Electronic Supplementary Material (ESI) for Chemical Science.

Supplementary Information

Dynamic-Dependent Selectivity in a Bisphosphine Iron Spin Crossover C-H Insertion/π-Coordination Reaction

Michael T. Davenport, Justin K. Kirkland, and Daniel H. Ess*

Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84604, United States

AUTHOR INFORMATION

Corresponding Author

*E-mail: dhe@chem.byu.edu

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1. Additional Computational Details

Geometry optimization and frequency calculations on local minima and transition-state structures were performed using density functional theory (DFT) with the Gaussian 16 software.[1] Unrestricted M06-L/6-31G**[LANL2DZ for Fe][2-4] was used to optimize structures and M06-L/def2-TZVP was used for single point energy evaluations. Continuum PCM solvation for mesitylene was included.[5]

Minimum energy crossing points (MECPs) with a degenerate open-shell singlet and triplet structure were located using MECPro 1.0.6.[6] MECPro interfaces with Gaussian 16. MECPs were optimized using PCM(mesitylene)-UM06-L/6-31G**[LANL2DZ for Fe].

Variational transition states (VTS) were optimized using the reaction-path variational transition state theory (RP-VTST). These calculations were performed using the Polyrate 17 program.[7] The program obtained energies, gradients, and Hessians from Gaussian 16 at the UM06-L/6-31G**[LANL2DZ for Fe] level of theory. Interface of these programs was done using the Gaussrate 17B program.

All metadynamics ab initio molecular dynamics simulations were performed using the QUICKSTEP module of CP2K 7.1 software package.[8] CP2K version 7.1 does not have the M06-L functional and therefore we used the PBE exchange-correlation functional.[9] The Gaussian/plane-wave basis function used was GTH-PBE/DZVP-MOLOPT-SR-GTH.[10] We used coordination number (CN) as the collective variable (CV), $CN = [1-(d/d_0)^6]/[1-(d/d_0)^{12}]$, where d is the distance between two atoms and d_0 is the reference distance.[11] The first collective, CN1, followed the breaking C-H bond distance (d_0 = 1.3 Å) and the second collective variable, CN2, followed bond forming coordinate between the leaving hydrogen and Fe (d_0 = 1.6 Å). The Gaussian potential hills with a height of 0.24 kcal/mol, and width of 0.1 were added to the potential every 50 steps to sample the free energy profile.

Quasiclassical direct dynamics simulations were initialized with normal mode and thermal sampling and propagated with the Verlet algorithm using Milo 1.0.1.[12] Milo interfaces with Gaussian 16 and energies and forces were calculated using PCM(mesitylene)-UM06-L/6-31G**[LANL2DZ for Fe]. Trajectories were sampled at the experimental temperature of 245.15 K. All trajectories were propagated in both forward and reverse directions.

To propagate adiabatic mixed spin trajectories, we implemented Truhlar's two state spin mixing model in our Milo program. The mixed spin energy and mixed spin gradients are defined in equations 1-3.[13]

$$E_{mixed} = min\left\{eigenvalue\begin{pmatrix} E_1 & \chi \\ \chi & \mathrm{E}_2 \end{pmatrix}\right\} \quad \textbf{(1)}$$

$$\mathrm{G}_i = \frac{\delta E_{mixed}}{\delta q_i} = \frac{(1-A)}{2}\frac{\delta E_1}{\delta q_i} + \frac{(1+A)}{2}\frac{\delta E_2}{\delta q_i} \quad \textbf{(2)}$$

$$A = \frac{(E_1 - E_2)}{\sqrt{4\chi^2 + (E_1 - E_2)^2}} \quad \textbf{(3)}$$

Where E_1 and E_2 are the energies from the two spin states, χ is the coupling constant, and A is based on the minimum eigenvalue from the mixed energy.

2. Additional Potential Energy Landscapes

Figure S1 shows the potential-energy surface for the singlet and triplet spin states for methane dissociation from $(DMPE)_2Fe(H)(CH_3)$ and formation of the weak coordinated solvent mesitylene.

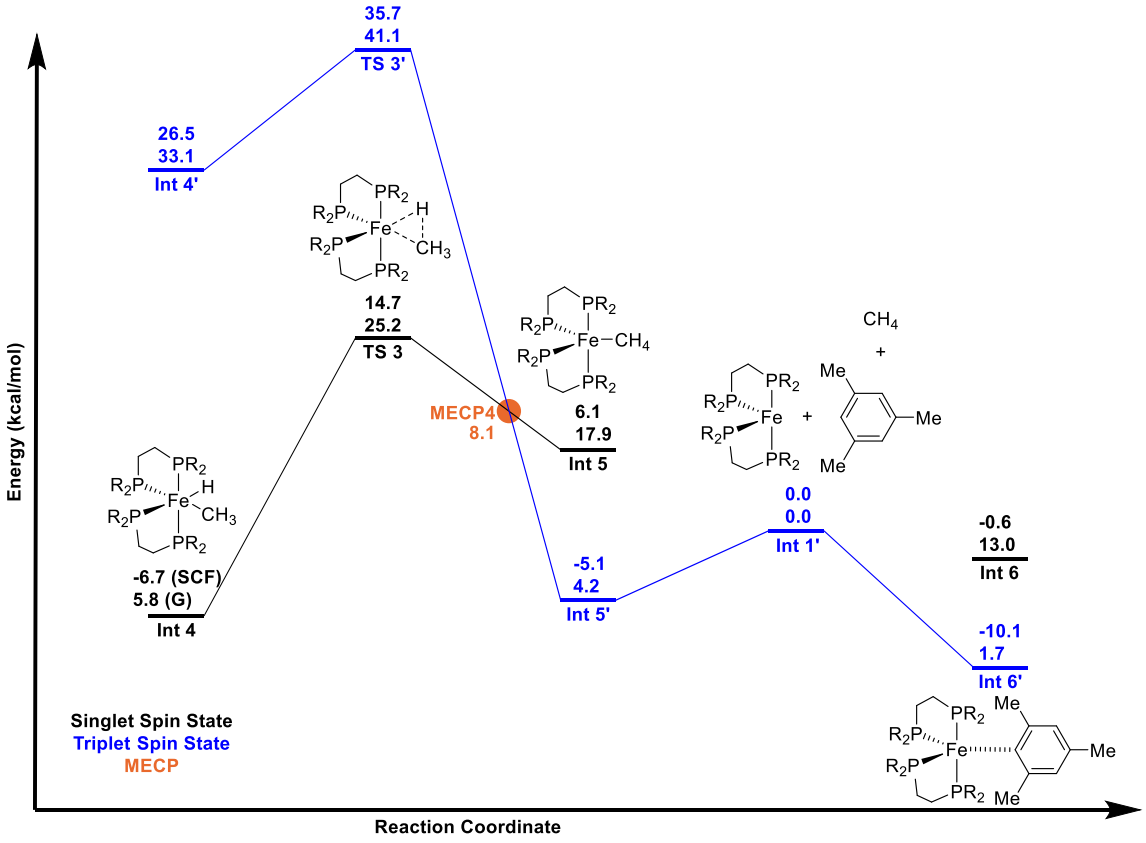

Figure S1. M06-L potential energy landscapes for reaction methane dissociation from $(DMPE)_2Fe(H)(CH_3)$ and mesitylene coordination to $(DMPE)_2Fe$. Black numbers and lines represent unrestricted singlet spin-state energies. Blue numbers and lines represent unrestricted triplet spin-state energies. The orange dot is the MECP. Energies are reported in kcal/mol. R = Me.

Figure S2 shows the potential-energy surface with *cis* and *trans* $(DMPE)_2Fe(H)(C_2H_3)$. Figure S2 also shows an estimate of the barrier for C-H activation/hydrogen atom transfer with *trans*-$(DMPE)_2Fe$.

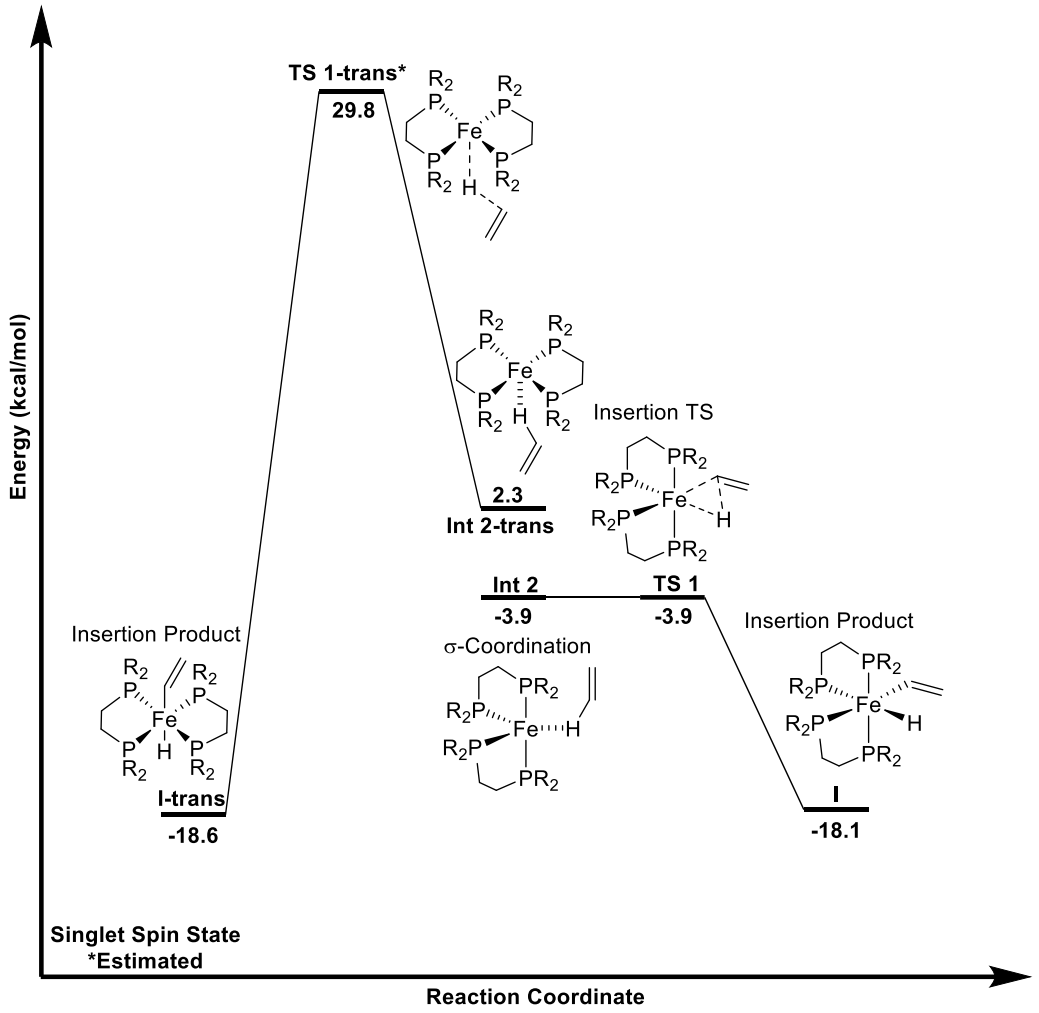

Figure S2. M06-L potential energy landscapes with *cis* and *trans* $(DMPE)_2Fe(H)(C_2H_3)$. TS 1-trans has restrained C-H and H-Fe bonds fixed at 1.5 Å and 1.7 Å, respectively. Energies are reported in kcal/mol relative to $(DMPE)_2Fe$ on the triplet spin state (R = Me).

3. Potential Energy Scan

Figure S3 plots the scan of $(DMPE)_2Fe(\eta^2\text{-}C_2H_4)$ **II** and shows no potential energy barrier for forming **II**.

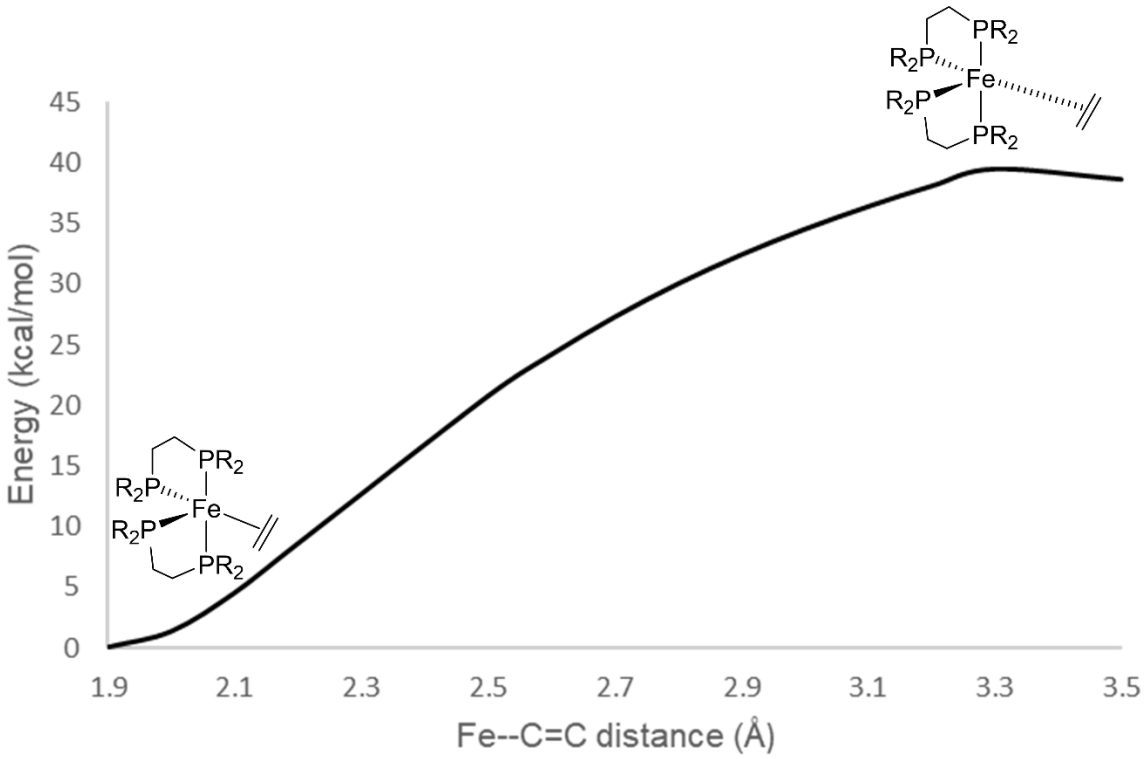

Figure S3. Potential energy scan of Fe-ethylene distance (Å) versus energy (kcal/mol).

4. Spin Orbit Coupling Calculations

RASSI calculations were performed using the output from CASPT2(18,11)/ANO-RCC-MB calculations at the singlet and triplet states to determine the spin-orbit coupling (SOC) between these two states. The overall value was obtained as the root sum of squares as shown below. The SOC value was calculated to be 0.821 kcal/mol. If we assume that the spin-orbit coupling parameter stabilize and destabilize equally in both directions, then the value will become 0.411 kcal/mol.[13] Figure S4 shows the 11 orbitals used in the CASSCF/CASPT2 calculations and contain a mixture of p and d orbitals from the iron, as well as p-orbital contribution from the phosphorus atoms, and the π/π* orbitals from the ethylene. The fractional occupancy is given as well for the singlet/triplet states.

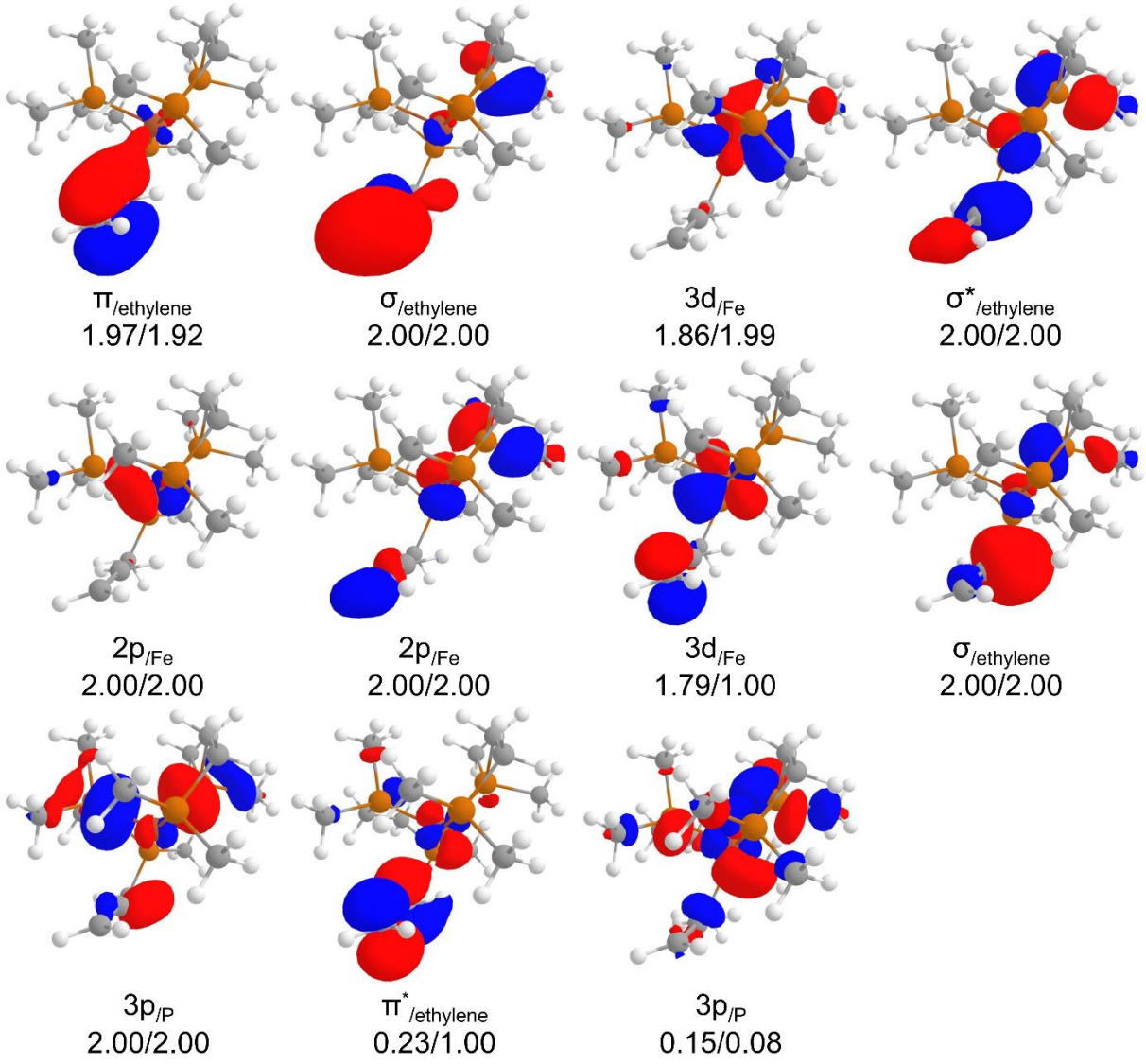

Figure S4. Orbitals that were generated by CASPT2 to calculate the spin orbit coupling. The first row visualizes the orbitals with the second describing the type of orbitals with the third row giving the occupancy of electrons for the singlet and triplet, respectively.

