Supporting Information

[2+2] cycloadditon or β-hydrogen elimination? --DFT study on the reactions of propylene catalyzed by (PDI)Fe-metallacycle

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Mingyang Jiao[a,b,c], Zichen Wang[a], BeiBei Zhang[a], and Bo-Zhen Chen[*,a]

[a.] School of Chemical Sciences, University of Chinese Academy of Sciences, No. 19A, YuQuan Road, Beijing 100049, P. R. China.

[b.] CAS Key Laboratory of Bio-based Materials, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao 266101, Shandong, China.

[c.] Shandong Energy Institute, Qingdao 266101, Shandong, China.

[*] corresponding author. Email: bozhenchen@hotmail.com.

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Computational methods

The calculations were mainly carried out using the Gaussian 09 program[1]. Considering that M052X is a proper calculation method for transition metal complexes[2-3], geometries were optimized at M052X[4-5]/BS1 level in the gas phase (BS1 denotes a mixed basis set of SDD[6-8] for metal atoms and 6-31G(d, p) for nonmetal atoms). The vibrational frequency was calculated at the same level to confirm whether the optimized geometry is a minimum (no imaginary frequencies) or a transition state (only one imaginary frequency). The intrinsic reaction coordinate (IRC)[9-10] pathways have been traced to confirm whether the transition state connects the reactant, intermediate, or product.

The improved energetic results were calculated by the single-point energy calculations with the solvent effects obtained by PCM[11-12] solvent model at M052X/BS2. BS2 designates a mixed basis set of SDD for the Fe atom and 6-311+G(d, p) for nonmetal atoms. Our calculation uses benzene as a solvent to replace the solvent benzene-d^6 used in the experiment. The enthalpies and Gibbs free energies at 298 K and 1 atm at M052X/BS2 level were gotten from M052X/BS1 frequency analysis calculations. The Gibbs free energies at the M052X/BS2 level were used in the following discussion unless otherwise specified.

Furthermore, the improved single point energetic results for the structure of Fe catalyst were calculated by CASPT2[13-14] code of Molcas[15] based on geometries optimized by M052X/BSI. ANO-S[16] was used as the basis set. The structure of the catalyst was simplified in this calculation (Figure S1). An active space of (12e, 12o) was used. The corrected energy was got according to the formula $E_{full}=E_{full}(DFT)+[E_{trun}(CASPT2)-E_{trun}(DFT)]$ (the E_{full} is the energy after rectification; the $E_{full}(DFT)$ is the energy of the unsimplified catalyst at the DFT level; the $E_{trun}(CASPT2)$ is the energy calculated by CASPT2 for the simplified catalyst. The $E_{trun}(DFT)$ is the energy of the simplified catalyst at the DFT level).

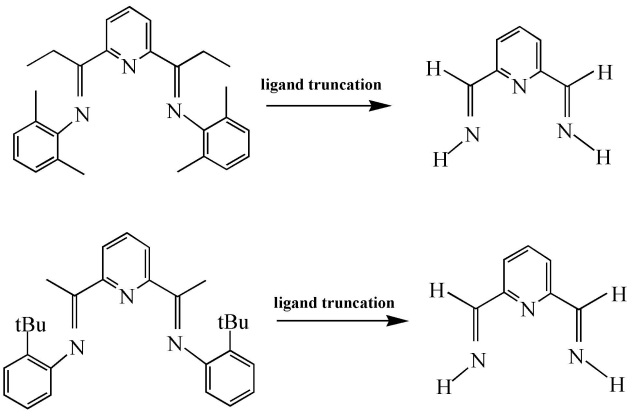


Figure S1 The truncation of Fe catalyst

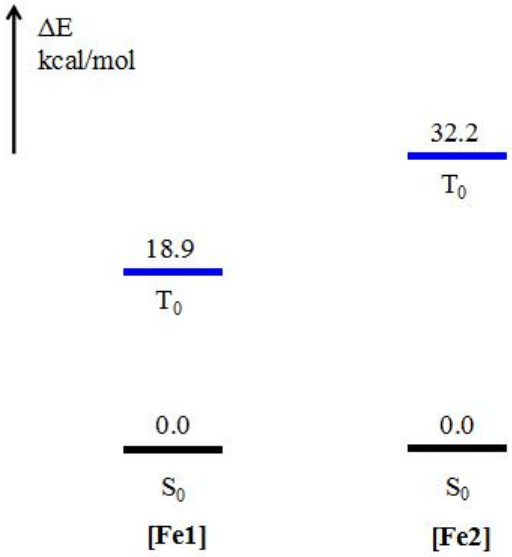


Figure S2. Energies of **[Fe1]** and **[Fe2]** in the singlet and triplet states after CASPT2 single point energy calculation correction.

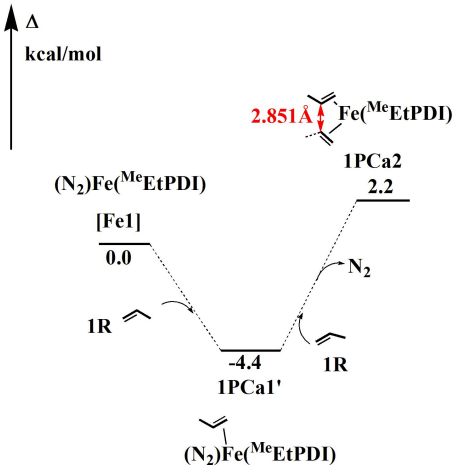


Figure S3. The association of **1PCa1'** with **[Fe1]** and **1PCa2**.

