188 -0.019477850701 2.252799828304
N 0.553711518310 0.527805242390 3.444641148078
C 1.292208721826 1.262642509697 4.453967478877
P -0.811481605923 1.056478112184 2.537345113137
Cl -0.125925685274 3.054909980160 1.778147312185
H 2.036556839154 0.600652878909 4.911367918445
H 1.800651363160 2.146123027402 4.038864767241
H 0.604109504443 1.592323398288 5.238912669149
H 0.525215094680 0.908685895278 -0.370591188253
H 0.508951764212 -0.881601788787 -0.370475550277
H -1.018884177955 0.017461284217 -0.372490866656
H 1.974873905408 0.669851728592 1.839907343204
H 1.654752408010 -1.015607133021 2.405555632892

E(M06-2X/6-31+G*) = -1030.02449232
Sum of electronic and zero-point Energies= -1029.903973
Sum of electronic and thermal Energies= -1029.895457
Sum of electronic and thermal Enthalpies= -1029.894513
Sum of electronic and thermal Free Energies=-1029.937406
C 0.004938413676 0.024381942820 0.023330701695
N -0.019808047935 -0.043387609093 1.468482186399
C 1.217580740357 -0.015614716705 2.251335087217
N 0.551783870099 0.511240030882 3.444600214461
C 1.282658437284 1.264131317481 4.440909778031
P -0.798608056300 1.039644042087 2.538353682921
Cl -0.079741828246 2.979371629213 1.786002368998
H 2.020307804762 0.611203862510 4.917737775493
H 1.794805220089 2.136115058208 4.009593992104
H 0.587517563432 1.611348715041 5.210115247231
H 0.536113549157 0.915026133206 -0.341756340913
H 0.490458067522 -0.873246729752 -0.372066900817
H -1.021421161776 0.050064139774 -0.352679424839
H 1.953359726110 0.697477807637 1.838370883607
H 1.677426080653 -1.001420684888 2.395005545671

**doubly hydrogenated 8a**

E(B3LYP-D3/6-31+G*) = -1031.40904244
Sum of electronic and zero-point Energies= -1031.268672
Sum of electronic and thermal Energies= -1031.259320
Sum of electronic and thermal Enthalpies= -1031.258376
Sum of electronic and thermal Free Energies=-1031.303517
C 0.001101607915 -0.014864951091 0.008420498831
N 0.004064662163 -0.007533419713 1.472517597165
C 1.322774780506 0.008437093251 2.090721369825
N 1.785792556262 -1.376974081516 2.099075093249
C 3.033967853702 -1.537959398562 2.843343360416
P 0.355333709223 -2.346876564949 2.567888276920
Cl 1.302489640696 -4.262511801153 2.781450554377
H 3.782006394047 -0.866034394169 2.404516924023
H 2.939987428410 -1.289836542616 3.917205755156
H 3.403214610609 -2.560048812993 2.751690896504
H 0.437500737494 0.900291314764 -0.424942131256
H 0.583588477275 -0.871749710357 -0.342320821340
H -1.026546271890 -0.123883584475 -0.351926906067
H 1.214024903138 0.425338305732 3.110428586366
H 2.058482152521 0.628550314599 1.549322112441
H -0.597692723408 0.718185954083 1.848763739260
H -0.114192121166 -2.641565858129 1.258491160532

E(M06-2X/6-31+G*) = -1031.20863717
Sum of electronic and zero-point Energies= -1031.066815
Sum of electronic and thermal Energies= -1031.057482
Sum of electronic and thermal Enthalpies= -1031.056538
Sum of electronic and thermal Free Energies=-1031.101988
C 0.030298332923 -0.053657203593 0.022984984763
N -0.017478461282 0.031752757054 1.478364776296
C 1.286724907290 -0.001268809744 2.106561489171
N 1.755712153170 -1.384129730848 2.082050797701
C 3.008271300572 -1.515721026074 2.818938884547

P 0.416659143193 -2.390622291989 2.643779259466
Cl 1.386079959346 -4.257555418989 2.595233735558
H 3.728220935110 -0.806297010282 2.397437011499
H 2.900000491701 -1.297119317622 3.896299714857
H 3.413223989677 -2.521007916465 2.701796877694
H 0.572109403405 0.787427726195 -0.437205957292
H 0.539331225431 -0.980089005270 -0.258037171660
H -0.987390098839 -0.081901407541 -0.373954627345
H 1.176111400571 0.376978380616 3.139215087313
H 2.041004254009 0.619071415575 1.591616056242
H -0.554696094236 0.834166814585 1.789332307034
H -0.208284444547 -2.579064092903 1.390232840557