$$SOC = \sqrt{\sum_{i=-1}^{1} s_i^2} \quad \textbf{(4)}$$

$$s_{-1} = 171.852\ cm^{-1} \quad \textbf{(5)}$$
$$s_0 = 152.981\ cm^{-1}$$
$$s_1 = 171.\ 852 cm^{-1}$$

$$SOC = 0.821\ kcal/mol \quad \textbf{(6)}$$

5. Variational Transition State Theory Energy Profile

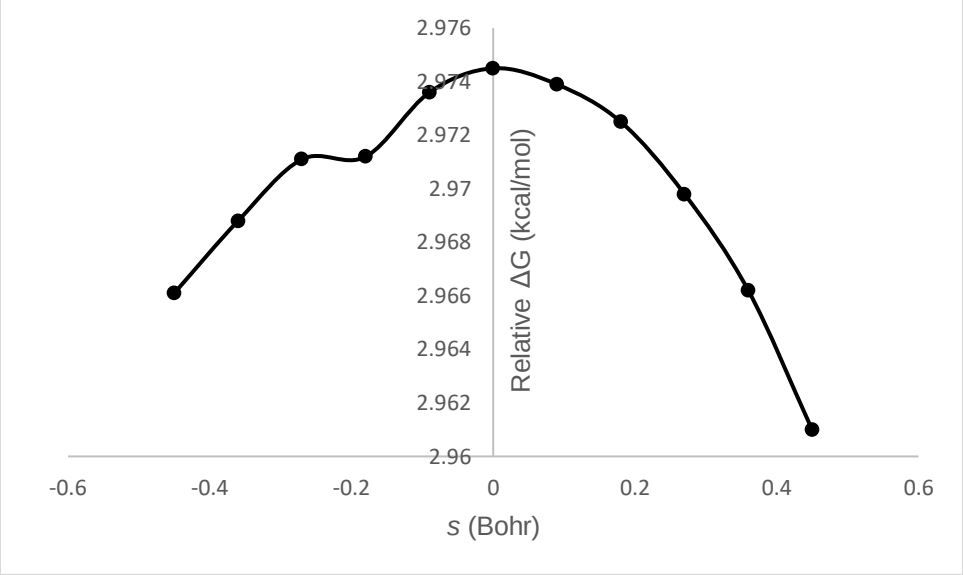

Figure S5. Relative free energy profile of **TS 2'** transition state calculated using Polyrate.

6. Mixed Spin Dynamics

Figure S6 plots mixed spin trajectories starting at **MECP2** (Figure S6a) and **MECP3** (Figure S6b) going forwards (left) and reverse (right).

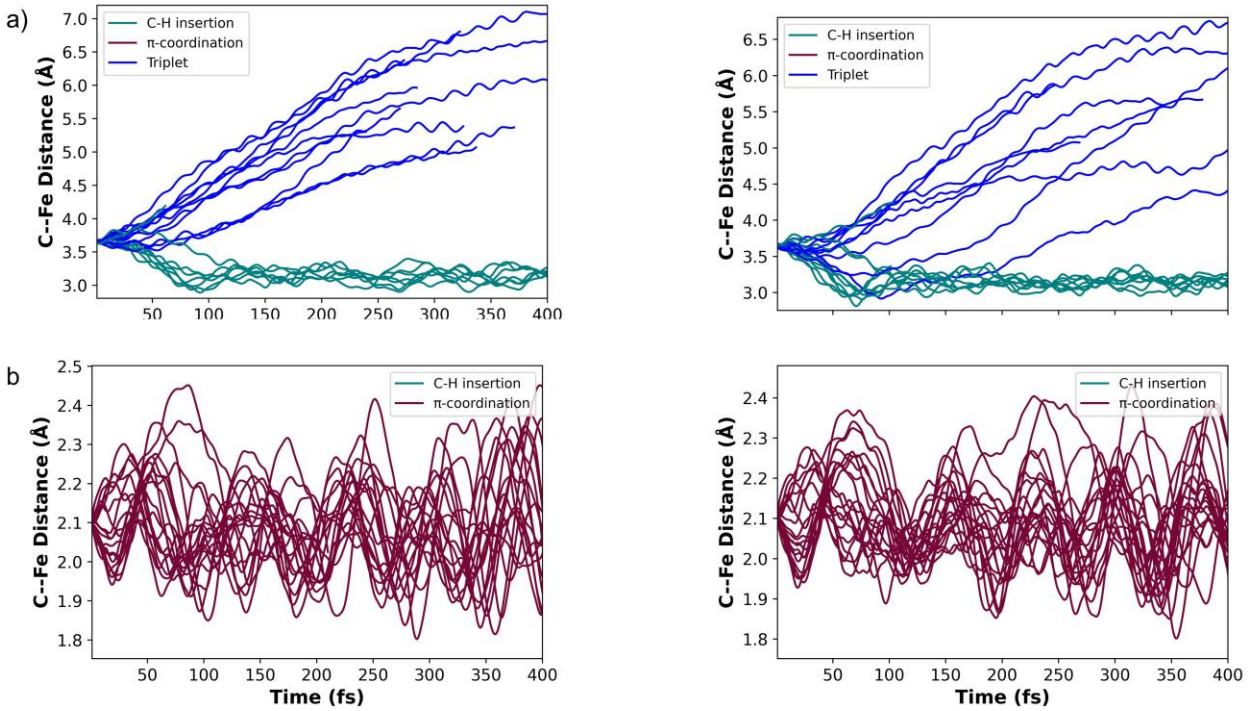

Figure S6. Plot of Fe-ethylene distance (Å) versus time (fs) for mixed spin surface forward (left) and reverse (right) direction trajectories starting from a) **MECP2** b) **MECP3**. The Fe-ethylene distance was measured from the distal carbon on ethylene to Fe. Trajectories plotted in teal color end at the insertion product **I**, trajectories plotted in burgundy end at the π-coordination structure **II**, and trajectories in blue form neither product **I** nor **II** and stays in the triplet state.

Figure S7 plots mixed spin trajectories starting at structure **C**. With no additional translation energy given to ethylene only one trajectory formed a product (Figure S7a). The other trajectories were repealed by the Fe metal center. Figures S7b and S7c show trajectories with 10 kcal/mol and 20 kcal/mol of added translational energy of ethylene (in the direction of the Fe metal center). This shows that increasing the translational energy only generated the π-coordination structure **II** on the singlet surface.

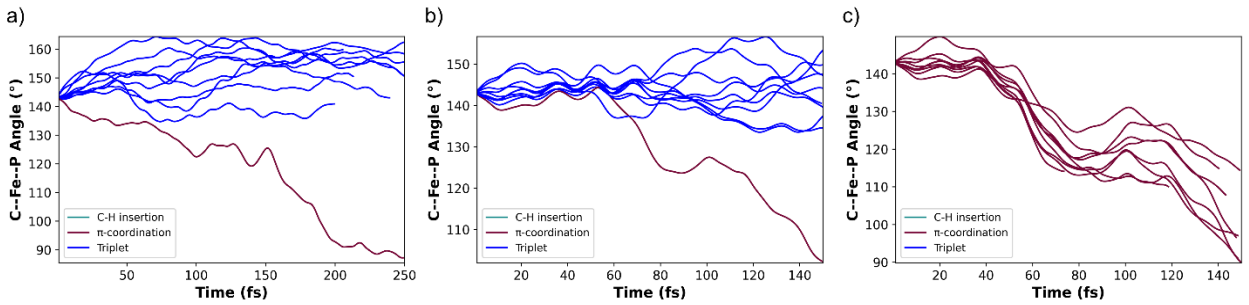

Figure S7. Plot of Fe-ethylene angle (°) versus time (fs) for mixed spin surface forward (left) and reverse (right) direction trajectories starting from the constraint optimized metadynamics structure **C**. The Fe-ethylene angle (°) was measured from the distal carbon on ethylene, Fe metal, and phosphine. a) Plot of trajectories with no added translational energy. b) Plot of trajectories with 10 kcal/mol of translational energy added to ethylene. c) Plot of trajectories with 20 kcal/mol of translational energy added to ethylene. Trajectories plotted in burgundy end at the π-coordination structure **II** in the singlet state. Blue trajectories stay on the triplet spin state surface. If the angle (°) becomes less than 130°**,** the spin state switched to be a singlet spin state leading to **II.** The y-axis is scaled for visual clarity.

7. Additional Trajectories

Figure S8 plots singlet spin trajectories starting at **TS1** (figure S8a) and **MECP3** (figure S8b) going forwards (left) and reverse (right). **TS1** forms **I** in the forward and reverse direction showed initial motion towards **Int 2** but reverted to the forward direction. **MECP3** resulted in the formation of **II** in both directions.

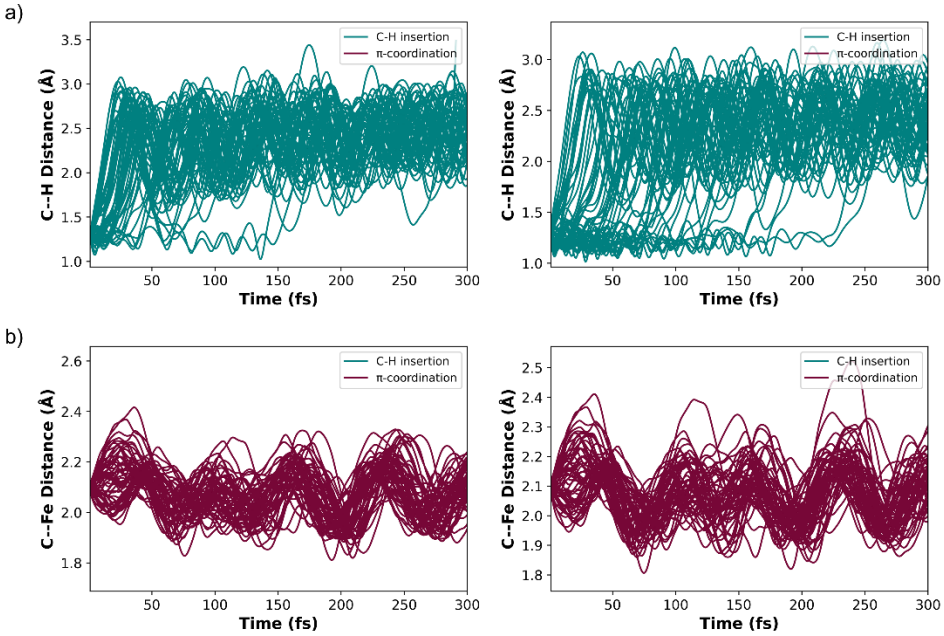

Figure S8. Plot of Fe-ethylene distance (Å) versus time (fs) for singlet surface forward (left) and reverse (right) direction trajectories starting from a) **TS 1** and b) **MECP3**. The Fe-ethylene distance was measured as the distance from the distal carbon on ethylene to the Fe. Trajectories plotted in teal color end at the insertion product **I** and trajectories plotted in burgundy end at the π-coordination structure **II**. The y-axis is scaled for visual clarity.

8. Energies and Cartesian Coordinates of Structures

Geometries optimized at PCM(mesitylene)-UM06L/6-31G**[LAML2DZ for Fe]

1. $(DMPE)_2Fe$

Charge = 0 Multiplicity = 1

Zero-point correction= 0.420804 (Hartree/Particle)
Thermal correction to Energy= 0.439974
Thermal correction to Enthalpy= 0.440750
Thermal correction to Gibbs Free Energy= 0.380103
Sum of electronic and zero-point Energies= -1964.949286
Sum of electronic and thermal Energies= -1964.930116
Sum of electronic and thermal Enthalpies= -1964.929340
Sum of electronic and thermal Free Energies= -1964.989987

Fe	-0.721469000000	-1.559543000000	1.294121000000
P	-0.702387000000	-0.303644000000	-0.511685000000
P	-0.890992000000	-3.281755000000	-0.027624000000
P	-2.685785000000	-1.187553000000	2.176928000000
P	-0.103297000000	-2.421890000000	3.223845000000
C	-1.629482000000	-2.652623000000	4.270562000000
C	-2.574980000000	-1.489108000000	4.020921000000
H	-1.369439000000	-2.767736000000	5.330882000000
H	-2.091630000000	-3.595033000000	3.946097000000
H	-2.171828000000	-0.571667000000	4.469767000000
H	-3.567031000000	-1.653244000000	4.461530000000
C	-1.012244000000	-2.708654000000	-1.813739000000
C	-1.540971000000	-1.283290000000	-1.856134000000
H	0.002439000000	-2.740148000000	-2.231289000000
H	-1.619354000000	-3.398912000000	-2.412059000000
H	-1.401951000000	-0.814170000000	-2.839408000000
H	-2.615766000000	-1.262460000000	-1.630764000000
C	-4.189032000000	-2.205305000000	1.800043000000

H	-5.053366000000	-1.903196000000	2.403377000000
H	-4.449998000000	-2.105516000000	0.741868000000
H	-3.976911000000	-3.260820000000	1.990265000000
C	-3.519817000000	0.465072000000	2.196873000000
H	-3.933145000000	0.684305000000	1.207659000000
H	-4.339273000000	0.503213000000	2.924429000000
H	-2.793437000000	1.246866000000	2.436130000000
C	0.941456000000	-1.409593000000	4.367603000000
H	1.045547000000	-1.872749000000	5.356028000000
H	1.936363000000	-1.275602000000	3.935423000000
H	0.497750000000	-0.417007000000	4.483918000000
C	0.701301000000	-4.063060000000	3.473401000000
H	1.688331000000	-4.073979000000	3.003289000000
H	0.815228000000	-4.306180000000	4.535962000000
H	0.095398000000	-4.841496000000	2.999955000000
C	0.513788000000	-4.476020000000	-0.207533000000
H	0.389523000000	-5.135142000000	-1.075253000000
H	1.450129000000	-3.919917000000	-0.314139000000
H	0.597720000000	-5.097096000000	0.688607000000
C	-2.264613000000	-4.524624000000	0.014460000000
H	-2.314393000000	-4.989095000000	1.004791000000
H	-3.219942000000	-4.025185000000	-0.166787000000
H	-2.130498000000	-5.312419000000	-0.736032000000
C	0.926101000000	0.040334000000	-1.320061000000
H	0.812729000000	0.468604000000	-2.323297000000
H	1.501331000000	0.737099000000	-0.705029000000
H	1.502695000000	-0.886512000000	-1.390691000000
C	-1.497572000000	1.342219000000	-0.754674000000

H	-1.403940000000	1.690790000000	-1.789340000000
H	-2.558481000000	1.280368000000	-0.499622000000
H	-1.038986000000	2.081409000000	-0.092716000000

1. $(DMPE)_2Fe$

Charge = 0 Multiplicity = 3

Zero-point correction= 0.420322 (Hartree/Particle)
Thermal correction to Energy= 0.439681
Thermal correction to Enthalpy= 0.440457
Thermal correction to Gibbs Free Energy= 0.378641
Sum of electronic and zero-point Energies= -1964.964898
Sum of electronic and thermal Energies= -1964.945539
Sum of electronic and thermal Enthalpies= -1964.944763
Sum of electronic and thermal Free Energies= -1965.006579

Fe	-0.695315000000	-1.540114000000	1.302614000000
P	-0.661793000000	-0.286090000000	-0.527433000000
P	-0.909601000000	-3.288476000000	-0.029256000000
P	-2.705311000000	-1.203358000000	2.169447000000
P	-0.077474000000	-2.395247000000	3.260993000000
C	-1.626151000000	-2.655281000000	4.265633000000
C	-2.583200000000	-1.500742000000	4.013969000000
H	-1.388984000000	-2.782001000000	5.330228000000
H	-2.069290000000	-3.598226000000	3.916981000000
H	-2.188687000000	-0.578857000000	4.461875000000
H	-3.571928000000	-1.674763000000	4.458113000000
C	-1.060892000000	-2.697010000000	-1.809142000000
C	-1.561948000000	-1.260705000000	-1.834647000000
H	-0.058696000000	-2.747271000000	-2.254278000000
H	-1.697746000000	-3.369998000000	-2.395890000000
H	-1.446550000000	-0.797575000000	-2.824110000000