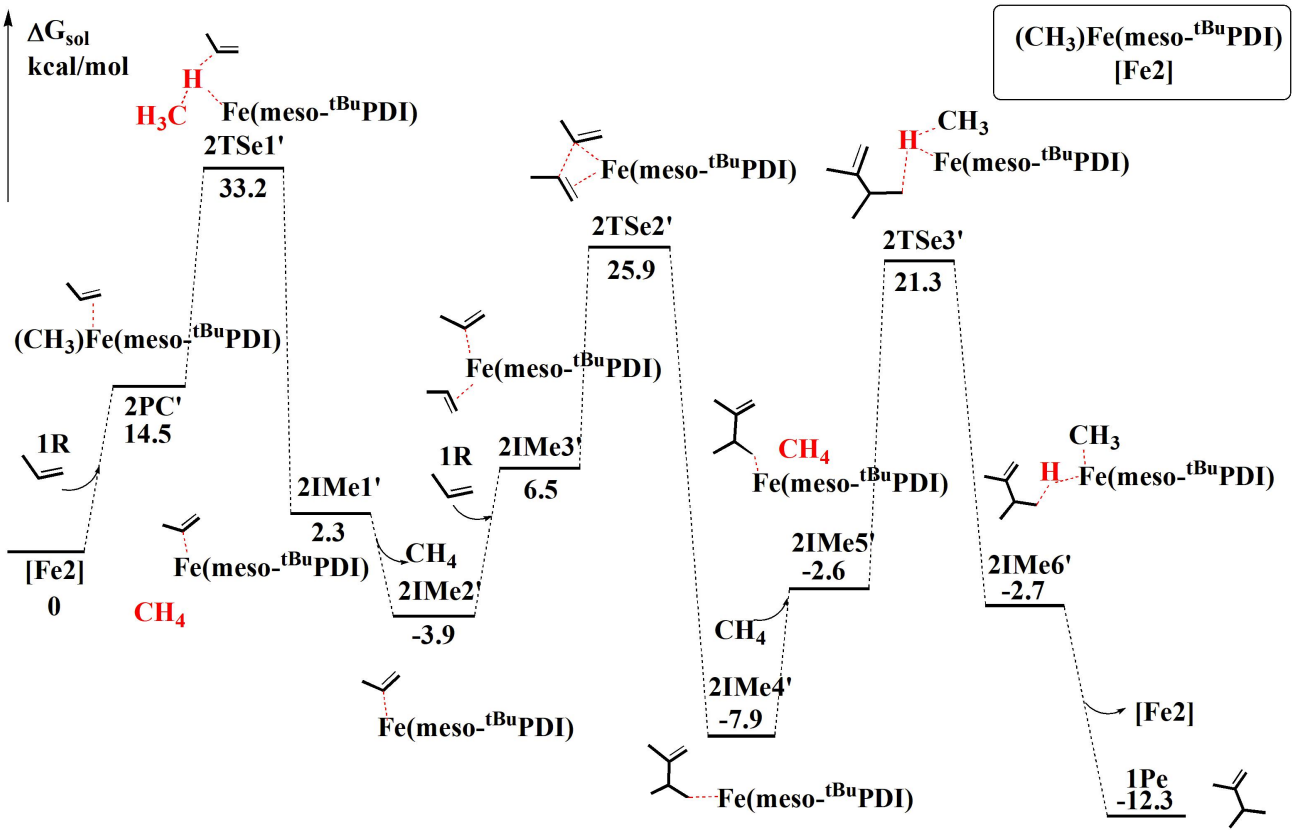


Figure S4. Free energy profiles for the β-hydrogen elimination reaction of **1R** under **[Fe2]** (**[Fe2]** = (CH$_3$)Fe(meso-^{tBu}PDI)). Energies are relative to **[Fe2]**+**1R** and are mass balanced. All energies are given in kcal/mol.

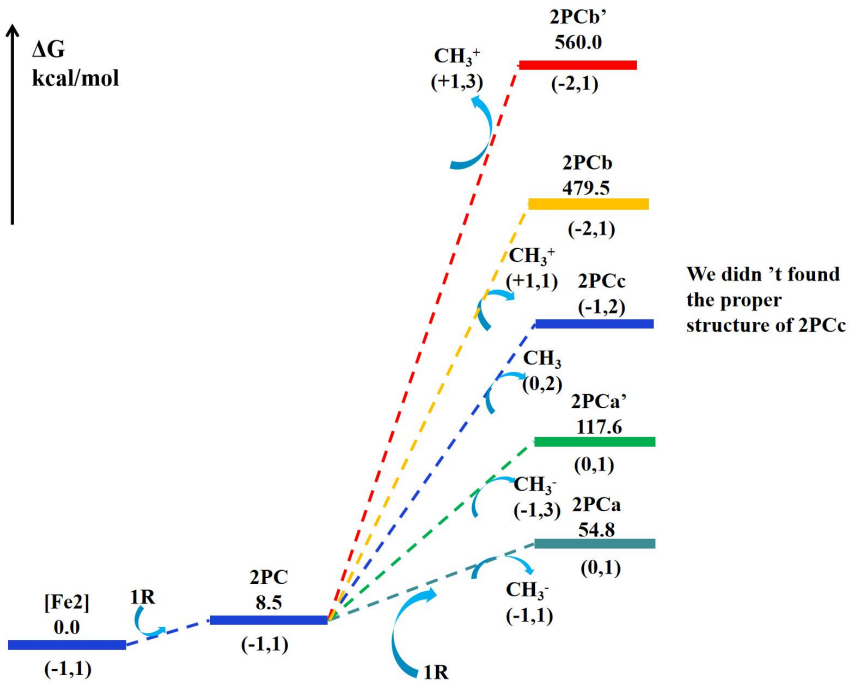


Figure S5. Free energy profiles for the reactions of **1R** and **2PC** to **2PCa**, **2PCa'**, **2PCb**, **2PCb'**, **2PCc** under **[Fe2]** (**[Fe2]**=(CH$_3$)Fe(meso-^{tBu}PDI)). Energies are relative to **[Fe2]**+**1R** and are mass balanced..