**8b**

E(B3LYP-D3/6-31+G*) = -1069.55898318
Sum of electronic and zero-point Energies= -1069.410249
Sum of electronic and thermal Energies= -1069.400532
Sum of electronic and thermal Enthalpies= -1069.399588
Sum of electronic and thermal Free Energies=-1069.445736
C -0.005409523866 0.008532676639 0.006522580362
N -0.017472080523 -0.068048112792 1.458763245761
C 1.283201950210 -0.010255776651 2.145601924257
C 0.995695878201 0.403507950248 3.602785865662
N -0.448008542216 0.208232710498 3.814116527326
C -0.966987649793 0.709034754842 5.082503763242
P -1.323000238714 0.461553734605 2.380991834294
Cl -1.169937040727 2.715251609102 2.176084093686
H 1.941501506730 0.721367925827 1.656701834026
H 1.258244088603 1.460136414270 3.767605209657
H 0.374701531330 0.980044808892 -0.344801753470
H 0.629795558927 -0.788565107630 -0.399031485997
H -1.017772069064 -0.130904027211 -0.384951228973
H -0.466146700182 0.189335795096 5.907410469437
H -0.804667643591 1.792900659643 5.191019188996
H -2.040083394413 0.506733896218 5.153355555008
H 1.554920347914 -0.206004931977 4.322111232734
H 1.762355180594 -0.996443640506 2.083187651561

E(M06-2X/6-31+G*) = -1069.34808520
Sum of electronic and zero-point Energies= -1069.197665
Sum of electronic and thermal Energies= -1069.188108
Sum of electronic and thermal Enthalpies= -1069.187164
Sum of electronic and thermal Free Energies=-1069.232774
C -0.026773810460 -0.040765704268 0.036389800107
N -0.026374988497 -0.144261375801 1.484932761593
C 1.269825667184 0.083463212892 2.131114823235
C 0.988040383823 0.319449965757 3.628556261370
N -0.463709469582 0.222313920597 3.808864648032
C -0.972483494218 0.751871933436 5.061741364891
P -1.310935354134 0.472599860243 2.377921844820
Cl -0.994133838142 2.649634310754 2.094074406406
H 1.756940391180 0.964022420776 1.687857603264
H 1.334668224214 1.317752378471 3.932529295969
H 0.274736391036 0.963456356233 -0.297094032894
H 0.667849318956 -0.777758143777 -0.379649514845
H -1.026288311957 -0.255965452677 -0.350796373163
H -0.513221043847 0.212044542528 5.896244623004
H -0.753260348653 1.825059836745 5.165691780991
H -2.054722510346 0.606005966031 5.114123653570
H 1.478559045828 -0.424769352207 4.265675925781
H 1.912214907035 -0.787743336621 1.961797635441

**doubly hydrogenated 8b**

E(B3LYP-D3/6-31+G*) = -1070.73603531
Sum of electronic and zero-point Energies= -1070.566969
Sum of electronic and thermal Energies= -1070.556150
Sum of electronic and thermal Enthalpies= -1070.555206
Sum of electronic and thermal Free Energies=-1070.604779
C 0.008710288504 0.000229536650 -0.003137675418
N -0.000253714610 0.032423326195 1.455241935620
C 1.330938510503 0.004215073457 2.043042915225
C 1.289959842367 0.024859535646 3.572126992379
N 0.546892103948 1.147999358809 4.168373604766
C 0.432275093269 1.025695045490 5.623991491596
P 0.626913424977 2.664963367749 3.418963646262
Cl 2.369518714090 3.643503829586 4.331687250521
H 1.886352373198 0.872293040088 1.663895438195
H 2.325482101548 0.008081371802 3.950940143455
H 0.475445464056 0.918643356298 -0.379097598640
H 0.559056304320 -0.859806726808 -0.430786058081
H -1.021058221251 -0.027344790395 -0.374166955989
H 0.038093923530 0.033619563199 5.876668717050
H 1.406065191784 1.155959180837 6.119807013747
H -0.257166449397 1.780538749334 6.011157581337
H 0.808920128520 -0.898121862144 3.927899373925
H 1.918627465405 -0.888609631353 1.748753881460
H -0.562159497079 -0.731836624074 1.825446281736
H -0.286219634762 3.285148834460 4.315637562156

E(M06-2X/6-31+G*) = -1070.51166711
Sum of electronic and zero-point Energies= -1070.340675
Sum of electronic and thermal Energies= -1070.329937
Sum of electronic and thermal Enthalpies= -1070.328993
Sum of electronic and thermal Free Energies=-1070.378345
C 0.022409929929 0.046436500397 0.030599280743
N 0.007777869145 0.063466963927 1.484003753126
C 1.336664471478 -0.014063235714 2.058807185449
C 1.289790849578 -0.002486898294 3.581295527755
N 0.530680666947 1.112577407674 4.150461560620
C 0.454239548308 1.037687159808 5.603763377630
P 0.591319927721 2.603692634998 3.368027237827
Cl 2.281832230248 3.584689924776 4.285326732782
H 1.912620153759 0.845676715630 1.690066298647
H 2.321297403115 -0.003453187127 3.969895502353
H 0.515200974453 0.956615360878 -0.327700959911
H 0.552692624576 -0.821244677895 -0.398770775519
H -1.003515327710 0.051066602174 -0.346073906614
H 0.082955649325 0.048959434311 5.895685296585
H 1.437535986367 1.199978954121 6.068351776320
H -0.237721112414 1.795308453557 5.978987758479
H 0.813661613019 -0.928086897020 3.935537569614
H 1.893828712877 -0.917782110917 1.749420587779
H -0.573561803035 -0.689262525881 1.845944432926
H -0.333316954764 3.222676955423 4.242817304714