H	-2.627846000000	-1.218257000000	-1.573143000000
C	-4.207329000000	-2.228532000000	1.807153000000
H	-5.069687000000	-1.928042000000	2.414160000000
H	-4.475329000000	-2.135393000000	0.750082000000
H	-3.989105000000	-3.282282000000	2.001190000000
C	-3.546797000000	0.446194000000	2.191116000000
H	-3.955117000000	0.665000000000	1.199428000000
H	-4.369848000000	0.483366000000	2.914645000000
H	-2.823397000000	1.229969000000	2.433969000000
C	0.927108000000	-1.402179000000	4.457281000000
H	1.005168000000	-1.884401000000	5.438792000000
H	1.933703000000	-1.253500000000	4.057814000000
H	0.475229000000	-0.414325000000	4.582763000000
C	0.735343000000	-4.033767000000	3.491675000000
H	1.730524000000	-4.028091000000	3.039185000000
H	0.832067000000	-4.298143000000	4.550833000000
H	0.143249000000	-4.805160000000	2.990213000000
C	0.507411000000	-4.464047000000	-0.241632000000
H	0.380370000000	-5.117298000000	-1.113232000000
H	1.435769000000	-3.896107000000	-0.356127000000
H	0.611318000000	-5.091949000000	0.647852000000
C	-2.266422000000	-4.550138000000	0.011712000000
H	-2.296159000000	-5.029967000000	0.995560000000
H	-3.230401000000	-4.059992000000	-0.148255000000
H	-2.134058000000	-5.325017000000	-0.752454000000
C	0.944914000000	0.010447000000	-1.396648000000
H	0.806593000000	0.422552000000	-2.403334000000
H	1.554749000000	0.706360000000	-0.814689000000

H	1.501501000000	-0.928302000000	-1.471146000000
C	-1.426459000000	1.374774000000	-0.759942000000
H	-1.367686000000	1.708643000000	-1.801991000000
H	-2.476789000000	1.340969000000	-0.459585000000
H	-0.923202000000	2.110665000000	-0.127480000000

MECP1. $(DMPE)_2Fe$

Charge = 0 Multiplicity = 1/3

Zero-point correction= 0.419745 (Hartree/Particle)
Thermal correction to Energy= 0.438582
Thermal correction to Enthalpy= 0.439359
Thermal correction to Gibbs Free Energy= 0.379601
Sum of electronic and zero-point Energies= -1964.946210
Sum of electronic and thermal Energies= -1964.927373
Sum of electronic and thermal Enthalpies= -1964.926597
Sum of electronic and thermal Free Energies= -1964.986355

Fe	-2.380200000000	-1.948003000000	2.108971000000
P	-2.572478000000	-0.797763000000	0.273606000000
P	-2.475357000000	-3.681135000000	0.853571000000
P	-4.067226000000	-1.164367000000	3.163379000000
P	-1.869602000000	-2.954942000000	3.962548000000
C	-3.361571000000	-3.030449000000	5.075791000000
C	-4.095915000000	-1.707084000000	4.957296000000
H	-3.077806000000	-3.272847000000	6.108218000000
H	-3.985838000000	-3.854743000000	4.706127000000
H	-3.568998000000	-0.933384000000	5.530590000000
H	-5.119383000000	-1.752606000000	5.349885000000
C	-2.825683000000	-3.224396000000	-0.927505000000
C	-2.188813000000	-1.869952000000	-1.199069000000
H	-2.479463000000	-4.001353000000	-1.620531000000

H	-3.916424000000	-3.160882000000	-1.037524000000
H	-1.097023000000	-1.964887000000	-1.254138000000
H	-2.530424000000	-1.416498000000	-2.139264000000
C	-5.777511000000	-1.673455000000	2.650261000000
H	-6.553233000000	-1.241189000000	3.294757000000
H	-5.966742000000	-1.365515000000	1.618248000000
H	-5.849480000000	-2.764319000000	2.687840000000
C	-4.414842000000	0.641246000000	3.430987000000
H	-4.592860000000	1.142909000000	2.475127000000
H	-5.286613000000	0.810283000000	4.074594000000
H	-3.540257000000	1.112900000000	3.889513000000
C	-0.659783000000	-2.053095000000	5.033270000000
H	-0.545260000000	-2.530402000000	6.013438000000
H	0.317298000000	-2.027979000000	4.544188000000
H	-0.986636000000	-1.020111000000	5.176169000000
C	-1.221583000000	-4.667427000000	4.190790000000
H	-0.216647000000	-4.747835000000	3.767832000000
H	-1.175266000000	-4.939635000000	5.251234000000
H	-1.862832000000	-5.388805000000	3.675932000000
C	-1.026709000000	-4.818549000000	0.584298000000
H	-1.250423000000	-5.628122000000	-0.121036000000
H	-0.180502000000	-4.239707000000	0.201717000000
H	-0.715575000000	-5.261683000000	1.533876000000
C	-3.769865000000	-4.985565000000	1.099378000000
H	-3.654441000000	-5.446905000000	2.084804000000
H	-4.757702000000	-4.516789000000	1.069793000000
H	-3.725723000000	-5.774951000000	0.338566000000
C	-1.508197000000	0.680214000000	-0.016410000000

H	-1.561865000000	1.020559000000	-1.056679000000
H	-1.834946000000	1.496384000000	0.634243000000
H	-0.468439000000	0.451301000000	0.227723000000
C	-4.190499000000	-0.117932000000	-0.309395000000
H	-4.081388000000	0.415517000000	-1.260110000000
H	-4.894986000000	-0.942568000000	-0.452584000000
H	-4.623387000000	0.564249000000	0.426843000000

Int 2'.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.471984 (Hartree/Particle)
Thermal correction to Energy= 0.494884
Thermal correction to Enthalpy= 0.495660
Thermal correction to Gibbs Free Energy= 0.425889
Sum of electronic and zero-point Energies= -2043.499773
Sum of electronic and thermal Energies= -2043.476874
Sum of electronic and thermal Enthalpies= -2043.476097
Sum of electronic and thermal Free Energies= -2043.545869

Fe	1.158318000000	-2.671397000000	-0.839903000000
P	-0.016086000000	-1.009051000000	-1.750328000000
P	1.913083000000	-3.106996000000	-2.868228000000
P	-0.324481000000	-4.272904000000	-0.462785000000
P	2.574888000000	-3.774292000000	0.466639000000
C	1.874892000000	-5.484948000000	0.711377000000
C	0.366923000000	-5.381065000000	0.879609000000
H	2.359165000000	-5.994162000000	1.555192000000
H	2.116928000000	-6.055824000000	-0.195455000000
H	0.126848000000	-4.906354000000	1.841763000000
H	-0.121696000000	-6.364300000000	0.880167000000
C	0.805859000000	-2.252978000000	-4.105569000000

C	0.435825000000	-0.881801000000	-3.559872000000
H	1.274720000000	-2.187804000000	-5.096654000000
H	-0.090776000000	-2.878778000000	-4.210917000000
H	1.302569000000	-0.210350000000	-3.619514000000
H	-0.372632000000	-0.405141000000	-4.128727000000
C	-0.761021000000	-5.565964000000	-1.717870000000
H	-1.488775000000	-6.293170000000	-1.338161000000
H	-1.175104000000	-5.089486000000	-2.612606000000
H	0.145019000000	-6.101038000000	-2.016487000000
C	-2.029511000000	-4.024976000000	0.222581000000
H	-2.697590000000	-3.662482000000	-0.563726000000
H	-2.446995000000	-4.955013000000	0.626004000000
H	-2.012072000000	-3.268913000000	1.013026000000
C	2.885118000000	-3.297609000000	2.230127000000
H	3.510942000000	-4.029497000000	2.753484000000
H	3.379050000000	-2.322716000000	2.268289000000
H	1.935919000000	-3.204048000000	2.765548000000
C	4.306492000000	-4.187800000000	-0.014731000000
H	4.907480000000	-3.275762000000	-0.065663000000
H	4.778076000000	-4.878282000000	0.693734000000
H	4.310178000000	-4.646639000000	-1.007898000000
C	3.531820000000	-2.316218000000	-3.310912000000
H	3.738303000000	-2.345138000000	-4.387728000000
H	3.532146000000	-1.274618000000	-2.975573000000
H	4.345816000000	-2.825299000000	-2.786467000000
C	2.162414000000	-4.717132000000	-3.745672000000
H	2.845411000000	-5.354992000000	-3.175656000000
H	1.208553000000	-5.244336000000	-3.830642000000

H	2.575187000000	-4.579430000000	-4.751912000000
C	0.109819000000	0.772840000000	-1.279304000000
H	-0.423876000000	1.423564000000	-1.981719000000
H	-0.314216000000	0.914677000000	-0.281396000000
H	1.160685000000	1.073417000000	-1.245952000000
C	-1.853069000000	-1.138137000000	-1.852332000000
H	-2.299015000000	-0.302844000000	-2.404567000000
H	-2.125039000000	-2.076665000000	-2.345066000000
H	-2.266696000000	-1.156695000000	-0.839325000000
H	0.736878000000	-0.653550000000	1.584320000000
C	-0.177207000000	-1.183866000000	1.845486000000
H	-0.074016000000	-2.263391000000	1.940776000000
C	-1.344607000000	-0.562987000000	2.014472000000
H	-2.253889000000	-1.106381000000	2.260862000000
H	-1.444893000000	0.514269000000	1.905415000000

TS I'.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.466302 (Hartree/Particle)
Thermal correction to Energy= 0.488898
Thermal correction to Enthalpy= 0.489675
Thermal correction to Gibbs Free Energy= 0.420312
Sum of electronic and zero-point Energies= -2043.457511
Sum of electronic and thermal Energies= -2043.434914
Sum of electronic and thermal Enthalpies= -2043.434137
Sum of electronic and thermal Free Energies= -2043.503501

Fe	-0.532390000000	-1.281007000000	0.700876000000
P	-1.824162000000	-0.177348000000	-0.821665000000
P	-0.979922000000	-3.157611000000	-0.632392000000
P	-1.878256000000	-1.094070000000	2.510444000000

P	0.061669000000	-3.891935000000	3.036124000000
C	-0.866211000000	-3.004058000000	4.388786000000
C	-1.124473000000	-1.519622000000	4.155605000000
H	-0.316485000000	-3.136261000000	5.331457000000
H	-1.819297000000	-3.534255000000	4.514810000000
H	-0.182646000000	-0.959115000000	4.206193000000
H	-1.769490000000	-1.130489000000	4.955836000000
C	-1.744928000000	-2.566138000000	-2.228454000000
C	-1.496014000000	-1.074053000000	-2.420225000000
H	-1.380481000000	-3.158019000000	-3.076489000000
H	-2.823001000000	-2.757537000000	-2.154674000000
H	-0.439926000000	-0.891593000000	-2.658286000000
H	-2.095672000000	-0.668149000000	-3.245698000000
C	-3.456955000000	-2.038761000000	2.636419000000
H	-3.961670000000	-1.884654000000	3.597547000000
H	-4.132090000000	-1.733666000000	1.831803000000
H	-3.254120000000	-3.106804000000	2.511814000000
C	-2.465958000000	0.604061000000	2.895056000000
H	-3.054176000000	0.990030000000	2.058030000000
H	-3.078112000000	0.634918000000	3.803387000000
H	-1.601517000000	1.260663000000	3.021683000000
C	1.679016000000	-3.013165000000	3.138920000000
H	2.025477000000	-2.905738000000	4.173940000000
H	2.433745000000	-3.571049000000	2.576773000000
H	1.595564000000	-2.023268000000	2.679383000000
C	0.495373000000	-5.404470000000	4.010455000000
H	1.176685000000	-6.037179000000	3.435406000000
H	0.973812000000	-5.160127000000	4.966391000000

H	-0.404929000000	-5.990786000000	4.214480000000
C	0.489997000000	-4.089879000000	-1.218944000000
H	0.239285000000	-4.836973000000	-1.979351000000
H	1.218055000000	-3.381157000000	-1.624241000000
H	0.957283000000	-4.591217000000	-0.365613000000
C	-2.109826000000	-4.530604000000	-0.178823000000
H	-1.725545000000	-5.030220000000	0.714803000000
H	-3.098205000000	-4.125146000000	0.055833000000
H	-2.209911000000	-5.261573000000	-0.988110000000
C	-1.526402000000	1.562226000000	-1.355437000000
H	-2.074946000000	1.821162000000	-2.267917000000
H	-1.829498000000	2.248134000000	-0.559095000000
H	-0.458205000000	1.712671000000	-1.533615000000
C	-3.675054000000	-0.179740000000	-0.839661000000
H	-4.089564000000	0.212970000000	-1.775632000000
H	-4.041471000000	-1.201271000000	-0.695079000000
H	-4.061157000000	0.424504000000	-0.012862000000
H	0.405683000000	-0.350946000000	1.530310000000
C	1.123641000000	-0.486692000000	0.050477000000
H	1.144324000000	0.538424000000	-0.338759000000
C	2.271929000000	-1.186614000000	-0.096912000000
H	3.133326000000	-0.787625000000	-0.635407000000
H	2.389486000000	-2.198796000000	0.291659000000

I’. $(DMPE)_2Fe(H)(C_2H_3)$

Charge = 0 Multiplicity = 3

Zero-point correction= 0.467596 (Hartree/Particle)
Thermal correction to Energy= 0.490402
Thermal correction to Enthalpy= 0.491178

Thermal correction to Gibbs Free Energy= 0.421319
Sum of electronic and zero-point Energies= -2043.464391
Sum of electronic and thermal Energies= -2043.441585
Sum of electronic and thermal Enthalpies= -2043.440809
Sum of electronic and thermal Free Energies= -2043.510668

Fe	-0.839990000000	-1.787055000000	1.059987000000
H	-0.491423000000	-0.946243000000	2.347248000000
C	1.042335000000	-1.623626000000	0.496034000000
H	1.307938000000	-1.917068000000	-0.539414000000
P	-1.592756000000	-0.862015000000	-1.018341000000
P	-1.051444000000	-3.906593000000	-0.020472000000
P	-2.758107000000	-1.655738000000	2.205629000000
P	-0.423376000000	-3.947976000000	3.565178000000
C	-2.127251000000	-3.568822000000	4.227021000000
C	-2.627156000000	-2.149245000000	3.987666000000
H	-2.134643000000	-3.782462000000	5.305446000000
H	-2.814157000000	-4.295854000000	3.770122000000
H	-1.943033000000	-1.426469000000	4.449346000000
H	-3.606608000000	-2.011719000000	4.466860000000
C	-1.653374000000	-3.559148000000	-1.741447000000
C	-1.140883000000	-2.204331000000	-2.220383000000
H	-1.368242000000	-4.366089000000	-2.427840000000
H	-2.750990000000	-3.554837000000	-1.697281000000
H	-0.044493000000	-2.212821000000	-2.279446000000
H	-1.513250000000	-1.962306000000	-3.224055000000
C	-4.327580000000	-2.530379000000	1.765056000000
H	-5.167516000000	-2.213150000000	2.393347000000
H	-4.582815000000	-2.341783000000	0.717817000000
H	-4.198669000000	-3.609674000000	1.885501000000

C	-3.409851000000	0.049502000000	2.415136000000
H	-3.732975000000	0.441636000000	1.446822000000
H	-4.257926000000	0.085224000000	3.107982000000
H	-2.609151000000	0.692823000000	2.786660000000
C	0.581275000000	-2.829171000000	4.628134000000
H	0.296342000000	-2.889110000000	5.685432000000
H	1.638801000000	-3.090052000000	4.533137000000
H	0.464685000000	-1.802095000000	4.271686000000
C	-0.176395000000	-5.534336000000	4.488524000000
H	0.848463000000	-5.889538000000	4.351518000000
H	-0.366047000000	-5.429188000000	5.563674000000
H	-0.846317000000	-6.305175000000	4.095172000000
C	0.513349000000	-4.815245000000	-0.316163000000
H	0.366614000000	-5.709793000000	-0.930217000000
H	1.237158000000	-4.155150000000	-0.800096000000
H	0.932654000000	-5.104305000000	0.651689000000
C	-2.148039000000	-5.297620000000	0.465433000000
H	-1.866241000000	-5.651255000000	1.461846000000
H	-3.187964000000	-4.964006000000	0.500837000000
H	-2.072071000000	-6.135338000000	-0.235737000000
C	-0.632873000000	0.548082000000	-1.691397000000
H	-0.774906000000	0.671485000000	-2.770335000000
H	-0.930632000000	1.471790000000	-1.189365000000
H	0.425490000000	0.379124000000	-1.476558000000
C	-3.289700000000	-0.440235000000	-1.606444000000
H	-3.304008000000	-0.188369000000	-2.672637000000
H	-3.964345000000	-1.284916000000	-1.440018000000
H	-3.681620000000	0.412597000000	-1.045703000000

C	2.100776000000	-1.182356000000	1.200444000000
H	3.115734000000	-1.135742000000	0.791517000000
H	2.000565000000	-0.846695000000	2.232927000000

MECP2.