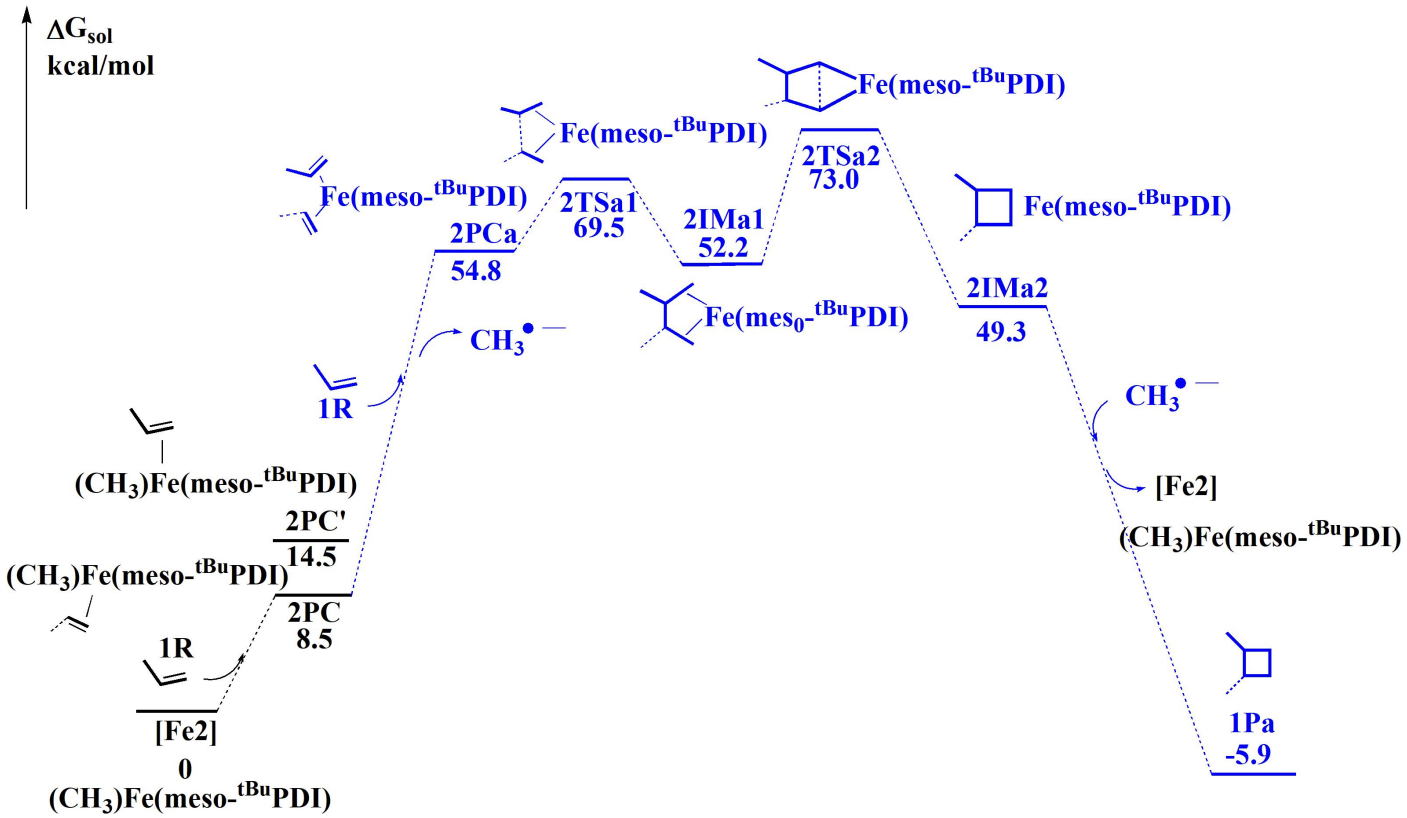
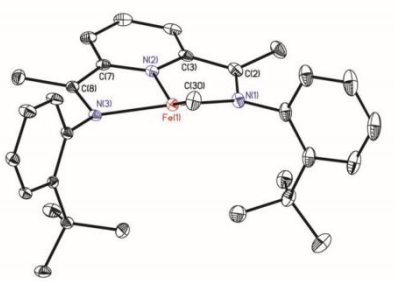


Figure S6. Free energy profiles for the [2+2] cycloaddition reaction of **1R** under **[Fe2]** (**[Fe2]** = (CH$_3$)Fe(meso-^{tBu}PDI)). Energies are relative to **[Fe2]**+**1R** and are mass balanced. In order to make the figure more concise, we only give the structure and energy of **2PC'**, and its association with other stationary points (**[Fe2]** and **2PCa**) is similar to **2PC**.

Table S1. The relative enthalpies and free energies for the stationary points along the reaction pathways of **1R** catalyzed by **[Fe1]** under M052X/6-31G(d, p) in gas. All values are given in kcal/mol. Energies are relative to **[Fe1](S$_0$)**+**1R(S$_0$)** and are mass balanced.

(0, 1)	ΔH	ΔG	(0, 3)	ΔH	ΔG	(0, 5)	ΔH	ΔG
[Fe1](S$_0$)	0	0	**[Fe1](T$_0$)**	0	0	**[Fe1](Q$_0$)**	0	0
1PCa1(S$_0$)	-21.9	-6.4	**1PCa1(T$_0$)**	-23.1	-11.9	**1PCa1(Q$_0$)**	-4.4	6.6
1PCa2(S$_0$)	-15.7	2.2	**1PCa2(T$_0$)**	-34.0	-19.6	**1PCa2(Q$_0$)**	-13.7	-0.7
1TSa1(S$_0$)	-2.9	18.3	**1TSa1(T$_0$)**	24.9	**43.1**	**1TSa1(Q$_0$)**	2.7	18.9
1IMa1(S$_0$)	-16.9	1.1	**1IMa1(T$_0$)**	-19.4	-0.9	**1IMa1(Q$_0$)**	-30.1	-14.9
1TSa2(S$_0$)	3.4	22.7	**1TSa2(T$_0$)**	9.1	27.1	**1TSa2(Q$_0$)**	9.6	**28.2**
1IMa2(S$_0$)	-24.3	-7.9	**1IMa2(T$_0$)**	-4.1	12.6	**1IMa2(Q$_0$)**	-14.7	1.5
1Pa(S$_0$)	-19.9	-5.9	**1Pa(S$_0$)**	-19.9	-5.9	**1Pa(S$_0$)**	-19.9	-5.9

Table S2. The structure parameter of **[Fe2]** based on different charge and spin multiplicity under M052x method. According to the calculation, the important parameter angle of N2-Fe1-C30 was close to the experimental value 149° .