**8c**

E(B3LYP-D3/6-31+G*) = -1108.88130847
Sum of electronic and zero-point Energies= -1108.702937
Sum of electronic and thermal Energies= -1108.692547
Sum of electronic and thermal Enthalpies= -1108.691603

Sum of electronic and thermal Free Energies=-1108.738638
C 0.001024694653 0.011157834658 -0.001258343171
N -0.008944256648 -0.036075321326 1.464169372029
C 1.336975940488 -0.008389571893 2.054023598695
C 1.303932518679 -0.364637523739 3.539229462719
C 0.400634189472 0.572299002078 4.339256522326
N -0.975487744316 0.563317757465 3.823111964194
C -1.934651405060 1.211512457884 4.722919281499
P -1.297561280287 0.805570374546 2.175954005440
Cl -0.578946862008 2.945960016024 1.926533126251
H 1.949004987399 -0.740033445857 1.512122390964
H 1.791897622677 0.984559710871 1.902247586755
H 0.950040285884 -1.396105874626 3.656330519988
H 2.322341421898 -0.309570727241 3.942512354789
H 0.362000359700 0.244190635464 5.385388131336
H 0.798452995580 1.600657859979 4.326801334580
H 0.521539503048 -0.872687323054 -0.388116125363
H -1.024553239937 -0.000146602720 -0.384326054138
H 0.502992395928 0.916255444281 -0.375964735973
H -2.937432107457 1.186087143686 4.284212885558
H -1.962512433802 0.667701317011 5.674376256473
H -1.665675990784 2.261089712960 4.916873252814

**doubly hydrogenated 8c**

E(B3LYP-D3/6-31+G*) = -1110.05520609
Sum of electronic and zero-point Energies= -1109.856841
Sum of electronic and thermal Energies= -1109.844920
Sum of electronic and thermal Enthalpies= -1109.843976
Sum of electronic and thermal Free Energies=-1109.896083
C -0.073180401697 -0.129986184007 0.073168009823
N 0.005819533790 -0.065106885878 1.533704418758
C 1.380927816237 0.000353305667 2.059586035253
C 2.047299120292 -1.379395631445 2.189155960028
C 1.713030879660 -2.126924410429 3.489311921454
N 0.277520848209 -2.293177071139 3.723828211983
C -0.381881487912 -3.214024522818 2.800589619111
P -1.343045594696 0.505574628758 2.364560462426
Cl -1.049505560574 2.673302223239 2.565315507227
H 1.973284524138 0.642837893628 1.391309816585
H 1.364974087241 0.497261047533 3.033933917166
H 1.796624168463 -1.995662317485 1.316408448796
H 3.137874445355 -1.249152535507 2.159740820113
H 2.248367339838 -3.097804835544 3.476192104384
H 2.113829690556 -1.550901659330 4.333915171756
H 0.510936133021 -0.981263150164 -0.297044343251
H -1.111946648058 -0.269010918837 -0.239883007872
H 0.317199726757 0.786724588485 -0.395093697536
H -1.410854530225 -3.384466421406 3.134263006695
H -0.429129168709 -2.762166718985 1.804926696195
H 0.125246820518 -4.193827297005 2.713293118435
H 0.133929753119 -2.609558446950 4.679988785155
H -0.840534965598 0.234072709348 3.659645189830

E(M06-2X/6-31+G*) = -1109.80672439
Sum of electronic and zero-point Energies= -1109.606597
Sum of electronic and thermal Energies= -1109.594736
Sum of electronic and thermal Enthalpies= -1109.593792
Sum of electronic and thermal Free Energies=-1109.645827
C -0.075319890229 -0.165283146831 0.106509191950
N 0.001041783917 -0.104092469310 1.560993154851
C 1.368152904977 -0.012118103031 2.081152276573
C 2.051059673893 -1.378980438656 2.183983049047
C 1.717557727128 -2.128767391882 3.475893896803
N 0.282877143581 -2.255624212157 3.708616469802
C -0.377366613523 -3.157398012646 2.774361913191
P -1.337200067695 0.481146178117 2.380445797266
Cl -1.018708751037 2.612032872019 2.504687302232
H 1.944964522021 0.656279436586 1.425294235898
H 1.340114415448 0.460723018054 3.068223163591
H 1.793753945455 -1.987878084473 1.307920216587
H 3.139127340584 -1.244161673015 2.149271097522
H 2.222272574391 -3.112973004741 3.452003895561
H 2.137426970893 -1.568161704676 4.320129025945
H 0.541512826700 -0.991000884677 -0.266311564573
H -1.107965561814 -0.343800012345 -0.204570098659
H 0.278331254970 0.768010243180 -0.355492196290
H -1.408558062382 -3.323434162940 3.098293542926
H -0.412592104862 -2.692797230043 1.783947952278
H 0.125462883398 -4.136074687045 2.682771274811
H 0.130894528939 -2.582591045642 4.658995291303
H -0.830052915025 0.244641905884 3.673697283900