Charge = 0 Multiplicity = 1/3

Zero-point correction= 0.471763 (Hartree/Particle)
Thermal correction to Energy= 0.493408
Thermal correction to Enthalpy= 0.494184
Thermal correction to Gibbs Free Energy= 0.429069
Sum of electronic and zero-point Energies= -2043.483416
Sum of electronic and thermal Energies= -2043.461771
Sum of electronic and thermal Enthalpies= -2043.460995
Sum of electronic and thermal Free Energies= -2043.526111

Fe	0.993038000000	-2.537058000000	-0.653590000000
P	-0.191476000000	-1.053653000000	-1.777167000000
P	1.970243000000	-2.916616000000	-2.542610000000
P	-0.432657000000	-4.129101000000	-0.352548000000
P	2.434865000000	-3.738254000000	0.500924000000
C	1.867254000000	-5.511036000000	0.387343000000
C	0.361638000000	-5.534739000000	0.605575000000
H	2.406944000000	-6.150133000000	1.098753000000
H	2.114335000000	-5.863995000000	-0.621893000000
H	0.134775000000	-5.355983000000	1.665671000000
H	-0.084394000000	-6.503942000000	0.349097000000
C	0.796971000000	-2.491673000000	-3.925909000000
C	0.159009000000	-1.149643000000	-3.609490000000
H	1.300744000000	-2.495112000000	-4.901582000000
H	0.040059000000	-3.286428000000	-3.943818000000
H	0.859561000000	-0.338218000000	-3.842824000000

H	-0.749153000000	-0.959515000000	-4.193725000000
C	-1.137471000000	-5.059906000000	-1.793293000000
H	-1.785206000000	-5.888120000000	-1.480588000000
H	-1.722266000000	-4.379024000000	-2.420547000000
H	-0.329239000000	-5.461472000000	-2.411807000000
C	-2.008717000000	-3.987808000000	0.613972000000
H	-2.721735000000	-3.358584000000	0.072596000000
H	-2.473024000000	-4.965608000000	0.790731000000
H	-1.811186000000	-3.506940000000	1.576166000000
C	2.598987000000	-3.590298000000	2.342046000000
H	3.365311000000	-4.274434000000	2.721820000000
H	2.869130000000	-2.569375000000	2.624504000000
H	1.651518000000	-3.833457000000	2.831394000000
C	4.230384000000	-3.903510000000	0.109656000000
H	4.736518000000	-2.963223000000	0.345187000000
H	4.702297000000	-4.708632000000	0.684019000000
H	4.379919000000	-4.099739000000	-0.954823000000
C	3.472622000000	-1.976586000000	-3.100955000000
H	3.779331000000	-2.228625000000	-4.123904000000
H	3.268695000000	-0.903348000000	-3.042856000000
H	4.306417000000	-2.182146000000	-2.423152000000
C	2.504748000000	-4.588750000000	-3.141846000000
H	3.339280000000	-4.976432000000	-2.550675000000
H	1.679994000000	-5.302110000000	-3.055416000000
H	2.822971000000	-4.550020000000	-4.190270000000
C	0.091684000000	0.753806000000	-1.506892000000
H	-0.492483000000	1.367330000000	-2.202992000000
H	-0.174478000000	1.037980000000	-0.486006000000

H	1.154224000000	0.971536000000	-1.645376000000
C	-2.038434000000	-1.061730000000	-1.738810000000
H	-2.477526000000	-0.262311000000	-2.346208000000
H	-2.407189000000	-2.025171000000	-2.104433000000
H	-2.372467000000	-0.946155000000	-0.702930000000
H	1.036330000000	-1.037613000000	0.875770000000
C	0.218385000000	-1.334174000000	1.557691000000
H	0.399887000000	-2.212072000000	2.168143000000
C	-0.846477000000	-0.551534000000	1.797843000000
H	-1.576574000000	-0.811173000000	2.560505000000
H	-1.048714000000	0.355537000000	1.234232000000

Int 2.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.472639 (Hartree/Particle)
Thermal correction to Energy= 0.493351
Thermal correction to Enthalpy= 0.494128
Thermal correction to Gibbs Free Energy= 0.431720
Sum of electronic and zero-point Energies= -2043.497620
Sum of electronic and thermal Energies= -2043.476907
Sum of electronic and thermal Enthalpies= -2043.476131
Sum of electronic and thermal Free Energies= -2043.538539

Fe	-0.526147000000	-1.396946000000	1.338663000000
P	-1.476063000000	-0.135147000000	-0.189374000000
P	-1.096347000000	-3.069947000000	0.075569000000
P	-2.000695000000	-0.897820000000	2.867230000000
P	0.413035000000	-2.582559000000	2.935714000000
C	-0.778033000000	-2.868871000000	4.327496000000
C	-1.529797000000	-1.568341000000	4.543775000000
H	-0.259229000000	-3.220714000000	5.228096000000

H	-1.463611000000	-3.666091000000	4.011320000000
H	-0.875833000000	-0.826996000000	5.019687000000
H	-2.408259000000	-1.683823000000	5.189947000000
C	-1.816075000000	-2.460679000000	-1.545897000000
C	-1.326409000000	-1.043238000000	-1.800240000000
H	-1.568890000000	-3.143356000000	-2.366797000000
H	-2.909222000000	-2.470974000000	-1.445887000000
H	-0.262455000000	-1.045989000000	-2.068026000000
H	-1.875010000000	-0.542340000000	-2.608004000000
C	-3.727830000000	-1.568681000000	2.784929000000
H	-4.338601000000	-1.247351000000	3.636834000000
H	-4.226098000000	-1.260613000000	1.862762000000
H	-3.675157000000	-2.661591000000	2.781050000000
C	-2.391920000000	0.842606000000	3.357522000000
H	-2.834152000000	1.395376000000	2.524010000000
H	-3.085568000000	0.886564000000	4.205301000000
H	-1.462383000000	1.350443000000	3.629115000000
C	1.772160000000	-1.729379000000	3.844246000000
H	2.232990000000	-2.371050000000	4.602950000000
H	2.536746000000	-1.397227000000	3.138198000000
H	1.364133000000	-0.838415000000	4.328924000000
C	1.129644000000	-4.272134000000	2.774621000000
H	1.929861000000	-4.281440000000	2.030332000000
H	1.531658000000	-4.621514000000	3.731339000000
H	0.355323000000	-4.972437000000	2.447795000000
C	0.239764000000	-4.176231000000	-0.553870000000
H	-0.069076000000	-4.708676000000	-1.459066000000
H	1.129550000000	-3.571124000000	-0.758796000000

H	0.509484000000	-4.918204000000	0.201437000000
C	-2.355067000000	-4.355774000000	0.501703000000
H	-2.042789000000	-4.897390000000	1.400620000000
H	-3.311937000000	-3.872492000000	0.721526000000
H	-2.503240000000	-5.082098000000	-0.305943000000
C	-0.834854000000	1.540193000000	-0.596889000000
H	-1.257984000000	1.920907000000	-1.532530000000
H	-1.094441000000	2.228548000000	0.212246000000
H	0.254027000000	1.521763000000	-0.681021000000
C	-3.284455000000	0.222346000000	-0.231857000000
H	-3.545014000000	0.801477000000	-1.123827000000
H	-3.847263000000	-0.714912000000	-0.250282000000
H	-3.603540000000	0.785236000000	0.648749000000
H	0.790516000000	-0.430291000000	1.426195000000
C	1.244276000000	-1.027660000000	0.411634000000
H	1.197656000000	-0.318923000000	-0.426242000000
C	2.459448000000	-1.653869000000	0.460969000000
H	3.222827000000	-1.475703000000	-0.294561000000
H	2.723217000000	-2.383264000000	1.225104000000

TS I.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.471908 (Hartree/Particle)
Thermal correction to Energy= 0.492125
Thermal correction to Enthalpy= 0.492901
Thermal correction to Gibbs Free Energy= 0.431643
Sum of electronic and zero-point Energies= -2043.498351
Sum of electronic and thermal Energies= -2043.478134
Sum of electronic and thermal Enthalpies= -2043.477357
Sum of electronic and thermal Free Energies= -2043.538616

Fe	-0.525448000000	-1.397938000000	1.337408000000
P	-1.475098000000	-0.135222000000	-0.189650000000
P	-1.101761000000	-3.070858000000	0.073617000000
P	-2.001539000000	-0.900964000000	2.866693000000
P	0.416135000000	-2.583811000000	2.934328000000
C	-0.773679000000	-2.867610000000	4.327903000000
C	-1.525469000000	-1.566996000000	4.543316000000
H	-0.253994000000	-3.218209000000	5.228466000000
H	-1.459576000000	-3.665279000000	4.013470000000
H	-0.870336000000	-0.824056000000	5.015135000000
H	-2.401837000000	-1.681172000000	5.192513000000
C	-1.809365000000	-2.458025000000	-1.551939000000
C	-1.317910000000	-1.040211000000	-1.801159000000
H	-1.556097000000	-3.139569000000	-2.371877000000
H	-2.903202000000	-2.468500000000	-1.460388000000
H	-0.252614000000	-1.042503000000	-2.063406000000
H	-1.862634000000	-0.537869000000	-2.610623000000
C	-3.729965000000	-1.568560000000	2.790853000000
H	-4.337155000000	-1.244698000000	3.644306000000
H	-4.230414000000	-1.260076000000	1.869951000000
H	-3.680246000000	-2.661613000000	2.788043000000
C	-2.386892000000	0.841941000000	3.351629000000
H	-2.832513000000	1.392112000000	2.518193000000
H	-3.075952000000	0.890690000000	4.202824000000
H	-1.454820000000	1.348916000000	3.616103000000
C	1.777305000000	-1.730891000000	3.839116000000
H	2.239930000000	-2.372354000000	4.596840000000
H	2.539380000000	-1.399630000000	3.129946000000

H	1.370761000000	-0.839565000000	4.324373000000
C	1.129021000000	-4.275290000000	2.775898000000
H	1.928135000000	-4.289160000000	2.030549000000
H	1.531669000000	-4.622662000000	3.733086000000
H	0.352403000000	-4.974683000000	2.452656000000
C	0.233105000000	-4.182587000000	-0.547523000000
H	-0.072176000000	-4.712743000000	-1.455251000000
H	1.126423000000	-3.580555000000	-0.746348000000
H	0.494493000000	-4.926487000000	0.208757000000
C	-2.369884000000	-4.349215000000	0.493600000000
H	-2.065902000000	-4.891667000000	1.394827000000
H	-3.325099000000	-3.860007000000	0.707551000000
H	-2.517827000000	-5.075344000000	-0.314235000000
C	-0.839486000000	1.543295000000	-0.591375000000
H	-1.261876000000	1.924748000000	-1.526999000000
H	-1.103495000000	2.228537000000	0.218962000000
H	0.249628000000	1.528940000000	-0.673069000000
C	-3.284895000000	0.214121000000	-0.234326000000
H	-3.547973000000	0.789594000000	-1.127933000000
H	-3.843185000000	-0.725915000000	-0.250062000000
H	-3.606842000000	0.777987000000	0.644639000000
H	0.767379000000	-0.422124000000	1.443386000000
C	1.235729000000	-1.028222000000	0.414251000000
H	1.197858000000	-0.304543000000	-0.411815000000
C	2.451438000000	-1.652222000000	0.462771000000
H	3.224993000000	-1.452007000000	-0.277109000000
H	2.708553000000	-2.399204000000	1.212292000000

I. $(DMPE)_2Fe(H)(C_2H_3)$

Charge = 0 Multiplicity = 1

Zero-point correction= 0.472185 (Hartree/Particle)
Thermal correction to Energy= 0.492733
Thermal correction to Enthalpy= 0.493509
Thermal correction to Gibbs Free Energy= 0.431393
Sum of electronic and zero-point Energies= -2043.519560
Sum of electronic and thermal Energies= -2043.499013
Sum of electronic and thermal Enthalpies= -2043.498236
Sum of electronic and thermal Free Energies= -2043.560353

Fe	-1.012878000000	-2.232066000000	1.298592000000
H	-0.749632000000	-0.864683000000	1.982453000000
C	0.973167000000	-2.271758000000	1.023335000000
H	1.415464000000	-3.191133000000	0.607434000000
P	-1.155120000000	-1.105384000000	-0.569747000000
P	-1.302629000000	-4.060221000000	0.084824000000
P	-3.027497000000	-1.882731000000	2.129885000000
P	-0.501538000000	-3.095590000000	3.223106000000
C	-2.036516000000	-3.391153000000	4.224831000000
C	-2.957152000000	-2.208954000000	3.966385000000
H	-1.815721000000	-3.530117000000	5.290287000000
H	-2.493294000000	-4.321307000000	3.860204000000
H	-2.547411000000	-1.302994000000	4.431424000000
H	-3.964292000000	-2.354448000000	4.375972000000
C	-1.735403000000	-3.552951000000	-1.654722000000
C	-0.940024000000	-2.296625000000	-1.980434000000
H	-1.552511000000	-4.366867000000	-2.367313000000
H	-2.812553000000	-3.338489000000	-1.676353000000
H	0.132165000000	-2.527443000000	-2.037071000000
H	-1.229711000000	-1.849387000000	-2.939174000000

C	-4.570276000000	-2.826048000000	1.726221000000
H	-5.442495000000	-2.404904000000	2.237945000000
H	-4.760690000000	-2.813850000000	0.648347000000
H	-4.460966000000	-3.868679000000	2.036289000000
C	-3.761968000000	-0.192297000000	2.157043000000
H	-4.237701000000	0.037426000000	1.201097000000
H	-4.522234000000	-0.112174000000	2.941503000000
H	-2.976332000000	0.545129000000	2.338218000000
C	0.479650000000	-2.059170000000	4.372526000000
H	0.687003000000	-2.575086000000	5.315796000000
H	1.417799000000	-1.791748000000	3.880768000000
H	-0.064745000000	-1.133293000000	4.574095000000
C	0.387198000000	-4.694813000000	3.370939000000
H	1.353824000000	-4.611351000000	2.865671000000
H	0.559712000000	-4.974406000000	4.415303000000
H	-0.185261000000	-5.489999000000	2.884053000000
C	0.128469000000	-5.170912000000	-0.289368000000
H	-0.189719000000	-6.017768000000	-0.905410000000
H	0.902145000000	-4.619839000000	-0.829034000000
H	0.579922000000	-5.552928000000	0.629865000000
C	-2.571840000000	-5.362922000000	0.386819000000
H	-2.428753000000	-5.808512000000	1.376193000000
H	-3.573253000000	-4.929778000000	0.355702000000
H	-2.514755000000	-6.159353000000	-0.362662000000
C	0.032765000000	0.220132000000	-0.996628000000
H	-0.105768000000	0.559602000000	-2.028170000000
H	-0.114064000000	1.066850000000	-0.320678000000
H	1.050534000000	-0.146348000000	-0.853722000000

C	-2.710738000000	-0.261835000000	-1.097006000000
H	-2.650124000000	0.071168000000	-2.138765000000
H	-3.570455000000	-0.930341000000	-0.990430000000
H	-2.884263000000	0.614226000000	-0.467232000000
C	1.900149000000	-1.346498000000	1.334410000000
H	2.971231000000	-1.494770000000	1.165645000000
H	1.622443000000	-0.383433000000	1.768228000000

Int 3'.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.474477 (Hartree/Particle)
Thermal correction to Energy= 0.497000
Thermal correction to Enthalpy= 0.497776
Thermal correction to Gibbs Free Energy= 0.428766
Sum of electronic and zero-point Energies= -2043.498012
Sum of electronic and thermal Energies= -2043.475490
Sum of electronic and thermal Enthalpies= -2043.474713
Sum of electronic and thermal Free Energies= -2043.543723

Fe	0.147739000000	-1.746071000000	1.210922000000
P	0.094346000000	-0.669297000000	-0.738335000000
P	-0.444902000000	-3.554952000000	0.100414000000
P	-1.726318000000	-1.121721000000	2.211373000000
P	0.810875000000	-2.590960000000	3.153091000000
C	-0.723383000000	-2.792848000000	4.191746000000
C	-1.593614000000	-1.556680000000	4.029156000000
H	-0.466724000000	-2.989655000000	5.241301000000
H	-1.245152000000	-3.681137000000	3.810632000000
H	-1.119436000000	-0.698338000000	4.524539000000
H	-2.584636000000	-1.678961000000	4.484935000000
C	-1.189476000000	-3.023134000000	-1.524403000000

C	-0.348149000000	-1.888422000000	-2.088227000000
H	-1.276518000000	-3.859934000000	-2.230507000000
H	-2.206567000000	-2.675749000000	-1.300835000000
H	0.600042000000	-2.284815000000	-2.474181000000
H	-0.837614000000	-1.373681000000	-2.924532000000
C	-3.372183000000	-1.886789000000	1.826864000000
H	-4.186315000000	-1.458497000000	2.423759000000
H	-3.608831000000	-1.756974000000	0.765203000000
H	-3.322938000000	-2.961189000000	2.025852000000
C	-2.320094000000	0.626493000000	2.399938000000
H	-2.692029000000	1.006558000000	1.444517000000
H	-3.127370000000	0.702518000000	3.138039000000
H	-1.495884000000	1.271826000000	2.718452000000
C	1.882911000000	-1.652737000000	4.334117000000
H	1.948952000000	-2.140517000000	5.313662000000
H	2.890256000000	-1.556506000000	3.919692000000
H	1.490753000000	-0.640011000000	4.462728000000
C	1.564549000000	-4.262348000000	3.351591000000
H	2.559582000000	-4.280277000000	2.898874000000
H	1.654367000000	-4.550728000000	4.405069000000
H	0.949397000000	-5.005627000000	2.835799000000
C	0.957843000000	-4.592464000000	-0.529964000000
H	0.640723000000	-5.322083000000	-1.285119000000
H	1.725860000000	-3.943278000000	-0.961631000000
H	1.419998000000	-5.131381000000	0.302409000000
C	-1.602873000000	-4.930286000000	0.537970000000
H	-1.271336000000	-5.423358000000	1.457030000000
H	-2.605607000000	-4.532750000000	0.715868000000

H	-1.664205000000	-5.683872000000	-0.255814000000
C	1.533229000000	0.159780000000	-1.549265000000
H	1.304727000000	0.472332000000	-2.574964000000
H	1.827748000000	1.036877000000	-0.966625000000
H	2.385027000000	-0.526508000000	-1.568996000000
C	-1.174448000000	0.641544000000	-1.026238000000
H	-1.161967000000	1.011539000000	-2.057981000000
H	-2.168338000000	0.240515000000	-0.805094000000
H	-0.994824000000	1.481909000000	-0.348899000000
C	2.778908000000	0.936356000000	1.791756000000
H	2.787687000000	-0.088791000000	1.418676000000
C	1.624748000000	1.540551000000	2.059997000000
H	0.682595000000	1.009588000000	1.908210000000
H	3.740440000000	1.425025000000	1.930250000000
H	1.573896000000	2.560773000000	2.433775000000

TS 2’

Charge = 0 Multiplicity = 3

Zero-point correction= 0.470680 (Hartree/Particle)
Thermal correction to Energy= 0.492924
Thermal correction to Enthalpy= 0.493701
Thermal correction to Gibbs Free Energy= 0.426004
Sum of electronic and zero-point Energies= -2043.496823
Sum of electronic and thermal Energies= -2043.474580
Sum of electronic and thermal Enthalpies= -2043.473803
Sum of electronic and thermal Free Energies= -2043.541500

Fe	0.341342000000	-1.511379000000	1.232610000000
P	0.113327000000	-0.572356000000	-0.825232000000
P	-0.318976000000	-3.438803000000	0.200413000000
P	-1.530078000000	-0.838597000000	2.233551000000