	Exp.	(-1, 1)[a]	(-1, 3)	(-1, 5)	(0, 2)	(0, 4)	(0, 6)
Fe(1)-N(1)/ Å	2.181	2.051	2.046	2.062	2.098	2.054	2.349
Fe(1)-N(3)/ Å	2.141	2.051	2.030	1.957	2.026	2.129	2.202
Fe(1)-N(2)/ Å	1.986	1.848	1.934	1.957	1.931	1.958	2.120
Fe(1)-C(30)/ Å	2.031	2.001	2.031	2.043	2.004	2.021	2.067
N(3)-Fe(1)-C(30)/ °	109.02	99.97	101.96	103.11	102.82	101.24	114.56
N(1)-Fe(1)-C(30)/ °	107.20	99.97	99.52	100.79	99.78	104.31	101.66
N(2)-Fe(1)-C(30)/ °	149.44	**149.09**	171.02	166.79	172.04	167.53	162.94

[a] ("-1" represents the charge and "1" represents the spin multiplicity)

Table S3. The relative enthalpies and free energies for the stationary points along the reaction pathways of **1R** catalyzed by **[Fe2]** under M052X/6-31G(d, p) in gas. All values are given in kcal/mol. Energies are relative to **[Fe2]**+**1R** and are mass balanced.

(-1, 1)	ΔH	ΔG	(-1, 3)	ΔH	ΔG	(-1, 5)	ΔH	ΔG
[Fe2](S_0)	0	0	**[Fe2](T_0)**	0	0	**[Fe2](Q_0)**	0	0
2PC(S_0)	-6.2	8.5	**2PC(T_0)**	-7.5	-7.5	**2PC(Q_0)**	12.9	21.8
2PC′(S_0)	-1.1	14.5	**2PC'(T_0)**	24.2	11.9	**2PC'(Q_0)**	30.1	39.7
2TSe1(S_0)	20.0	33.5	**2TSe1(T_0)**	36.8	**48.7**	**2TSe1(Q_0)**	27.7	**39.3**
2IMe5(S_0)	-29.2	-5.2	**2IMe5(T_0)**	-41.1	-42.3	**2IMe5(Q_0)**	7.5	29.0
2TSe3(S_0)	-7.3	20.2	**2TSe3(T_0)**	13.8	**14.5**	**2TSe3(Q_0)**	41.2	**67.8**
2IMe6(S_0)	-25.1	1.0	**2IMe6(T_0)**	-31.2	-35.0	**2IMe6(Q_0)**	4.7	28.7
1Pe(S_0)	-24.9	-12.3	**1Pe(S_0)**	-24.9	-12.3	**1Pe(S_0)**	-24.9	-12.3

(0, 2)	ΔH	ΔG	(0, 4)	ΔH	ΔG
[Fe2](D_0)	0.0	0.0	**[Fe2](Q_0)**	0.0	0.0
2PC(D_0)	5.6	20.0	**2PC(Q_0)**	-5.8	4.1
2PC'(D_0)	-4.1	7.7	**2PC'(Q_0)**	6.2	18.7
2TSe1(D_0)	60.4	**73.1**	**2TSe1(Q_0)**	32.7	**45.8**
2IMe5(D_0)	10.0	32.1	**2IMe5(Q_0)**	-27.7	-4.0
2TSe3(D_0)	17.9	**44.4**	**2TSe3(Q_0)**	5.9	**34.2**
2IMe6(D_0)	-28.1	-4.2	**2IMe6(Q_0)**	-20.7	5.0
1Pe(S_0)	-24.9	-12.3	**1Pe(S_0)**	-24.9	-12.3

Table S4 The NBO charge of the key stationary point along the reaction pathway catalyzed by **[Fe1]** and **[Fe2]**

Catalysts	Reactions	Atoms	1PCa1	1TSa1	1IMa1	1TSa2	1IMa2
[Fe1]	**1PCa1 → 1IMa2** [2+2] cycloaddition	C1-C4	-1.235	-1.409	-1.865	-1.221	-1.258
		Fe	0.353	0.162	0.454	0.318	0.494
		N1	-0.547	-0.474	-0.432	-0.553	-0.601
		N2	-0.515	-0.367	-0.372	-0.520	-0.567
		N3	-0.560	-0.475	-0.433	-0.545	-0.587
	Reactions	**Atoms**	**1PCa1**	**1TSa1**	**1IMa1**	**1TSe2**	**1IMa2**
	1PCa → 1IMa2 β-hydrogen elimination reaction	C1-C4	-1.235	-1.409	-1.865	-1.240	-1.258
		Fe	0.353	0.162	0.454	-0.097	0.494
		N1	-0.547	-0.474	-0.432	-0.470	-0.601
		N2	-0.515	-0.367	-0.372	-0.445	-0.567
		N3	-0.560	-0.475	-0.433	-0.474	-0.587
[Fe2]	**Reactions**	**Atoms**	**2PCa1**	**2TSa1**	**2IMa1**	**2TSa2**	**2IMa2**
	2PCa1 → 2IMa2 [2+2] cycloaddition	C1-C4	-1.153	-0.909	-1.871	-1.230	-1.258
		Fe	0.116	-0.002	0.451	0.311	0.507
		N1	-0.576	-0.493	-0.436	-0.547	-0.599
		N2	-0.524	-0.366	-0.379	-0.516	-0.576
		N3	-0.670	-0.590	-0.444	-0.555	-0.603
	Reactions	**Atoms**	**2IMe5**	**2TSe**	**2IMe6**		
	2PCe → 2IMe6 β-hydrogen elimination reaction	C1-C4	-1.568	-1.478	-1.298		
		Fe	0.708	0.394	0.599		
		N1	-0.600	-0.565	-0.585		
		N2	-0.706	-0.657	-0.667		
		N3	-0.654	-0.610	-0.608		

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Optimized coordinates

[Fe1]

0 1

Fe	0.08497600	-0.09189000	-0.11809100
N	0.04184400	-1.68035400	-1.24335200
N	0.03656100	-2.53623500	-1.93348800
N	2.02558000	0.23984900	-0.20225300
C	1.27847000	2.40641000	-0.11029300
C	-1.13065200	2.39812000	0.04010300
C	1.27188200	3.79740600	-0.05429300
C	-1.14159100	3.77843700	0.09721600
C	0.06738200	4.49250000	0.03541000
H	2.20894100	4.34057400	-0.07330700
H	-2.08052200	4.30964500	0.19546900
H	0.06274200	5.57258300	0.07631900
N	0.06861100	1.70733000	-0.09543500
C	2.38710300	1.52432500	-0.12468700
C	3.78818400	1.98332900	0.17361400
H	4.51554700	1.33522000	-0.30997400
H	3.93699100	2.98747200	-0.22674700
C	4.03846800	1.97900300	1.68953200
H	3.91689400	0.96951900	2.08718600
H	5.05015800	2.31737000	1.91936300
H	3.32564500	2.63432700	2.19189000
C	2.89615400	-0.85221800	-0.03719300
C	2.53276600	-1.73941600	0.99958600
C	3.28314100	-2.88558900	1.22350200
C	4.37822800	-3.17713900	0.41283400
C	4.69297200	-2.33131800	-0.64123800
C	3.95850800	-1.16953800	-0.89808900
H	3.00565500	-3.55571500	2.02924800
H	4.96170600	-4.07224200	0.58654600
H	5.51243700	-2.58261200	-1.30610900
C	1.32088300	-1.41573700	1.83802300
H	1.37024400	-0.41378500	2.26541900
H	0.36557900	-1.50573200	1.26640100
H	1.19476600	-2.14116000	2.64242600
C	4.26185300	-0.35790700	-2.13379900
H	3.46252700	0.35193500	-2.34217500
H	5.19816300	0.19742400	-2.03886700
H	4.36663200	-1.02297700	-2.99279000
C	-2.23917900	1.50005100	0.11628900
C	-3.66052800	1.98200800	0.23391000
H	-4.26711600	1.20671100	0.70438000
H	-3.68304600	2.85432000	0.88988400
C	-4.26027200	2.34416900	-1.13194200
H	-4.29322700	1.46619900	-1.77674500
H	-5.27660200	2.72389200	-1.01754000
H	-3.65552100	3.10550200	-1.62623900
N	-1.89624900	0.22331300	0.02594600
C	-2.87007600	-0.80424200	0.14058800
C	-3.22041900	-1.25231600	1.42855000
C	-3.39104200	-1.42578800	-1.00327900
C	-4.10807600	-2.31708300	1.55303500
C	-4.27859200	-2.49216500	-0.83677900
C	-4.63926100	-2.93841700	0.42619600
H	-4.38070900	-2.66262700	2.54370100
H	-4.68555000	-2.97410200	-1.71905800
H	-5.32674200	-3.76778700	0.53526500
C	-3.02225900	-0.97648600	-2.39660400
H	-2.63424500	-1.81593600	-2.97742700
H	-3.90109000	-0.59869000	-2.92433700
H	-2.26840100	-0.19061800	-2.37551700
C	-2.64055400	-0.57802100	2.64510800
H	-1.55313800	-0.50291200	2.57191400
H	-3.01557400	0.44302000	2.75196100
H	-2.89791900	-1.13127300	3.54808000

Zero-point correction= 0.536035 Hartree

Sum of electronic and thermal Free Energies= -1444.595171 Hartree

Number of imaginary frequencies= 0

1R

0 1

C	1.27427900	-0.22320200	-0.00004800
H	1.27811700	-1.30779700	0.00004700
H	2.23509900	0.27555100	0.00019700
C	0.13488900	0.46014000	-0.00003400
H	0.17031800	1.54630800	0.00010100
C	-1.22951900	-0.16311900	-0.00003400
H	-1.16111400	-1.25136600	-0.00123000
H	-1.79956000	0.14609700	0.87959500
H	-1.80075500	0.14828500	-0.87801300

Zero-point correction= 0.081048 Hartree

Sum of electronic and thermal Free Energies= -117.829839 Hartree

Number of imaginary frequencies= 0

1PCa1

0 1			
0 1			
Fe	0.03363700	-0.08602100	0.30930100
N	-2.00626800	0.32851400	0.01859900
C	-1.09773600	2.45405700	0.01131800
C	1.28595500	2.39288000	0.01451900
C	-1.07548500	3.83953700	0.04294500
C	1.32558000	3.78337700	0.04630500
C	0.14525000	4.52316000	0.04690000
H	-2.00677800	4.39143000	0.06373600
H	2.28264900	4.28915700	0.07957300
H	0.17083700	5.60341900	0.06811100
N	0.07453600	1.71411300	-0.05211800
C	-2.26360400	1.62460800	-0.00253300
C	-3.64732600	2.22013900	-0.09541100
H	-4.37407000	1.50656900	0.29239800
H	-3.68644100	3.09783400	0.55272200
C	-4.03666900	2.61798800	-1.52522400
H	-4.11968800	1.73363100	-2.15516800
H	-4.99988200	3.13030500	-1.52946700
H	-3.28696000	3.27953700	-1.96119500
C	-3.07773500	-0.58185900	-0.20586800
C	-3.29921400	-1.05490600	-1.51505000
C	-4.25842600	-2.04715800	-1.71937600
C	-5.01393900	-2.54787400	-0.66704800
C	-4.83136300	-2.02841300	0.60740400
C	-3.87770800	-1.04116200	0.85626500
H	-4.41307000	-2.42272800	-2.72503100
H	-5.75075600	-3.32174900	-0.84198400
H	-5.43954900	-2.38456500	1.43195000
C	-2.55465200	-0.50435000	-2.71087900
H	-1.73111100	0.14187500	-2.40999300
H	-2.15675200	-1.31644800	-3.32319600
H	-3.23306000	0.06907700	-3.34667300
C	-3.77883900	-0.46808000	2.25014300
H	-3.01746900	0.30531100	2.32005900
H	-4.73644100	-0.02812700	2.53891600
H	-3.54841800	-1.24755600	2.98001800
C	2.39811800	1.51078600	-0.03192200
C	3.81183000	2.02457700	-0.15170500
H	4.42087100	1.29354500	-0.68419700
H	3.81545500	2.93901900	-0.74717700
C	4.43349900	2.29654800	1.22608600
H	4.47292300	1.37841000	1.81303200
H	5.44959400	2.68096300	1.12351200
H	3.83989600	3.02595600	1.77970100
N	2.07766900	0.21954800	0.01803500
C	3.04254700	-0.71004800	-0.46404300
C	3.21612800	-0.80231000	-1.86386200
C	3.77476400	-1.54399100	0.39042900
C	4.07614000	-1.76956100	-2.37643400
C	4.63041700	-2.50092600	-0.16119900
C	4.77647600	-2.62739700	-1.53383600
H	4.19708200	-1.84667000	-3.45121900
H	5.19329400	-3.14344800	0.50744300
H	5.43911300	-3.37758300	-1.94689800
C	3.70126900	-1.39489700	1.88645500
H	3.03758100	-0.57654800	2.15523500
H	3.33683100	-2.30893700	2.35910100
H	4.69378000	-1.18892100	2.29468900
C	2.50168400	0.14703900	-2.79400600
H	1.48165800	0.34681700	-2.45737300
H	3.01603600	1.11179500	-2.83475200
H	2.47750400	-0.25982400	-3.80525500
C	-0.07180300	0.57170900	2.36965000
H	0.88893800	0.99447500	2.65031200
H	-0.87622400	1.27913900	2.22005000
C	-0.29760300	-0.76652700	2.49632800
H	-1.30874600	-1.12595800	2.35737900
C	0.62416200	-1.67435200	3.27032000
H	0.11345900	-1.97792600	4.18883900
H	0.90228800	-2.58487800	2.74129900
H	1.53162200	-1.14978000	3.56016700
C	0.14560600	-2.41433400	0.21234300
H	1.14033000	-2.55796300	0.62409900
C	0.03877200	-1.83859300	-1.01850200
H	0.91076400	-1.58150700	-1.60002100
H	-0.91131700	-1.87777100	-1.53135900
C	-0.97057200	-3.26046100	0.77554900
H	-1.03751800	-3.22836800	1.86284000
H	-1.93326300	-2.96130800	0.35927100
H	-0.79423600	-4.30360500	0.49669700