P	0.928332000000	-2.468828000000	3.219911000000
C	-0.673127000000	-2.628554000000	4.163047000000
C	-1.458624000000	-1.333351000000	4.035850000000
H	-0.484544000000	-2.903715000000	5.209366000000
H	-1.229667000000	-3.457020000000	3.703446000000
H	-0.940818000000	-0.524491000000	4.570178000000
H	-2.464150000000	-1.409744000000	4.469983000000
C	-1.088887000000	-3.012670000000	-1.444608000000
C	-0.287955000000	-1.890549000000	-2.087963000000
H	-1.155465000000	-3.894196000000	-2.096926000000
H	-2.116602000000	-2.683268000000	-1.239569000000
H	0.672147000000	-2.279952000000	-2.451439000000
H	-0.800560000000	-1.455338000000	-2.955374000000
C	-3.144680000000	-1.624730000000	1.772922000000
H	-3.980895000000	-1.265313000000	2.384821000000
H	-3.373937000000	-1.428642000000	0.720478000000
H	-3.061513000000	-2.708754000000	1.894709000000
C	-2.158651000000	0.893504000000	2.443071000000
H	-2.496241000000	1.288801000000	1.480717000000
H	-2.997511000000	0.942576000000	3.147448000000
H	-1.356006000000	1.541153000000	2.806950000000
C	1.975158000000	-1.678620000000	4.534878000000
H	1.873395000000	-2.182192000000	5.502971000000
H	3.028441000000	-1.710195000000	4.241417000000
H	1.698671000000	-0.627242000000	4.657653000000
C	1.555132000000	-4.197814000000	3.395470000000
H	2.582304000000	-4.265625000000	3.026120000000
H	1.535390000000	-4.542395000000	4.435731000000

H	0.939339000000	-4.873616000000	2.793846000000
C	1.158493000000	-4.386212000000	-0.393940000000
H	0.906411000000	-5.120391000000	-1.168907000000
H	1.902927000000	-3.688596000000	-0.790247000000
H	1.621479000000	-4.910814000000	0.446895000000
C	-1.392641000000	-4.881429000000	0.654119000000
H	-1.024992000000	-5.354187000000	1.570266000000
H	-2.415277000000	-4.542596000000	0.843939000000
H	-1.422231000000	-5.640035000000	-0.137605000000
C	1.389611000000	0.364765000000	-1.789234000000
H	1.049715000000	0.607384000000	-2.802964000000
H	1.632641000000	1.300192000000	-1.275511000000
H	2.308356000000	-0.225140000000	-1.860207000000
C	-1.304616000000	0.581470000000	-1.107417000000
H	-1.420475000000	0.854497000000	-2.163111000000
H	-2.231800000000	0.116871000000	-0.757784000000
H	-1.153512000000	1.495287000000	-0.524495000000
C	2.390159000000	0.171342000000	1.633244000000
H	2.714223000000	0.143794000000	0.597621000000
C	1.363341000000	0.943141000000	2.038283000000
H	0.782819000000	1.544592000000	1.343571000000
H	2.991925000000	-0.391593000000	2.339212000000
H	1.068733000000	1.004642000000	3.083439000000

II'. $(DMPE)_2Fe(\eta^2\text{-}C_2H_4)$

Charge = 0 Multiplicity = 3

Zero-point correction= 0.472192 (Hartree/Particle)
Thermal correction to Energy= 0.494552
Thermal correction to Enthalpy= 0.495329

Thermal correction to Gibbs Free Energy= 0.426529
Sum of electronic and zero-point Energies= -2043.508406
Sum of electronic and thermal Energies= -2043.486046
Sum of electronic and thermal Enthalpies= -2043.485269
Sum of electronic and thermal Free Energies= -2043.554069

Fe	-0.133639000000	-1.962219000000	0.975939000000
P	-1.872990000000	-1.039517000000	-0.120553000000
P	-0.121628000000	-3.512358000000	-0.686855000000
P	-0.914597000000	-2.050968000000	3.101216000000
P	1.404314000000	-4.553120000000	2.958060000000
C	0.810552000000	-3.802906000000	4.561172000000
C	0.298572000000	-2.368617000000	4.475790000000
H	1.626112000000	-3.858673000000	5.296015000000
H	0.015178000000	-4.460099000000	4.936134000000
H	1.135290000000	-1.678009000000	4.305937000000
H	-0.152907000000	-2.081403000000	5.435663000000
C	-1.370449000000	-3.022617000000	-1.987833000000
C	-1.645282000000	-1.526799000000	-1.907624000000
H	-1.043567000000	-3.336149000000	-2.987094000000
H	-2.288885000000	-3.582370000000	-1.767272000000
H	-0.775277000000	-0.962021000000	-2.268802000000
H	-2.503345000000	-1.233726000000	-2.527049000000
C	-2.212777000000	-3.290538000000	3.512507000000
H	-2.476780000000	-3.288505000000	4.576594000000
H	-3.110907000000	-3.081254000000	2.924970000000
H	-1.860056000000	-4.288683000000	3.234907000000
C	-1.680254000000	-0.506570000000	3.736832000000
H	-2.530075000000	-0.234502000000	3.104626000000
H	-2.024059000000	-0.605382000000	4.772456000000

H	-0.950313000000	0.305436000000	3.679535000000
C	2.819133000000	-3.422051000000	2.606079000000
H	3.471976000000	-3.287947000000	3.477154000000
H	3.416550000000	-3.819218000000	1.780258000000
H	2.434889000000	-2.447289000000	2.291577000000
C	2.345789000000	-5.963031000000	3.702391000000
H	2.913049000000	-6.485008000000	2.927111000000
H	3.044465000000	-5.634174000000	4.481013000000
H	1.652051000000	-6.684462000000	4.142998000000
C	1.393306000000	-3.773133000000	-1.698791000000
H	1.236407000000	-4.490130000000	-2.511768000000
H	1.712721000000	-2.817064000000	-2.122801000000
H	2.201356000000	-4.136861000000	-1.057205000000
C	-0.619614000000	-5.254592000000	-0.372459000000
H	0.122099000000	-5.734913000000	0.270864000000
H	-1.574719000000	-5.265779000000	0.161532000000
H	-0.723353000000	-5.827584000000	-1.300530000000
C	-1.989405000000	0.794130000000	-0.314739000000
H	-2.702843000000	1.094512000000	-1.090432000000
H	-2.292716000000	1.250688000000	0.632382000000
H	-1.002612000000	1.192188000000	-0.570687000000
C	-3.675115000000	-1.422556000000	0.084035000000
H	-4.301796000000	-0.961685000000	-0.688798000000
H	-3.824251000000	-2.506873000000	0.057333000000
H	-4.019633000000	-1.071350000000	1.061976000000
H	1.042769000000	-0.309240000000	-0.795496000000
C	1.326556000000	-0.817673000000	0.128028000000
H	2.259744000000	-1.379396000000	0.043515000000

C	0.958871000000	-0.277746000000	1.391135000000
H	1.634425000000	-0.404377000000	2.241176000000
H	0.362068000000	0.633015000000	1.446302000000

MECP3.

Charge = 0 Multiplicity = 1/3

Zero-point correction= 0.471869 (Hartree/Particle)
Thermal correction to Energy= 0.493257
Thermal correction to Enthalpy= 0.494033
Thermal correction to Gibbs Free Energy= 0.429442
Sum of electronic and zero-point Energies= -2043.499603
Sum of electronic and thermal Energies= -2043.478215
Sum of electronic and thermal Enthalpies= -2043.477439
Sum of electronic and thermal Free Energies= -2043.542030

Fe	0.451524000000	-1.277054000000	1.313108000000
P	0.098441000000	-0.573126000000	-0.814389000000
P	-0.399105000000	-3.526993000000	0.242342000000
P	-1.515663000000	-0.757401000000	2.273105000000
P	0.920016000000	-2.435556000000	3.245383000000
C	-0.691245000000	-2.581691000000	4.169774000000
C	-1.445261000000	-1.264835000000	4.066260000000
H	-0.524590000000	-2.891511000000	5.209806000000
H	-1.262920000000	-3.385653000000	3.683500000000
H	-0.901936000000	-0.473414000000	4.600710000000
H	-2.449547000000	-1.321289000000	4.506206000000
C	-1.138979000000	-3.005163000000	-1.384450000000
C	-0.307676000000	-1.913774000000	-2.043732000000
H	-1.253177000000	-3.877951000000	-2.041287000000
H	-2.151555000000	-2.637189000000	-1.167246000000
H	0.649431000000	-2.329937000000	-2.384018000000

H	-0.806903000000	-1.503721000000	-2.931535000000
C	-3.057824000000	-1.649900000000	1.769820000000
H	-3.919480000000	-1.386343000000	2.393922000000
H	-3.301541000000	-1.422071000000	0.727158000000
H	-2.889183000000	-2.729097000000	1.839745000000
C	-2.200763000000	0.942249000000	2.451299000000
H	-2.522465000000	1.325826000000	1.479381000000
H	-3.056598000000	0.968710000000	3.134944000000
H	-1.420222000000	1.606119000000	2.831822000000
C	1.975408000000	-1.655947000000	4.545397000000
H	1.874920000000	-2.156743000000	5.514250000000
H	3.025017000000	-1.693156000000	4.241946000000
H	1.707928000000	-0.601828000000	4.663162000000
C	1.505998000000	-4.182505000000	3.403308000000
H	2.539185000000	-4.263754000000	3.054117000000
H	1.455919000000	-4.545612000000	4.436173000000
H	0.889853000000	-4.836980000000	2.778162000000
C	1.156455000000	-4.324053000000	-0.350095000000
H	0.984153000000	-4.999435000000	-1.196648000000
H	1.875409000000	-3.552586000000	-0.641827000000
H	1.606564000000	-4.894874000000	0.467438000000
C	-1.423479000000	-5.054637000000	0.512022000000
H	-1.078295000000	-5.592116000000	1.400454000000
H	-2.465193000000	-4.767981000000	0.686629000000
H	-1.394516000000	-5.741653000000	-0.342823000000
C	1.378559000000	0.341389000000	-1.780717000000
H	1.036992000000	0.577630000000	-2.794542000000
H	1.634546000000	1.276292000000	-1.273389000000

H	2.289747000000	-0.260017000000	-1.845838000000
C	-1.329493000000	0.562896000000	-1.106762000000
H	-1.439596000000	0.842614000000	-2.161222000000
H	-2.256351000000	0.086839000000	-0.770497000000
H	-1.192727000000	1.472239000000	-0.513573000000
C	2.199591000000	-0.131652000000	1.503791000000
H	2.641430000000	0.084023000000	0.531824000000
C	1.129926000000	0.663617000000	1.975498000000
H	0.723170000000	1.466148000000	1.359270000000
H	2.907652000000	-0.550615000000	2.217007000000
H	1.003511000000	0.829861000000	3.046539000000

II. $(DMPE)_2Fe(\eta^2\text{-}C_2H_4)$

Charge = 0 Multiplicity = 1

Zero-point correction= 0.476859 (Hartree/Particle)
Thermal correction to Energy= 0.496794
Thermal correction to Enthalpy= 0.497570
Thermal correction to Gibbs Free Energy= 0.436916
Sum of electronic and zero-point Energies= -2043.542665
Sum of electronic and thermal Energies= -2043.522729
Sum of electronic and thermal Enthalpies= -2043.521953
Sum of electronic and thermal Free Energies= -2043.582607

Fe	-0.434227000000	-1.394696000000	1.420540000000
P	-0.889656000000	-0.409986000000	-0.498677000000
P	-0.537505000000	-3.238162000000	0.269873000000
P	-2.281512000000	-0.801883000000	2.391290000000
P	0.008821000000	-2.442674000000	3.311721000000
C	-1.539070000000	-2.611995000000	4.321434000000
C	-2.287525000000	-1.296712000000	4.193004000000
H	-1.313647000000	-2.879250000000	5.361735000000

H	-2.124168000000	-3.435157000000	3.889769000000
H	-1.760258000000	-0.508015000000	4.745508000000
H	-3.306827000000	-1.344347000000	4.594748000000
C	-0.952869000000	-2.918267000000	-1.523107000000
C	-0.405798000000	-1.547787000000	-1.882329000000
H	-0.566351000000	-3.715807000000	-2.168954000000
H	-2.046603000000	-2.929396000000	-1.619166000000
H	0.691155000000	-1.565290000000	-1.915239000000
H	-0.761834000000	-1.183008000000	-2.854075000000
C	-3.966545000000	-1.421846000000	1.926208000000
H	-4.756613000000	-0.985902000000	2.548861000000
H	-4.188217000000	-1.201166000000	0.879217000000
H	-3.988374000000	-2.509568000000	2.045676000000
C	-2.666515000000	0.994871000000	2.580317000000
H	-2.844371000000	1.458703000000	1.605638000000
H	-3.543639000000	1.172722000000	3.212987000000
H	-1.796676000000	1.488897000000	3.022024000000
C	1.114555000000	-1.632473000000	4.550718000000
H	1.274029000000	-2.281650000000	5.417258000000
H	2.083051000000	-1.402621000000	4.097808000000
H	0.677684000000	-0.690603000000	4.891492000000
C	0.711467000000	-4.141994000000	3.461055000000
H	1.755198000000	-4.137622000000	3.133524000000
H	0.680991000000	-4.482904000000	4.501165000000
H	0.165892000000	-4.859856000000	2.843966000000
C	1.034521000000	-4.180784000000	0.004951000000
H	0.894651000000	-5.038210000000	-0.663188000000
H	1.770128000000	-3.500699000000	-0.434148000000

H	1.448764000000	-4.538301000000	0.949265000000
C	-1.696136000000	-4.647540000000	0.578046000000
H	-1.540924000000	-5.075167000000	1.572812000000
H	-2.723355000000	-4.272124000000	0.540704000000
H	-1.586383000000	-5.448449000000	-0.162346000000
C	-0.068325000000	1.155542000000	-1.009709000000
H	-0.225292000000	1.348991000000	-2.075347000000
H	-0.475491000000	1.994660000000	-0.438569000000
H	1.004926000000	1.103442000000	-0.810141000000
C	-2.609934000000	-0.026181000000	-1.052557000000
H	-2.610585000000	0.434236000000	-2.046201000000
H	-3.196166000000	-0.948267000000	-1.098198000000
H	-3.111113000000	0.652189000000	-0.357258000000
C	1.519582000000	-0.877407000000	1.197335000000
H	2.244532000000	-1.498707000000	1.732129000000
C	0.800111000000	0.141832000000	1.919292000000
H	1.003813000000	0.286226000000	2.979781000000
H	1.863601000000	-0.672687000000	0.178433000000
H	0.595736000000	1.094887000000	1.430387000000

Metadynamics A.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.473528 (Hartree/Particle)
Thermal correction to Energy= 0.493756
Thermal correction to Enthalpy= 0.494533
Thermal correction to Gibbs Free Energy= 0.431997
Sum of electronic and zero-point Energies= -2043.475039
Sum of electronic and thermal Energies= -2043.454811
Sum of electronic and thermal Enthalpies= -2043.454035
Sum of electronic and thermal Free Energies= -2043.516571

Fe	9.203303000000	8.747892000000	8.723274000000
P	7.440537000000	7.734268000000	9.355052000000

P	7.976438000000	10.583899000000	8.857969000000
P	10.414576000000	6.918368000000	8.780321000000
P	9.568043000000	8.665784000000	6.610867000000
C	9.706385000000	6.874207000000	6.095484000000
C	10.566534000000	6.114329000000	7.091197000000
H	10.083007000000	6.783718000000	5.067964000000
H	8.680958000000	6.485981000000	6.099175000000
H	11.622995000000	6.158830000000	6.800373000000
H	10.302943000000	5.052281000000	7.150583000000
C	6.322851000000	10.217231000000	9.632320000000
C	5.928409000000	8.817785000000	9.205069000000
H	6.464484000000	10.258411000000	10.719937000000
H	5.576248000000	10.978046000000	9.371057000000
H	5.085908000000	8.414089000000	9.780335000000
H	5.634344000000	8.810046000000	8.146830000000
C	10.095021000000	5.452293000000	9.861540000000
H	9.084324000000	5.061105000000	9.723170000000
H	10.809887000000	4.649093000000	9.653239000000
H	10.200884000000	5.748940000000	10.908860000000
C	12.203245000000	7.112939000000	9.203720000000
H	12.313369000000	7.489470000000	10.223751000000
H	12.730783000000	6.156972000000	9.117697000000
H	12.671883000000	7.832937000000	8.527303000000
C	11.118559000000	9.323457000000	5.817133000000
H	11.153670000000	10.411402000000	5.933320000000
H	11.996329000000	8.914227000000	6.328111000000
H	11.191039000000	9.082191000000	4.749297000000
C	8.397976000000	9.193361000000	5.273962000000

H	8.684001000000	8.740905000000	4.317426000000
H	7.378171000000	8.879666000000	5.517978000000
H	8.400034000000	10.278093000000	5.149824000000
C	8.488429000000	12.029428000000	9.881013000000
H	8.704674000000	11.711239000000	10.902377000000
H	9.395144000000	12.485513000000	9.477501000000
H	7.689197000000	12.778091000000	9.901568000000
C	7.411889000000	11.533110000000	7.373342000000
H	8.276210000000	11.885757000000	6.802957000000
H	6.814904000000	10.893104000000	6.719774000000
H	6.806664000000	12.398331000000	7.664413000000
C	7.127688000000	7.035987000000	11.053388000000
H	7.186727000000	7.847736000000	11.784564000000
H	6.146588000000	6.552193000000	11.136711000000
H	7.899090000000	6.307644000000	11.315893000000
C	6.819784000000	6.292224000000	8.365443000000
H	7.552795000000	5.480676000000	8.330703000000
H	5.879356000000	5.890932000000	8.762017000000
H	6.652922000000	6.625501000000	7.336309000000
C	11.226402000000	10.578991000000	11.083897000000
H	10.454893000000	10.511730000000	11.849447000000
C	11.074273000000	9.945921000000	9.924365000000
H	10.167550000000	9.253445000000	9.887968000000
H	12.105169000000	11.186821000000	11.365058000000
H	11.824337000000	9.948057000000	9.141762000000