Zero-point correction= 0.696885 Hartree

Sum of electronic and thermal Free Energies= -1570.727036 Hartree

Number of imaginary frequencies= 0

1PCa2

0 1

Fe	-0.01719500	-0.05197400	0.27463300
N	-2.00533700	0.29941000	0.07934300
C	-1.18759300	2.44927900	-0.04955700
C	1.20804100	2.41484900	-0.14019800
C	-1.17930500	3.83232100	-0.16948800
C	1.22818000	3.79522700	-0.27740300
C	0.03145400	4.51814700	-0.29135500
H	-2.11517900	4.37720800	-0.18326500
H	2.17393600	4.31180800	-0.38277600
H	0.04320800	5.59374800	-0.39717200
N	0.00259000	1.73351800	-0.05896300
C	-2.32125000	1.58564800	-0.00289400
C	-3.72573000	2.09936200	-0.18012900
H	-4.42769700	1.42618000	0.31152100
H	-3.81448000	3.07012900	0.31057100
C	-4.09929700	2.22711800	-1.66391300
H	-4.07992500	1.24800000	-2.14299700
H	-5.10189800	2.64288600	-1.77519800
H	-3.39122200	2.87552600	-2.18182800
C	-3.02204100	-0.69238700	-0.00193300
C	-3.18538600	-1.39505000	-1.21139200
C	-4.11490200	-2.43333900	-1.26718000
C	-4.87629800	-2.77936300	-0.15894300
C	-4.72086600	-2.06805400	1.02334100
C	-3.80650800	-1.01935800	1.12055900
H	-4.23684400	-2.97347400	-2.19980300
H	-5.58842400	-3.59293300	-0.21730700
H	-5.31772200	-2.32168700	1.89268000
C	-2.40350200	-1.04533400	-2.45624200
H	-1.72579300	-0.21083000	-2.28226800
H	-1.81584600	-1.90150400	-2.79478100
H	-3.08523400	-0.78056900	-3.26779600
C	-3.71862700	-0.24443800	2.41357200
H	-2.81565300	0.35892800	2.46354000
H	-4.57322200	0.43006200	2.51542500
H	-3.73473300	-0.92182000	3.26897500
C	2.32042200	1.52151200	-0.17909000
C	3.72370000	2.01456900	-0.43352300
H	4.34804100	1.17073200	-0.72915600
H	3.70317000	2.70887900	-1.27723100
C	4.34830800	2.71413100	0.78412300
H	4.38953800	2.04073800	1.63899200
H	5.36480800	3.03834000	0.55534400
H	3.76730200	3.58725100	1.08017300
N	1.98821200	0.24348500	-0.04029100
C	2.94596700	-0.77509500	-0.31583700
C	2.97076600	-1.29767200	-1.62573600
C	3.80602000	-1.28633600	0.66666500
C	3.81209700	-2.36890000	-1.91049800
C	4.63476100	-2.36435500	0.34224500
C	4.63434600	-2.91516400	-0.92945100
H	3.82422600	-2.77373900	-2.91597800
H	5.29161100	-2.76365900	1.10749200
H	5.27849800	-3.75386400	-1.16187900
C	3.91226500	-0.67988200	2.04420200
H	3.12356000	0.04717700	2.22265600
H	3.86100000	-1.44892300	2.81725900
H	4.87374900	-0.17273800	2.15597100
C	2.13658700	-0.66971300	-2.71226500
H	1.09185700	-0.56979100	-2.41345900
H	2.49165400	0.34108900	-2.93173100
H	2.19637100	-1.25851800	-3.62744800
C	0.05794800	0.22782100	2.37931200
H	1.07018800	0.54049900	2.60549700
H	-0.70802300	0.98499200	2.48969200
C	-0.25511200	-1.09421700	2.23652600
H	-1.30323800	-1.37340300	2.19668700
C	0.71573500	-2.22317700	2.47285200
H	0.75021700	-2.46869700	3.53796000
H	0.41383600	-3.12597100	1.94174400
H	1.71948800	-1.95910800	2.14677600
N	-0.03988800	-2.88942400	-0.80659100
N	-0.04774000	-1.86706700	-0.39572100

Zero-point correction= 0.621118 Hartree

Sum of electronic and thermal Free Energies= -1562.434338 Hartree

Number of imaginary frequencies= 0

1TSa1

0 1

Fe	-0.01932200	-0.03878400	-0.19663200
N	2.02327100	0.36930200	-0.06023500
C	1.10871600	2.48503500	-0.13709000
C	-1.26048500	2.43415000	-0.08427900
C	1.08926700	3.87020500	-0.21939700
C	-1.30215700	3.82068400	-0.14465300
C	-0.12264700	4.55888000	-0.21467000
H	2.02379600	4.41267900	-0.28206100
H	-2.25978300	4.32467300	-0.13861100

H	-0.14672200	5.63795100	-0.26835800
N	-0.05946700	1.75020500	-0.05100000
C	2.27893900	1.65636800	-0.09137500
C	3.65760000	2.26781700	-0.02674700
H	4.39844100	1.51337700	-0.28883400
H	3.71923100	3.05577200	-0.78134900
C	3.99063600	2.84892800	1.35452500
H	4.00944400	2.05998300	2.10451400
H	4.97109700	3.32664800	1.33755400
H	3.24921400	3.58713200	1.66108400
C	3.11140000	-0.53598700	0.11365200
C	3.45200100	-0.96900200	1.40586800
C	4.43568000	-1.95178600	1.54405000
C	5.09484800	-2.47227100	0.44112600
C	4.80053600	-1.97782500	-0.82515800
C	3.82227100	-1.00360500	-1.00980900
H	4.68336500	-2.30155100	2.54032400
H	5.84985300	-3.23823800	0.56567800
H	5.34338000	-2.34354200	-1.68918100
C	2.82680500	-0.39140600	2.65437400
H	2.00091700	0.27875700	2.42264700
H	2.45152500	-1.18902600	3.29847900
H	3.57846800	0.15592500	3.22821500
C	3.59282700	-0.42821800	-2.38601400
H	2.63477000	-0.72735400	-2.80922900
H	3.60340200	0.66328100	-2.36629100
H	4.38011200	-0.76244300	-3.06163900
C	-2.38845400	1.55580700	0.01727400
C	-3.78880400	2.10332000	0.14710000
H	-4.44025000	1.32759900	0.54882700
H	-3.78447500	2.92642000	0.86522000
C	-4.34598400	2.59178300	-1.19961200
H	-4.35695700	1.77978100	-1.92546100
H	-5.36648900	2.95741600	-1.07784300
H	-3.73804400	3.39608900	-1.61377100
N	-2.08003400	0.27864000	0.01237600
C	-3.07965300	-0.66008000	0.40695800
C	-3.27702700	-0.85664900	1.78970400
C	-3.83763600	-1.37867700	-0.52770700
C	-4.14788300	-1.85975500	2.20767100
C	-4.69993000	-2.37702400	-0.06795900
C	-4.84180800	-2.63738300	1.28685100
H	-4.28564800	-2.02351600	3.27042100
H	-5.27583300	-2.94108200	-0.79349300
H	-5.50682500	-3.42169800	1.62591800
C	-3.84609700	-1.02474100	-1.99328600
H	-2.98714300	-0.41626400	-2.26698400
H	-3.86290800	-1.91986500	-2.61649900
H	-4.75115000	-0.45696600	-2.22546500
C	-2.62462600	0.05187200	2.80307500
H	-1.61118600	0.32571700	2.50892200
H	-3.19988900	0.97764900	2.90315400
H	-2.59735000	-0.42781200	3.78180800
C	0.01098300	-0.13948800	-2.12723400
H	-0.93252000	0.13219400	-2.59337100
H	0.84887600	0.44861600	-2.48758600
C	0.22646900	-1.55408800	-1.86011300
H	1.27022300	-1.84516100	-1.91493400
C	-0.67763200	-2.51356400	-2.61638400
H	-0.45415500	-2.45117700	-3.68434200
H	-0.55790900	-3.55094600	-2.30379800
H	-1.71976800	-2.23946200	-2.47586200
C	-0.05613800	-2.31198400	-0.04084600
H	-1.05715100	-2.68552400	-0.24310100
C	-0.00197700	-1.48872800	1.15333800
H	-0.89528100	-1.47569400	1.76106000
H	0.91500000	-1.56504400	1.72197700
C	1.01671100	-3.39199700	-0.10761900
H	1.06921400	-3.90037600	-1.07133100
H	1.99738200	-2.96506300	0.10625400
H	0.80519200	-4.14202800	0.65809600

Zero-point correction= 0.700356 Hartree

Sum of electronic and thermal Free Energies= -1570.703645 Hartree

Number of imaginary frequencies= 1

1IMa1

0 1

Fe	-0.00062900	0.00689800	0.10714000
N	2.04230300	0.41842200	0.10953900
C	1.17206700	2.53923700	-0.29401000
C	-1.16634900	2.55280800	-0.16691800
C	1.19762900	3.91128400	-0.53297900
C	-1.20383600	3.92607900	-0.38812900
C	-0.00573900	4.60972600	-0.58494000
H	2.13793400	4.42887100	-0.66490200
H	-2.14755600	4.45430900	-0.40575100
H	-0.00983700	5.67604000	-0.76579400
N	0.00455200	1.88182500	-0.13758600

C	2.33678700	1.65575200	-0.12820800
C	3.72401800	2.24227300	-0.11680600
H	4.45020000	1.46316900	-0.33438500
H	3.80535100	2.99720300	-0.90128400
C	4.03812500	2.85371200	1.25747400
H	4.04357700	2.07145100	2.01753400
H	5.02066500	3.32599600	1.24749300
H	3.29690700	3.60255400	1.54070800
C	3.08073100	-0.52556900	0.36145500
C	3.20100200	-0.99927600	1.67760400
C	4.17912300	-1.94875900	1.95617000
C	5.00355000	-2.44060300	0.94940000
C	4.85210500	-1.97746300	-0.34971600
C	3.89513200	-1.01208600	-0.67017600
H	4.28055900	-2.31536900	2.97093200
H	5.75186700	-3.18965900	1.17594700
H	5.48043900	-2.36801000	-1.14214900
C	2.26175600	-0.51295700	2.74837500
H	1.24810200	-0.85544800	2.51865100
H	2.55229700	-0.90786400	3.72174900
H	2.23657600	0.57744300	2.80788000
C	3.77525200	-0.52477600	-2.09352300
H	4.48847400	0.27924400	-2.29940700
H	3.99342800	-1.33995100	-2.78402600
H	2.77469300	-0.15633200	-2.30986900
C	-2.32025000	1.67847300	0.10338500
C	-3.69108200	2.28030000	0.27794500
H	-4.31141100	1.57975800	0.83691000
H	-3.58053800	3.18002900	0.88905300
C	-4.38061200	2.64035200	-1.04703700
H	-4.63947800	1.74162400	-1.60267200
H	-5.29904500	3.19330300	-0.84875000
H	-3.73923500	3.25471500	-1.68043600
N	-2.02291600	0.42618300	0.23681700
C	-3.03976500	-0.51677700	0.57588200
C	-3.15176400	-0.86850300	1.93135000
C	-3.85166600	-1.10323400	-0.40119500
C	-4.10661900	-1.80950500	2.30036100
C	-4.79613100	-2.04682300	0.01280900
C	-4.92951500	-2.40082900	1.34654200
H	-4.19884000	-2.08258600	3.34509100
H	-5.42851000	-2.50876400	-0.73714700
H	-5.66700200	-3.13556800	1.64409600
C	-3.72227200	-0.79791400	-1.87307200
H	-3.13036200	0.09407300	-2.06145200
H	-3.22690600	-1.62508400	-2.38578100
H	-4.70930800	-0.67043800	-2.32251500
C	-2.24488400	-0.23546900	2.95182600
H	-1.20174200	-0.46404800	2.71514100
H	-2.34878700	0.85255600	2.96725200
H	-2.46599200	-0.61577500	3.94868700
C	0.02548800	-0.28234600	-1.86008800
H	-0.97024300	-0.09232300	-2.27984500
H	0.72422400	0.36875800	-2.40575400
C	0.37420300	-1.76558300	-2.02821100
H	1.43902100	-1.90725400	-1.79234300
C	0.13732800	-2.25067400	-3.46151100
H	0.64123000	-1.59419700	-4.17658100
H	0.50031600	-3.26841000	-3.62321700
H	-0.93307100	-2.23266800	-3.69379900
C	-0.39470500	-2.56129400	-0.96019000
H	-1.46568800	-2.37107200	-1.12370100
C	-0.00863500	-1.99588300	0.42007500
H	-0.70162200	-2.39610600	1.17562300
H	0.98964400	-2.38781100	0.67162400
C	-0.16388400	-4.07186900	-1.06063600
H	-0.54764400	-4.50159800	-1.99060800
H	0.90813400	-4.28808600	-1.00243500
H	-0.65158600	-4.58187300	-0.22662500