Metadynamics B.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.473214 (Hartree/Particle)
Thermal correction to Energy= 0.493772
Thermal correction to Enthalpy= 0.494548
Thermal correction to Gibbs Free Energy= 0.431314
Sum of electronic and zero-point Energies= -2043.478099
Sum of electronic and thermal Energies= -2043.457542
Sum of electronic and thermal Enthalpies= -2043.456765
Sum of electronic and thermal Free Energies= -2043.520000

Fe	9.157120000000	8.836468000000	8.631001000000
P	7.438050000000	7.823274000000	9.343329000000
P	7.923770000000	10.657796000000	8.670605000000
P	10.493640000000	7.098891000000	8.741573000000
P	9.507216000000	8.696545000000	6.531974000000
C	9.672434000000	6.885029000000	6.102185000000
C	10.589870000000	6.199761000000	7.100714000000
H	10.007206000000	6.746337000000	5.065394000000
H	8.657623000000	6.476288000000	6.173278000000
H	11.631399000000	6.239976000000	6.760344000000
H	10.346361000000	5.140014000000	7.237931000000
C	6.288045000000	10.307178000000	9.501403000000
C	5.904660000000	8.877158000000	9.165685000000
H	6.454148000000	10.411302000000	10.581771000000
H	5.520611000000	11.039078000000	9.218793000000
H	5.079103000000	8.501889000000	9.783690000000
H	5.585932000000	8.803635000000	8.116956000000
C	10.312009000000	5.691226000000	9.929007000000
H	9.321794000000	5.234980000000	9.844238000000
H	11.068714000000	4.918003000000	9.756992000000
H	10.423599000000	6.064564000000	10.951587000000
C	12.289931000000	7.425503000000	9.032233000000
H	12.446875000000	7.794752000000	10.047411000000

H	12.881572000000	6.515018000000	8.885544000000
H	12.639133000000	8.194921000000	8.338225000000
C	10.961698000000	9.360317000000	5.570129000000
H	10.961371000000	10.453784000000	5.617850000000
H	11.894263000000	9.015707000000	6.028001000000
H	10.953382000000	9.055116000000	4.515783000000
C	8.216073000000	9.111050000000	5.267952000000
H	8.427101000000	8.588134000000	4.328056000000
H	7.228066000000	8.805129000000	5.626302000000
H	8.190045000000	10.182120000000	5.058287000000
C	8.507589000000	12.093153000000	9.673288000000
H	8.804018000000	11.758853000000	10.670604000000
H	9.376736000000	12.556636000000	9.198720000000
H	7.719458000000	12.847665000000	9.769837000000
C	7.328283000000	11.607032000000	7.200357000000
H	8.176092000000	11.930029000000	6.589360000000
H	6.679507000000	10.984543000000	6.580317000000
H	6.764215000000	12.491448000000	7.514736000000
C	7.195931000000	7.249912000000	11.099556000000
H	7.273948000000	8.113089000000	11.768382000000
H	6.226811000000	6.761583000000	11.261565000000
H	7.989769000000	6.551103000000	11.378976000000
C	6.833671000000	6.292801000000	8.490213000000
H	7.587415000000	5.499896000000	8.525533000000
H	5.906289000000	5.908949000000	8.932168000000
H	6.651492000000	6.525110000000	7.436485000000
C	11.059324000000	9.460369000000	11.777006000000
H	10.503128000000	8.662999000000	12.265332000000

C	10.718444000000	9.923799000000	10.577570000000
H	9.785169000000	9.524797000000	10.093707000000
H	11.925346000000	9.853193000000	12.281214000000
H	11.265106000000	10.719388000000	10.081217000000

Metadynamics C.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.472173 (Hartree/Particle)
Thermal correction to Energy= 0.494598
Thermal correction to Enthalpy= 0.495374
Thermal correction to Gibbs Free Energy= 0.427836
Sum of electronic and zero-point Energies= -2043.479005
Sum of electronic and thermal Energies= -2043.456580
Sum of electronic and thermal Enthalpies= -2043.455804
Sum of electronic and thermal Free Energies= -2043.523342

Fe	9.118144000000	8.730125000000	8.836361000000
P	7.239344000000	7.680536000000	9.205489000000
P	7.963837000000	10.601906000000	9.163807000000
P	10.455974000000	6.982842000000	9.030470000000
P	9.337664000000	8.549546000000	6.695508000000
C	9.866722000000	6.798557000000	6.314218000000
C	10.938084000000	6.394148000000	7.314637000000
H	10.209772000000	6.694582000000	5.276186000000
H	8.975577000000	6.167520000000	6.429382000000
H	11.882797000000	6.898339000000	7.070540000000
H	11.143994000000	5.316477000000	7.306395000000
C	6.203766000000	10.191779000000	9.617660000000
C	5.825579000000	8.872013000000	8.968163000000
H	6.173641000000	10.096225000000	10.710709000000
H	5.525206000000	11.011155000000	9.348399000000

H	4.883963000000	8.465621000000	9.359901000000
H	5.699804000000	9.000735000000	7.884514000000
C	9.945737000000	5.390783000000	9.816727000000
H	9.014022000000	5.026955000000	9.374782000000
H	10.712419000000	4.616968000000	9.698698000000
H	9.770337000000	5.551460000000	10.884041000000
C	12.137742000000	7.106514000000	9.790005000000
H	12.048064000000	7.221521000000	10.873669000000
H	12.738221000000	6.213294000000	9.582746000000
H	12.664382000000	7.982867000000	9.401066000000
C	10.674384000000	9.470152000000	5.789600000000
H	10.456956000000	10.542680000000	5.808598000000
H	11.633151000000	9.323825000000	6.297368000000
H	10.776582000000	9.154198000000	4.744258000000
C	8.005379000000	8.761076000000	5.429510000000
H	7.096109000000	8.239407000000	5.742527000000
H	7.760237000000	9.821796000000	5.322814000000
H	8.308761000000	8.380821000000	4.446893000000
C	8.355979000000	11.825427000000	10.490416000000
H	8.512250000000	11.301377000000	11.437013000000
H	9.279628000000	12.357577000000	10.251514000000
H	7.546654000000	12.554790000000	10.609972000000
C	7.682636000000	11.790187000000	7.773115000000
H	8.644216000000	12.149129000000	7.393530000000
H	7.174048000000	11.273272000000	6.954195000000
H	7.077607000000	12.653715000000	8.073002000000
C	6.777196000000	6.977668000000	10.861060000000
H	6.902961000000	7.745804000000	11.629269000000

H	5.745306000000	6.606229000000	10.889718000000
H	7.450740000000	6.153426000000	11.112139000000
C	6.604203000000	6.284553000000	8.165933000000
H	7.227842000000	5.393494000000	8.284414000000
H	5.574506000000	6.016258000000	8.430004000000
H	6.630972000000	6.566591000000	7.109096000000
C	11.843854000000	10.717919000000	10.511624000000
H	11.955979000000	9.851488000000	11.161150000000
C	11.317260000000	10.580526000000	9.292844000000
H	11.039786000000	9.603165000000	8.887166000000
H	12.249532000000	11.665568000000	10.920921000000
H	11.197123000000	11.421829000000	8.611406000000

Int 4.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.467531 (Hartree/Particle)
Thermal correction to Energy= 0.487128
Thermal correction to Enthalpy= 0.487905
Thermal correction to Gibbs Free Energy= 0.428192
Sum of electronic and zero-point Energies= -2005.441989
Sum of electronic and thermal Energies= -2005.422392
Sum of electronic and thermal Enthalpies= -2005.421615
Sum of electronic and thermal Free Energies= -2005.481328

Fe	-0.660887000000	-1.494894000000	1.279555000000
P	-0.814265000000	-0.351022000000	-0.563079000000
P	-0.843811000000	-3.290072000000	0.028916000000
P	-2.632686000000	-1.117170000000	2.184100000000
P	-0.085495000000	-2.445570000000	3.161375000000
C	-1.561478000000	-2.562113000000	4.292369000000
C	-2.468425000000	-1.374735000000	4.025263000000
H	-1.259985000000	-2.637966000000	5.344494000000

H	-2.076542000000	-3.498704000000	4.037667000000
H	-2.018113000000	-0.456365000000	4.423964000000
H	-3.454192000000	-1.479070000000	4.495256000000
C	-0.610330000000	-2.792533000000	-1.756009000000
C	-1.259018000000	-1.442108000000	-1.995885000000
H	0.474194000000	-2.722322000000	-1.909793000000
H	-0.982130000000	-3.572167000000	-2.432365000000
H	-0.976266000000	-0.996829000000	-2.957622000000
H	-2.353524000000	-1.536734000000	-1.990401000000
C	-4.156966000000	-2.099812000000	1.832927000000
H	-5.000304000000	-1.785559000000	2.457629000000
H	-4.438303000000	-1.976027000000	0.781984000000
H	-3.969512000000	-3.163388000000	2.001605000000
C	-3.394871000000	0.561568000000	2.211841000000
H	-3.885161000000	0.783889000000	1.261635000000
H	-4.143984000000	0.635087000000	3.007570000000
H	-2.619766000000	1.313126000000	2.382819000000
C	1.148841000000	-1.597737000000	4.229486000000
H	1.323367000000	-2.154197000000	5.155812000000
H	2.091435000000	-1.506461000000	3.683322000000
H	0.813640000000	-0.588526000000	4.475560000000
C	0.551320000000	-4.164565000000	3.329522000000
H	1.483629000000	-4.286465000000	2.772916000000
H	0.736643000000	-4.407427000000	4.381150000000
H	-0.179124000000	-4.876136000000	2.935291000000
C	0.399235000000	-4.654901000000	0.056258000000
H	0.365345000000	-5.216850000000	-0.883396000000
H	1.399825000000	-4.234243000000	0.183350000000

H	0.213742000000	-5.354281000000	0.873327000000
C	-2.365672000000	-4.333056000000	-0.109592000000
H	-2.590025000000	-4.785456000000	0.861997000000
H	-3.223057000000	-3.716771000000	-0.392389000000
H	-2.248062000000	-5.134873000000	-0.846899000000
C	0.743431000000	0.438286000000	-1.128921000000
H	0.617129000000	1.001398000000	-2.059845000000
H	1.099720000000	1.112586000000	-0.345625000000
H	1.503844000000	-0.333843000000	-1.265996000000
C	-1.987320000000	1.040606000000	-0.829223000000
H	-1.837927000000	1.503906000000	-1.810017000000
H	-3.014971000000	0.671419000000	-0.771080000000
H	-1.855637000000	1.804532000000	-0.058374000000
H	0.840156000000	-1.667649000000	0.895398000000
C	-0.092482000000	0.354565000000	2.129009000000
H	-0.478745000000	0.523003000000	3.146616000000
H	1.000930000000	0.399264000000	2.192322000000
H	-0.413457000000	1.238304000000	1.555114000000

Int 4’.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.461817 (Hartree/Particle)
Thermal correction to Energy= 0.483660
Thermal correction to Enthalpy= 0.484437
Thermal correction to Gibbs Free Energy= 0.417332
Sum of electronic and zero-point Energies= -2005.396714
Sum of electronic and thermal Energies= -2005.374871
Sum of electronic and thermal Enthalpies= -2005.374094
Sum of electronic and thermal Free Energies= -2005.441199

Fe	-0.401742000000	-1.142673000000	1.481003000000

P	-0.636343000000	-0.283641000000	-0.513435000000
P	-1.309054000000	-3.744391000000	-0.126136000000
P	-2.648284000000	-1.093423000000	2.308096000000
P	0.103805000000	-2.164478000000	3.358112000000
C	-1.418458000000	-2.424562000000	4.401840000000
C	-2.422527000000	-1.312158000000	4.139800000000
H	-1.158312000000	-2.507687000000	5.464320000000
H	-1.840844000000	-3.393133000000	4.102046000000
H	-2.040147000000	-0.356693000000	4.520404000000
H	-3.385204000000	-1.496316000000	4.633229000000
C	-0.649939000000	-2.862768000000	-1.631681000000
C	-1.238978000000	-1.469543000000	-1.808677000000
H	0.437305000000	-2.795844000000	-1.503373000000
H	-0.832174000000	-3.483145000000	-2.519567000000
H	-1.014220000000	-1.064119000000	-2.804400000000
H	-2.335079000000	-1.500701000000	-1.726410000000
C	-4.004924000000	-2.292612000000	1.962075000000
H	-4.879717000000	-2.128379000000	2.600666000000
H	-4.310764000000	-2.202392000000	0.915042000000
H	-3.640314000000	-3.313648000000	2.104014000000
C	-3.580075000000	0.487675000000	2.271634000000
H	-4.040196000000	0.634460000000	1.291125000000
H	-4.370611000000	0.509745000000	3.029340000000
H	-2.885985000000	1.312946000000	2.449427000000
C	1.238455000000	-1.319948000000	4.532170000000
H	1.376270000000	-1.895011000000	5.453573000000
H	2.211849000000	-1.174543000000	4.056753000000
H	0.841195000000	-0.332040000000	4.777827000000

C	0.808066000000	-3.860432000000	3.379051000000
H	1.801333000000	-3.851041000000	2.923564000000
H	0.884831000000	-4.261372000000	4.395736000000
H	0.172945000000	-4.519963000000	2.781401000000
C	-0.065488000000	-5.105234000000	-0.064596000000
H	0.101156000000	-5.559411000000	-1.048128000000
H	0.881650000000	-4.698310000000	0.301369000000
H	-0.388149000000	-5.889205000000	0.626373000000
C	-2.705133000000	-4.659402000000	-0.940005000000
H	-3.186418000000	-5.328625000000	-0.220790000000
H	-3.465180000000	-3.947414000000	-1.277076000000
H	-2.380645000000	-5.251388000000	-1.804050000000
C	0.916731000000	0.342492000000	-1.269528000000
H	0.753601000000	0.774213000000	-2.262832000000
H	1.347029000000	1.106981000000	-0.616655000000
H	1.638430000000	-0.474406000000	-1.342057000000
C	-1.759460000000	1.133872000000	-0.850746000000
H	-1.703382000000	1.458390000000	-1.895382000000
H	-2.790608000000	0.845138000000	-0.629474000000
H	-1.500997000000	1.977027000000	-0.204874000000
H	0.727381000000	-2.049182000000	0.784751000000
C	-0.182125000000	0.773941000000	2.370225000000
H	-0.529843000000	0.892885000000	3.408536000000
H	0.911071000000	0.913076000000	2.395556000000
H	-0.597852000000	1.619332000000	1.801722000000

TS 3.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.464787 (Hartree/Particle)
Thermal correction to Energy= 0.485074
Thermal correction to Enthalpy= 0.485850
Thermal correction to Gibbs Free Energy= 0.424245
Sum of electronic and zero-point Energies= -2005.412741
Sum of electronic and thermal Energies= -2005.392453
Sum of electronic and thermal Enthalpies= -2005.391677
Sum of electronic and thermal Free Energies= -2005.453282

Fe	-0.581169000000	-1.455232000000	1.298071000000
P	-0.956597000000	-0.436169000000	-0.590318000000
P	-0.610126000000	-3.242522000000	0.101616000000
P	-2.503811000000	-0.971143000000	2.170425000000
P	-0.222753000000	-2.539824000000	3.154804000000
C	-1.848500000000	-3.011290000000	3.924148000000
C	-2.759588000000	-1.800934000000	3.834567000000
H	-1.718158000000	-3.373182000000	4.952347000000
H	-2.251055000000	-3.842824000000	3.331627000000
H	-2.483942000000	-1.068037000000	4.603620000000
H	-3.815210000000	-2.048191000000	3.997311000000
C	-1.055788000000	-2.903799000000	-1.691142000000
C	-1.802237000000	-1.583980000000	-1.772571000000
H	-0.113656000000	-2.835441000000	-2.249348000000
H	-1.618180000000	-3.740286000000	-2.122037000000
H	-1.837828000000	-1.173063000000	-2.789604000000
H	-2.836542000000	-1.699769000000	-1.424759000000
C	-4.111267000000	-1.386756000000	1.346905000000
H	-4.979161000000	-1.074693000000	1.939457000000
H	-4.171520000000	-0.904093000000	0.366105000000
H	-4.167143000000	-2.467457000000	1.184540000000
C	-2.926796000000	0.761333000000	2.684925000000

H	-3.051418000000	1.409870000000	1.813732000000
H	-3.846699000000	0.798837000000	3.279173000000
H	-2.108513000000	1.170098000000	3.287353000000
C	0.555048000000	-1.618328000000	4.552514000000
H	0.485153000000	-2.177450000000	5.491576000000
H	1.610572000000	-1.434435000000	4.335892000000
H	0.069687000000	-0.645768000000	4.674675000000
C	0.691225000000	-4.131336000000	3.340654000000
H	1.728774000000	-4.008447000000	3.019032000000
H	0.684084000000	-4.472344000000	4.381530000000
H	0.235981000000	-4.909548000000	2.721779000000
C	0.880756000000	-4.300548000000	-0.211443000000
H	0.675263000000	-5.090986000000	-0.943696000000
H	1.689203000000	-3.667102000000	-0.587008000000
H	1.230164000000	-4.767720000000	0.712261000000
C	-1.809891000000	-4.613016000000	0.462074000000
H	-1.634789000000	-5.022181000000	1.462256000000
H	-2.827798000000	-4.211516000000	0.446518000000
H	-1.741036000000	-5.434109000000	-0.261295000000
C	0.507654000000	0.070541000000	-1.592973000000
H	0.218197000000	0.465506000000	-2.572938000000
H	1.074885000000	0.839342000000	-1.062325000000
H	1.168711000000	-0.789234000000	-1.729768000000
C	-1.964885000000	1.096094000000	-0.767566000000
H	-2.014291000000	1.432319000000	-1.808611000000
H	-2.983707000000	0.923057000000	-0.409505000000
H	-1.527428000000	1.896338000000	-0.162879000000
H	0.906472000000	-1.007273000000	1.261800000000

C	0.696592000000	0.242544000000	1.879514000000
H	-0.136727000000	0.835317000000	2.270891000000
H	1.420157000000	0.119733000000	2.690267000000
H	1.182032000000	0.845193000000	1.104451000000

TS 3'.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.460599 (Hartree/Particle)
Thermal correction to Energy= 0.482891
Thermal correction to Enthalpy= 0.483667
Thermal correction to Gibbs Free Energy= 0.414985
Sum of electronic and zero-point Energies= -2005.383303
Sum of electronic and thermal Energies= -2005.361011
Sum of electronic and thermal Enthalpies= -2005.360235
Sum of electronic and thermal Free Energies= -2005.428917

Fe	-0.550447000000	-0.867572000000	0.939090000000
P	-1.194623000000	-0.074888000000	-1.065157000000
P	-0.367000000000	-2.865520000000	-0.084079000000
P	-2.335320000000	-0.978732000000	2.355053000000
P	-0.722385000000	-3.773576000000	3.631659000000
C	-1.818210000000	-2.657965000000	4.646870000000
C	-1.957203000000	-1.217263000000	4.167170000000
H	-1.452809000000	-2.659381000000	5.683633000000
H	-2.805593000000	-3.137096000000	4.670706000000
H	-1.024269000000	-0.667487000000	4.349952000000
H	-2.734957000000	-0.715756000000	4.759475000000
C	-0.170175000000	-2.516781000000	-1.903248000000
C	-1.194757000000	-1.467810000000	-2.309616000000
H	0.848593000000	-2.135401000000	-2.049213000000
H	-0.264101000000	-3.436461000000	-2.495702000000

H	-1.024173000000	-1.084765000000	-3.323814000000
H	-2.202299000000	-1.904443000000	-2.300545000000
C	-3.798062000000	-2.077918000000	2.166092000000
H	-4.542602000000	-1.908128000000	2.952440000000
H	-4.263606000000	-1.896657000000	1.193041000000
H	-3.479304000000	-3.123692000000	2.195405000000
C	-3.174326000000	0.660130000000	2.465872000000
H	-3.599109000000	0.918319000000	1.492312000000
H	-3.971877000000	0.670997000000	3.217573000000
H	-2.440467000000	1.429841000000	2.722701000000
C	0.886308000000	-2.886777000000	3.798647000000
H	1.064756000000	-2.528887000000	4.819813000000
H	1.702974000000	-3.559175000000	3.519282000000
H	0.909606000000	-2.040369000000	3.104472000000
C	-0.467456000000	-5.078038000000	4.918144000000
H	0.263422000000	-5.811428000000	4.566999000000
H	-0.113110000000	-4.662713000000	5.868978000000
H	-1.404600000000	-5.610733000000	5.101986000000
C	0.971174000000	-4.104576000000	0.168277000000
H	0.950825000000	-4.896099000000	-0.589393000000
H	1.944270000000	-3.606690000000	0.140569000000
H	0.851379000000	-4.564346000000	1.153977000000
C	-1.815255000000	-4.008324000000	-0.143680000000
H	-1.962108000000	-4.438974000000	0.851179000000
H	-2.717774000000	-3.449028000000	-0.407751000000
H	-1.673764000000	-4.819782000000	-0.866972000000
C	-0.017068000000	1.097055000000	-1.880204000000
H	-0.307136000000	1.343170000000	-2.908178000000

H	0.041966000000	2.022855000000	-1.300432000000
H	0.982849000000	0.653530000000	-1.888238000000
C	-2.778823000000	0.752526000000	-1.544270000000
H	-2.856804000000	0.917564000000	-2.625404000000
H	-3.624483000000	0.136716000000	-1.221300000000
H	-2.860432000000	1.721055000000	-1.042096000000
H	0.989340000000	-0.840841000000	0.747508000000
C	0.878590000000	0.460310000000	1.589043000000
H	0.108177000000	1.224933000000	1.793258000000
H	1.335077000000	0.163189000000	2.540646000000
H	1.649585000000	0.947985000000	0.986094000000

MECP4.

Charge = 0 Multiplicity = 1/3

Zero-point correction= 0.465636 (Hartree/Particle)
Thermal correction to Energy= 0.487058
Thermal correction to Enthalpy= 0.487834
Thermal correction to Gibbs Free Energy= 0.421151
Sum of electronic and zero-point Energies= -2005.420306
Sum of electronic and thermal Energies= -2005.398885
Sum of electronic and thermal Enthalpies= -2005.398108
Sum of electronic and thermal Free Energies= -2005.464792

Fe	-2.296731000000	-1.894931000000	2.120224000000
P	-2.556614000000	-0.755881000000	0.247144000000
P	-2.446375000000	-3.650427000000	0.863449000000
P	-4.029409000000	-1.125803000000	3.155989000000
P	-1.836498000000	-2.960437000000	3.996343000000
C	-3.382150000000	-3.028628000000	5.033272000000
C	-4.064605000000	-1.675785000000	4.944107000000
H	-3.149653000000	-3.324106000000	6.064567000000

H	-4.020291000000	-3.812087000000	4.603620000000
H	-3.506317000000	-0.931568000000	5.526693000000
H	-5.087831000000	-1.691070000000	5.339730000000
C	-2.779945000000	-3.200751000000	-0.922430000000
C	-2.144329000000	-1.848749000000	-1.201811000000
H	-2.430990000000	-3.984711000000	-1.605984000000
H	-3.869540000000	-3.135842000000	-1.042465000000
H	-1.050431000000	-1.936446000000	-1.238575000000
H	-2.474813000000	-1.411724000000	-2.153563000000
C	-5.758548000000	-1.620616000000	2.685897000000
H	-6.511764000000	-1.153072000000	3.332383000000
H	-5.973938000000	-1.351855000000	1.648701000000
H	-5.847739000000	-2.707797000000	2.771556000000
C	-4.342046000000	0.687888000000	3.410088000000
H	-4.501654000000	1.186016000000	2.448624000000
H	-5.212375000000	0.886160000000	4.047896000000
H	-3.456954000000	1.141296000000	3.867260000000
C	-0.665826000000	-2.210464000000	5.222332000000
H	-0.729771000000	-2.716311000000	6.192723000000
H	0.361384000000	-2.292351000000	4.857220000000
H	-0.888694000000	-1.148961000000	5.358500000000
C	-1.276690000000	-4.712843000000	4.174768000000
H	-0.245632000000	-4.818014000000	3.825863000000
H	-1.321025000000	-5.037162000000	5.220722000000
H	-1.904412000000	-5.381446000000	3.579107000000
C	-0.977819000000	-4.764153000000	0.608358000000
H	-1.183764000000	-5.584339000000	-0.090962000000
H	-0.145597000000	-4.169036000000	0.220446000000

H	-0.655683000000	-5.191593000000	1.561225000000
C	-3.737215000000	-4.963596000000	1.072196000000
H	-3.638790000000	-5.446040000000	2.049738000000
H	-4.726061000000	-4.496693000000	1.033442000000
H	-3.678670000000	-5.736659000000	0.296146000000
C	-1.639656000000	0.784282000000	-0.196057000000
H	-1.911340000000	1.142594000000	-1.195398000000
H	-1.857562000000	1.572849000000	0.530243000000
H	-0.563917000000	0.594517000000	-0.172452000000
C	-4.255241000000	-0.245964000000	-0.277434000000
H	-4.251741000000	0.232802000000	-1.263135000000
H	-4.895428000000	-1.131388000000	-0.321280000000
H	-4.698529000000	0.445533000000	0.444083000000
C	0.282066000000	-0.347412000000	2.502226000000
H	-0.710270000000	-0.022887000000	2.839370000000
H	0.941900000000	-0.458287000000	3.363662000000
H	0.691388000000	0.391504000000	1.811912000000
H	0.179251000000	-1.313305000000	1.990996000000

Int 5.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.468247 (Hartree/Particle)
Thermal correction to Energy= 0.489542
Thermal correction to Enthalpy= 0.490318
Thermal correction to Gibbs Free Energy= 0.424947
Sum of electronic and zero-point Energies= -2005.423341
Sum of electronic and thermal Energies= -2005.402046
Sum of electronic and thermal Enthalpies= -2005.401270
Sum of electronic and thermal Free Energies= -2005.466641

Fe	-2.243085000000	-1.885840000000	2.112863000000

P	-2.599013000000	-0.777925000000	0.260711000000
P	-2.294901000000	-3.615895000000	0.872408000000
P	-3.916816000000	-1.060820000000	3.162792000000
P	-1.878871000000	-2.997057000000	3.958980000000
C	-3.403323000000	-3.002711000000	5.024931000000
C	-3.991972000000	-1.606352000000	4.950999000000
H	-3.172011000000	-3.323206000000	6.048986000000
H	-4.096460000000	-3.739430000000	4.597647000000
H	-3.382020000000	-0.905757000000	5.536054000000
H	-5.014481000000	-1.552071000000	5.344541000000
C	-2.661137000000	-3.212127000000	-0.922705000000
C	-2.133858000000	-1.817884000000	-1.208919000000
H	-2.244946000000	-3.972678000000	-1.594058000000
H	-3.751460000000	-3.236998000000	-1.049259000000
H	-1.037576000000	-1.823399000000	-1.263459000000
H	-2.511795000000	-1.396602000000	-2.149957000000
C	-5.636574000000	-1.579540000000	2.675258000000
H	-6.401780000000	-1.114790000000	3.309521000000
H	-5.847148000000	-1.328270000000	1.633797000000
H	-5.711235000000	-2.666900000000	2.772100000000
C	-4.263043000000	0.749296000000	3.411126000000
H	-4.432042000000	1.241711000000	2.448061000000
H	-5.138644000000	0.930553000000	4.046412000000
H	-3.389724000000	1.223050000000	3.870922000000
C	-0.668157000000	-2.263635000000	5.153592000000
H	-0.722145000000	-2.764351000000	6.126466000000
H	0.348978000000	-2.369176000000	4.767494000000
H	-0.866484000000	-1.197215000000	5.289662000000

C	-1.347253000000	-4.756674000000	4.143616000000
H	-0.316040000000	-4.871488000000	3.798633000000
H	-1.395833000000	-5.068844000000	5.192459000000
H	-1.976550000000	-5.427966000000	3.553834000000
C	-0.883777000000	-4.806805000000	0.609628000000
H	-1.147154000000	-5.630649000000	-0.065195000000
H	-0.033887000000	-4.262117000000	0.186640000000
H	-0.559097000000	-5.231626000000	1.562976000000
C	-3.629502000000	-4.880452000000	1.137531000000
H	-3.549212000000	-5.331725000000	2.130995000000
H	-4.600249000000	-4.378164000000	1.085524000000
H	-3.602581000000	-5.683012000000	0.389688000000
C	-1.714407000000	0.796967000000	-0.122336000000
H	-2.006600000000	1.186496000000	-1.103193000000
H	-1.938483000000	1.551743000000	0.637133000000
H	-0.634899000000	0.630760000000	-0.123251000000
C	-4.294872000000	-0.277334000000	-0.280486000000
H	-4.266667000000	0.227234000000	-1.252110000000
H	-4.927905000000	-1.164891000000	-0.366526000000
H	-4.758621000000	0.394038000000	0.447247000000
C	-0.040719000000	-0.447533000000	2.490829000000
H	-0.961556000000	0.027591000000	2.845095000000
H	0.640534000000	-0.592160000000	3.328244000000
H	0.426472000000	0.179811000000	1.732635000000
H	-0.254309000000	-1.442927000000	2.034699000000

Int 5’.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.466484 (Hartree/Particle)
Thermal correction to Energy= 0.489243
Thermal correction to Enthalpy= 0.490019
Thermal correction to Gibbs Free Energy= 0.420630
Sum of electronic and zero-point Energies= -2005.439092
Sum of electronic and thermal Energies= -2005.416333
Sum of electronic and thermal Enthalpies= -2005.415557
Sum of electronic and thermal Free Energies= -2005.484946

Fe	-2.477041000000	-1.712890000000	2.245127000000
P	-2.474591000000	-0.451873000000	0.413888000000
P	-2.705895000000	-3.465411000000	0.928577000000
P	-4.478600000000	-1.397221000000	3.134890000000
P	-1.848930000000	-2.581987000000	4.187425000000
C	-3.389759000000	-2.939396000000	5.169603000000
C	-4.381061000000	-1.805089000000	4.960740000000
H	-3.155967000000	-3.105271000000	6.229579000000
H	-3.798579000000	-3.879975000000	4.775648000000
H	-4.028559000000	-0.898893000000	5.471192000000
H	-5.372220000000	-2.037012000000	5.371715000000
C	-3.121161000000	-2.873761000000	-0.793119000000
C	-2.343428000000	-1.593602000000	-1.060726000000
H	-2.920437000000	-3.644616000000	-1.549023000000
H	-4.201301000000	-2.674636000000	-0.811455000000
H	-1.275456000000	-1.820529000000	-1.184805000000
H	-2.670133000000	-1.085058000000	-1.977056000000
C	-5.950122000000	-2.430590000000	2.679079000000
H	-6.848930000000	-2.160150000000	3.246355000000
H	-6.163968000000	-2.322308000000	1.610475000000
H	-5.721948000000	-3.484165000000	2.865063000000
C	-5.360051000000	0.228669000000	3.260974000000

H	-5.768503000000	0.509409000000	2.286090000000
H	-6.186022000000	0.193395000000	3.981297000000
H	-4.657285000000	1.009421000000	3.566006000000
C	-0.886971000000	-1.576878000000	5.407636000000
H	-0.780651000000	-2.079349000000	6.376253000000
H	0.110073000000	-1.374479000000	5.005660000000
H	-1.380540000000	-0.613138000000	5.559848000000
C	-0.954887000000	-4.184053000000	4.373266000000
H	0.050496000000	-4.102278000000	3.950570000000
H	-0.868113000000	-4.487868000000	5.422693000000
H	-1.487031000000	-4.966393000000	3.823784000000
C	-1.133734000000	-4.376177000000	0.554570000000
H	-1.256740000000	-5.119731000000	-0.242076000000
H	-0.361673000000	-3.661038000000	0.255950000000
H	-0.772896000000	-4.883210000000	1.454317000000
C	-3.836710000000	-4.924454000000	1.041209000000
H	-3.672078000000	-5.451334000000	1.986444000000
H	-4.877349000000	-4.590380000000	1.023259000000
H	-3.682048000000	-5.631383000000	0.217724000000
C	-1.198597000000	0.799459000000	-0.056424000000
H	-1.327626000000	1.151718000000	-1.086542000000
H	-1.258852000000	1.659456000000	0.615657000000
H	-0.199981000000	0.366675000000	0.046037000000
C	-3.983477000000	0.507850000000	-0.047034000000
H	-3.913661000000	0.927675000000	-1.057237000000
H	-4.861569000000	-0.142663000000	0.008716000000
H	-4.129958000000	1.325642000000	0.663695000000
C	1.426530000000	-1.693805000000	1.776136000000

H	2.018069000000	-0.889786000000	2.216507000000
H	1.739063000000	-2.651193000000	2.197120000000
H	1.581435000000	-1.709184000000	0.695468000000
H	0.364536000000	-1.531908000000	1.990533000000

Int 6.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.605957 (Hartree/Particle)
Thermal correction to Energy= 0.632162
Thermal correction to Enthalpy= 0.632938
Thermal correction to Gibbs Free Energy= 0.557607
Sum of electronic and zero-point Energies= -2314.949993
Sum of electronic and thermal Energies= -2314.923788
Sum of electronic and thermal Enthalpies= -2314.923012
Sum of electronic and thermal Free Energies= -2314.998343

Fe	-0.457483000000	-1.564538000000	1.436854000000
P	-0.463245000000	-0.258664000000	-0.331606000000
P	-0.525810000000	-3.198364000000	0.034340000000
P	-2.417159000000	-1.067416000000	2.188377000000
P	-0.233035000000	-2.783226000000	3.248019000000
C	-1.936787000000	-3.280156000000	3.807076000000
C	-2.842671000000	-2.063623000000	3.724795000000
H	-1.912937000000	-3.723736000000	4.811122000000
H	-2.273329000000	-4.060546000000	3.112654000000
H	-2.665090000000	-1.408522000000	4.587245000000
H	-3.906262000000	-2.329568000000	3.745792000000
C	-0.844496000000	-2.595221000000	-1.716938000000
C	-1.376015000000	-1.171883000000	-1.670059000000
H	0.117509000000	-2.616110000000	-2.244600000000
H	-1.513308000000	-3.276695000000	-2.255863000000

H	-1.286192000000	-0.657330000000	-2.635906000000
H	-2.437043000000	-1.164548000000	-1.391298000000
C	-3.937776000000	-1.332930000000	1.157101000000
H	-4.861238000000	-1.147610000000	1.718655000000
H	-3.919624000000	-0.655717000000	0.296533000000
H	-3.956576000000	-2.356229000000	0.771163000000
C	-2.902407000000	0.605009000000	2.845110000000
H	-2.815659000000	1.367659000000	2.065195000000
H	-3.930233000000	0.615550000000	3.229117000000
H	-2.224660000000	0.885471000000	3.657500000000
C	0.431525000000	-1.991614000000	4.784693000000
H	0.290219000000	-2.618864000000	5.672236000000
H	1.501814000000	-1.795321000000	4.665686000000
H	-0.063228000000	-1.027862000000	4.942073000000
C	0.628673000000	-4.411331000000	3.375048000000
H	1.696957000000	-4.290535000000	3.172605000000
H	0.509394000000	-4.859781000000	4.367743000000
H	0.223339000000	-5.104067000000	2.631206000000
C	0.927389000000	-4.299195000000	-0.332377000000
H	0.715284000000	-5.011853000000	-1.139226000000
H	1.782363000000	-3.681769000000	-0.624817000000
H	1.217198000000	-4.861921000000	0.560038000000
C	-1.789521000000	-4.549733000000	0.180678000000
H	-1.621561000000	-5.114696000000	1.103757000000
H	-2.793083000000	-4.118195000000	0.237040000000
H	-1.750837000000	-5.250503000000	-0.661756000000
C	1.124816000000	0.122280000000	-1.193442000000
H	0.956413000000	0.549658000000	-2.188942000000

H	1.707569000000	0.829684000000	-0.596173000000
H	1.719667000000	-0.791263000000	-1.289196000000
C	-1.263082000000	1.399164000000	-0.456438000000
H	-1.231129000000	1.791221000000	-1.479218000000
H	-2.308834000000	1.331464000000	-0.141535000000
H	-0.756572000000	2.109013000000	0.204358000000
C	3.946607000000	1.802015000000	0.867792000000
C	4.139060000000	0.418433000000	0.892882000000
C	2.823801000000	2.333331000000	1.513922000000
H	4.999818000000	-0.007865000000	0.377599000000
H	2.655586000000	3.410201000000	1.491672000000
C	3.242459000000	-0.431720000000	1.545526000000
C	1.913290000000	1.513174000000	2.182054000000
C	2.136470000000	0.132414000000	2.184590000000
H	1.411668000000	-0.521815000000	2.674387000000
C	3.434557000000	-1.917921000000	1.555147000000
H	4.086890000000	-2.250675000000	0.741849000000
H	3.886523000000	-2.262042000000	2.494222000000
H	2.466397000000	-2.427063000000	1.456263000000
C	0.712960000000	2.074322000000	2.882021000000
H	-0.178118000000	1.474687000000	2.658520000000
H	0.838574000000	2.054787000000	3.971516000000
H	0.517491000000	3.111640000000	2.594552000000
C	4.926018000000	2.702135000000	0.176001000000
H	5.611584000000	3.173022000000	0.890458000000
H	5.539663000000	2.153937000000	-0.543934000000
H	4.423814000000	3.514644000000	-0.357852000000

Int 6'.

Charge = 0 Multiplicity = 3

Zero-point correction= 0.604885 (Hartree/Particle)
Thermal correction to Energy= 0.632327
Thermal correction to Enthalpy= 0.633103
Thermal correction to Gibbs Free Energy= 0.552043
Sum of electronic and zero-point Energies= -2314.964485
Sum of electronic and thermal Energies= -2314.937043
Sum of electronic and thermal Enthalpies= -2314.936267
Sum of electronic and thermal Free Energies= -2315.017327

Fe	-0.596312000000	-1.699149000000	1.303946000000
P	-0.336079000000	-0.472014000000	-0.539057000000
P	-1.168919000000	-3.343412000000	-0.048477000000
P	-2.520239000000	-0.959398000000	2.090711000000
P	-0.276768000000	-2.712130000000	3.260354000000
C	-1.887295000000	-2.629636000000	4.196116000000
C	-2.540453000000	-1.280429000000	3.933850000000
H	-1.733746000000	-2.823259000000	5.265708000000
H	-2.521423000000	-3.438525000000	3.808149000000
H	-1.956691000000	-0.478240000000	4.406616000000
H	-3.557773000000	-1.223968000000	4.342998000000
C	-1.464037000000	-2.661351000000	-1.782347000000
C	-1.597431000000	-1.143720000000	-1.731027000000
H	-0.600018000000	-2.935946000000	-2.401028000000
H	-2.339097000000	-3.135819000000	-2.241692000000
H	-1.491663000000	-0.688456000000	-2.725265000000
H	-2.580850000000	-0.854145000000	-1.338090000000
C	-4.159798000000	-1.712936000000	1.658432000000
H	-4.990821000000	-1.236905000000	2.192704000000
H	-4.340752000000	-1.627016000000	0.582115000000

H	-4.146897000000	-2.777617000000	1.907651000000
C	-3.076954000000	0.808417000000	2.078901000000
H	-3.395265000000	1.082758000000	1.067766000000
H	-3.919352000000	0.981164000000	2.759083000000
H	-2.253371000000	1.471475000000	2.360171000000
C	0.870251000000	-2.044271000000	4.557364000000
H	0.768699000000	-2.574536000000	5.511064000000
H	1.907870000000	-2.129113000000	4.220396000000
H	0.666191000000	-0.981109000000	4.720912000000
C	0.138575000000	-4.500392000000	3.432612000000
H	1.147331000000	-4.680076000000	3.048049000000
H	0.095551000000	-4.840334000000	4.473621000000
H	-0.557126000000	-5.098553000000	2.836744000000
C	0.120672000000	-4.617581000000	-0.440534000000
H	-0.166902000000	-5.264644000000	-1.278025000000
H	1.061937000000	-4.117175000000	-0.688589000000
H	0.302214000000	-5.245397000000	0.437079000000
C	-2.612400000000	-4.498419000000	0.097542000000
H	-2.593175000000	-5.003556000000	1.068782000000
H	-3.545858000000	-3.933727000000	0.035061000000
H	-2.611641000000	-5.259241000000	-0.691702000000
C	1.187360000000	-0.607161000000	-1.577104000000
H	1.042039000000	-0.185404000000	-2.578657000000
H	2.009142000000	-0.077988000000	-1.086090000000
H	1.482492000000	-1.656567000000	-1.674029000000
C	-0.606007000000	1.344318000000	-0.693048000000
H	-0.641790000000	1.664087000000	-1.740654000000
H	-1.536760000000	1.634723000000	-0.199082000000

H	0.218127000000	1.868325000000	-0.198797000000
C	4.044588000000	1.664542000000	0.457264000000
C	4.221161000000	0.276759000000	0.490599000000
C	2.964099000000	2.219892000000	1.150234000000
H	5.041527000000	-0.168762000000	-0.072272000000
H	2.802989000000	3.297423000000	1.110849000000
C	3.351635000000	-0.550344000000	1.204648000000
C	2.084867000000	1.420396000000	1.884959000000
C	2.297322000000	0.041092000000	1.904120000000
H	1.588448000000	-0.593667000000	2.432677000000
C	3.486622000000	-2.043098000000	1.192541000000
H	4.143491000000	-2.387444000000	0.388361000000
H	3.895356000000	-2.426058000000	2.135533000000
H	2.500951000000	-2.513984000000	1.061887000000
C	0.919836000000	1.996600000000	2.632219000000
H	0.070605000000	1.300700000000	2.606509000000
H	1.161728000000	2.169654000000	3.687798000000
H	0.593759000000	2.954165000000	2.214186000000
C	5.000572000000	2.539166000000	-0.297334000000
H	5.850665000000	2.835863000000	0.328590000000
H	5.414974000000	2.028096000000	-1.171094000000
H	4.522026000000	3.461047000000	-0.639692000000

Int 2-trans.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.474311 (Hartree/Particle)
Thermal correction to Energy= 0.495464
Thermal correction to Enthalpy= 0.496240
Thermal correction to Gibbs Free Energy= 0.432652
Sum of electronic and zero-point Energies= -2043.486871

Sum of electronic and thermal Energies= -2043.465718
Sum of electronic and thermal Enthalpies= -2043.464941
Sum of electronic and thermal Free Energies= -2043.528530

Fe	-1.217784000000	-2.112675000000	1.317546000000
H	0.104369000000	-0.935026000000	1.348627000000
C	0.709312000000	-1.248638000000	2.253935000000
H	1.453555000000	-2.029929000000	2.114405000000
P	-1.818389000000	-1.102437000000	-0.520601000000
P	-0.274632000000	-3.546243000000	-0.014430000000
P	-2.650527000000	-0.985081000000	2.495691000000
P	-1.398132000000	-3.547145000000	2.937511000000
C	-2.316126000000	-2.850763000000	4.420130000000
C	-2.391522000000	-1.339892000000	4.297522000000
H	-1.839893000000	-3.183917000000	5.349452000000
H	-3.325076000000	-3.281129000000	4.412798000000
H	-1.439035000000	-0.876868000000	4.580789000000
H	-3.183366000000	-0.902049000000	4.918504000000
C	-0.913934000000	-3.387345000000	-1.754875000000
C	-1.094349000000	-1.910893000000	-2.040013000000
H	-0.244196000000	-3.881851000000	-2.470608000000
H	-1.877937000000	-3.909850000000	-1.787456000000
H	-0.119776000000	-1.437817000000	-2.216608000000
H	-1.711283000000	-1.713223000000	-2.924297000000
C	-4.450408000000	-1.401014000000	2.378042000000
H	-5.050985000000	-0.826106000000	3.093594000000
H	-4.824175000000	-1.208857000000	1.370515000000
H	-4.586610000000	-2.468187000000	2.572586000000
C	-2.800365000000	0.856987000000	2.498041000000
H	-3.240216000000	1.197527000000	1.555329000000

H	-3.438614000000	1.208869000000	3.315845000000
H	-1.814180000000	1.320310000000	2.592042000000
C	0.159283000000	-4.124929000000	3.763886000000
H	-0.036091000000	-4.843863000000	4.567205000000
H	0.826045000000	-4.591455000000	3.030890000000
H	0.679151000000	-3.256951000000	4.178877000000
C	-2.267152000000	-5.182806000000	2.860925000000
H	-1.707865000000	-5.907074000000	2.266690000000
H	-2.394046000000	-5.595027000000	3.868926000000
H	-3.251529000000	-5.055704000000	2.402189000000
C	1.545953000000	-3.332449000000	-0.327748000000
H	1.905984000000	-3.963620000000	-1.148064000000
H	1.761034000000	-2.284995000000	-0.560184000000
H	2.108633000000	-3.589691000000	0.575311000000
C	-0.277437000000	-5.388224000000	0.110797000000
H	0.198766000000	-5.724564000000	1.036342000000
H	-1.303610000000	-5.763189000000	0.095842000000
H	0.267193000000	-5.827459000000	-0.731883000000
C	-1.241864000000	0.632926000000	-0.828394000000
H	-1.503693000000	0.984620000000	-1.833402000000
H	-1.678692000000	1.318283000000	-0.096975000000
H	-0.154604000000	0.673906000000	-0.711739000000
C	-3.576900000000	-0.859511000000	-1.055212000000
H	-3.631842000000	-0.432650000000	-2.062937000000
H	-4.112385000000	-1.812224000000	-1.036930000000
H	-4.085122000000	-0.173520000000	-0.370657000000
C	0.860806000000	-0.380755000000	3.270736000000
H	1.645593000000	-0.494297000000	4.015562000000

H	0.185048000000	0.461284000000	3.408922000000

TS 1-trans.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.466546 (Hartree/Particle)
Thermal correction to Energy= 0.488202
Thermal correction to Enthalpy= 0.488978
Thermal correction to Gibbs Free Energy= 0.423932
Sum of electronic and zero-point Energies= -2043.456793
Sum of electronic and thermal Energies= -2043.435137
Sum of electronic and thermal Enthalpies= -2043.434361
Sum of electronic and thermal Free Energies= -2043.499407

Fe	-1.560120000000	-2.286297000000	1.290854000000
H	-0.158176000000	-1.457566000000	1.778451000000
C	0.789829000000	-0.422730000000	2.307973000000
H	0.365351000000	0.575346000000	2.433856000000
P	-1.793271000000	-1.077234000000	-0.498508000000
P	-0.459707000000	-3.631987000000	0.014127000000
P	-2.950596000000	-1.093188000000	2.463642000000
P	-1.470391000000	-3.557495000000	3.050284000000
C	-2.491042000000	-2.876695000000	4.466338000000
C	-2.659969000000	-1.380693000000	4.275996000000
H	-2.039077000000	-3.136136000000	5.431296000000
H	-3.469038000000	-3.373920000000	4.430980000000
H	-1.736178000000	-0.847526000000	4.536492000000
H	-3.467877000000	-0.963882000000	4.891360000000
C	-0.900999000000	-3.347240000000	-1.773384000000
C	-0.968420000000	-1.846585000000	-1.987323000000
H	-0.185203000000	-3.837939000000	-2.446052000000
H	-1.881491000000	-3.810362000000	-1.942552000000

H	0.044907000000	-1.428638000000	-2.044528000000
H	-1.481211000000	-1.566817000000	-2.915448000000
C	-4.729872000000	-1.569714000000	2.327472000000
H	-5.359796000000	-1.040614000000	3.053511000000
H	-5.099180000000	-1.352072000000	1.321175000000
H	-4.836900000000	-2.647366000000	2.481173000000
C	-3.132904000000	0.740303000000	2.435982000000
H	-3.518206000000	1.076378000000	1.468120000000
H	-3.824041000000	1.086798000000	3.212858000000
H	-2.162823000000	1.219102000000	2.597795000000
C	0.170176000000	-3.746483000000	3.874427000000
H	0.110926000000	-4.354941000000	4.784948000000
H	0.882403000000	-4.217284000000	3.188875000000
H	0.564451000000	-2.757870000000	4.127676000000
C	-2.037554000000	-5.314708000000	3.126306000000
H	-1.353045000000	-5.977286000000	2.591948000000
H	-2.101418000000	-5.658304000000	4.165455000000
H	-3.025219000000	-5.409309000000	2.664919000000
C	1.370680000000	-3.370255000000	-0.068620000000
H	1.844675000000	-3.948915000000	-0.871357000000
H	1.587280000000	-2.307535000000	-0.213531000000
H	1.825605000000	-3.663416000000	0.882575000000
C	-0.463782000000	-5.476644000000	0.047800000000
H	0.069856000000	-5.847013000000	0.928305000000
H	-1.487472000000	-5.859954000000	0.081108000000
H	0.033186000000	-5.884510000000	-0.839911000000
C	-1.098844000000	0.627957000000	-0.605669000000
H	-1.209102000000	1.051720000000	-1.611046000000

H	-1.591621000000	1.295894000000	0.106507000000
H	-0.035018000000	0.596348000000	-0.350294000000
C	-3.486573000000	-0.753225000000	-1.163141000000
H	-3.458260000000	-0.211659000000	-2.116013000000
H	-4.015930000000	-1.699267000000	-1.309950000000
H	-4.064596000000	-0.157802000000	-0.448907000000
C	2.053801000000	-0.706428000000	2.595079000000
H	2.756180000000	0.039411000000	2.979022000000
H	2.466379000000	-1.707315000000	2.463740000000

I-trans.

Charge = 0 Multiplicity = 1

Zero-point correction= 0.471417 (Hartree/Particle)
Thermal correction to Energy= 0.492157
Thermal correction to Enthalpy= 0.492934
Thermal correction to Gibbs Free Energy= 0.430303
Sum of electronic and zero-point Energies= -2043.519538
Sum of electronic and thermal Energies= -2043.498798
Sum of electronic and thermal Enthalpies= -2043.498021
Sum of electronic and thermal Free Energies= -2043.560652

Fe	-1.742854000000	-2.386977000000	1.253239000000
H	-0.523671000000	-1.545412000000	1.845632000000
C	-3.365588000000	-3.350842000000	0.548556000000
H	-4.287316000000	-2.743571000000	0.552981000000
P	-1.839906000000	-1.094196000000	-0.512088000000
P	-0.305813000000	-3.539472000000	0.072553000000
P	-2.890907000000	-1.047534000000	2.543414000000
P	-1.553882000000	-3.682737000000	3.002470000000
C	-2.531137000000	-2.990543000000	4.424736000000
C	-2.531603000000	-1.475994000000	4.312248000000

H	-2.143014000000	-3.348786000000	5.385593000000
H	-3.552713000000	-3.379522000000	4.323607000000
H	-1.538592000000	-1.070287000000	4.541531000000
H	-3.250276000000	-1.000159000000	4.990723000000
C	-0.764578000000	-3.367901000000	-1.710263000000
C	-0.987243000000	-1.888667000000	-1.979224000000
H	-0.007636000000	-3.804695000000	-2.373413000000
H	-1.698849000000	-3.928604000000	-1.829697000000
H	-0.025438000000	-1.377779000000	-2.110210000000
H	-1.564563000000	-1.709251000000	-2.892813000000
C	-4.734454000000	-1.103058000000	2.558728000000
H	-5.152109000000	-0.444020000000	3.326742000000
H	-5.131724000000	-0.802594000000	1.584960000000
H	-5.071086000000	-2.127176000000	2.740055000000
C	-2.645086000000	0.772222000000	2.572369000000
H	-3.094856000000	1.230288000000	1.686633000000
H	-3.110670000000	1.218554000000	3.457212000000
H	-1.576321000000	0.999122000000	2.573360000000
C	0.111608000000	-3.850836000000	3.767391000000
H	0.092339000000	-4.467206000000	4.672736000000
H	0.808151000000	-4.302465000000	3.054458000000
H	0.494124000000	-2.856267000000	4.009543000000
C	-2.112839000000	-5.430597000000	3.033577000000
H	-1.454605000000	-6.056257000000	2.425947000000
H	-2.119490000000	-5.823469000000	4.055607000000
H	-3.115324000000	-5.488550000000	2.603626000000
C	1.425646000000	-2.917834000000	0.072077000000
H	2.060760000000	-3.444394000000	-0.649582000000

H	1.428336000000	-1.848071000000	-0.151370000000
H	1.848938000000	-3.033495000000	1.073509000000
C	0.043542000000	-5.344545000000	0.186932000000
H	0.496929000000	-5.583981000000	1.153485000000
H	-0.875849000000	-5.925760000000	0.089247000000
H	0.739770000000	-5.651724000000	-0.600354000000
C	-1.040865000000	0.564178000000	-0.566837000000
H	-1.042270000000	0.972226000000	-1.583527000000
H	-1.557169000000	1.268223000000	0.088998000000
H	-0.009397000000	0.478039000000	-0.214911000000
C	-3.483327000000	-0.676422000000	-1.224460000000
H	-3.390691000000	-0.085135000000	-2.140973000000
H	-4.022918000000	-1.601940000000	-1.439981000000
H	-4.072750000000	-0.105837000000	-0.499587000000
C	-3.591530000000	-4.579779000000	0.042319000000
H	-4.572702000000	-4.919209000000	-0.304158000000
H	-2.804228000000	-5.333530000000	-0.046269000000

8. References

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