Zero-point correction= 0.696978 Hartree

Sum of electronic and thermal Free Energies= -1570.729831 Hartree

Number of imaginary frequencies= 0

1TSa2

0 1

Fe	-0.08632800	0.02251000	-0.04488000
N	1.86988200	0.56876300	0.15963500
C	0.90375000	2.60363200	-0.34018200
C	-1.48405300	2.43061700	-0.28375000
C	0.80099000	3.96496600	-0.60471100
C	-1.59916200	3.78618800	-0.54129900
C	-0.45101400	4.56779500	-0.71930400
H	1.69860300	4.56154600	-0.70873400
H	-2.58018500	4.24073400	-0.60351600
H	-0.53430800	5.62538700	-0.92581100
N	-0.23939700	1.82439500	-0.19071600
C	2.08688900	1.86073800	-0.07497400
C	3.40777800	2.55004300	0.15089700

H	4.23428500	1.88176600	-0.07788700
H	3.49053700	3.40467800	-0.52214100
C	3.53098300	3.01417200	1.61011400
H	3.50660500	2.15353600	2.28062600
H	4.47134100	3.54429100	1.76936900
H	2.70494900	3.67705300	1.87091700
C	2.94146700	-0.27144700	0.56015800
C	2.89715200	-0.81631800	1.86027300
C	3.88750000	-1.71264700	2.25573800
C	4.91184600	-2.07943700	1.39039200
C	4.95680600	-1.52732000	0.11850800
C	3.99040400	-0.61786500	-0.31555600
H	3.85227200	-2.12234900	3.25898000
H	5.67097600	-2.78290900	1.70836300
H	5.75444400	-1.80117200	-0.56360900
C	1.80670400	-0.43368400	2.83063400
H	0.92483400	-1.06959600	2.71172700
H	2.15932800	-0.55194100	3.85618100
H	1.48004100	0.59516500	2.67863700
C	4.11669300	-0.05289300	-1.71300100
H	4.96507900	0.63317700	-1.77773800
H	4.29516800	-0.85703000	-2.42982100
H	3.22181100	0.48794400	-2.01682200
C	-2.54142900	1.50494700	-0.03888500
C	-3.98070000	1.94997900	0.04269700
H	-4.52739600	1.27578500	0.70352900
H	-4.00821300	2.93958700	0.50179800
C	-4.67771700	2.00123000	-1.32441200
H	-4.76800100	1.00265800	-1.74996100
H	-5.68086800	2.41843700	-1.22417400
H	-4.11235900	2.61986700	-2.02300100
N	-2.13128900	0.25733700	0.13993100
C	-3.09166900	-0.72216800	0.51655300
C	-3.33182200	-0.91352900	1.89054200
C	-3.73737700	-1.51860200	-0.44032300
C	-4.23236600	-1.89783500	2.28707000
C	-4.63740700	-2.49457600	-0.00350700
C	-4.88768300	-2.68783700	1.34677700
H	-4.42107000	-2.04312100	3.34463800
H	-5.14197200	-3.10720900	-0.74266300
H	-5.58765600	-3.44897800	1.66794700
C	-3.45792600	-1.37344000	-1.91642200
H	-2.96228000	-0.43058600	-2.13839500
H	-2.80993600	-2.18254300	-2.26677500
H	-4.38506400	-1.42998100	-2.48974500
C	-2.63146500	-0.04555200	2.90235500
H	-1.55118100	-0.05192100	2.74022500
H	-2.95098000	0.99636400	2.81649900
H	-2.84486100	-0.38799000	3.91475600
C	0.21649200	-0.62799300	-2.01793700
H	-0.70683100	-0.82711500	-2.56150900
H	0.57936700	0.36880200	-2.27724700
C	1.22393400	-1.76145700	-2.19116300
H	2.15119000	-1.47358100	-1.69896700
C	1.50990700	-2.16257200	-3.63080500
H	1.95687400	-1.33414100	-4.18570500
H	2.19949100	-3.00944800	-3.67418500
H	0.58586600	-2.45071000	-4.13948400
C	0.56118300	-2.80973500	-1.29738300
H	-0.12112200	-3.42401200	-1.89615100
C	-0.27881400	-1.85538700	-0.44973700
H	-1.32952700	-2.11625500	-0.37803600
H	0.13563200	-1.69381600	0.59730600
C	1.51304500	-3.71124400	-0.52028200
H	2.12452200	-4.30255700	-1.20600200
H	2.18397600	-3.10960200	0.09865300
H	0.96924800	-4.40157100	0.12839000

Zero-point correction= 0.697883 Hartree

Sum of electronic and thermal Free Energies= -1570.696698 Hartree

Number of imaginary frequencies= 1

1IMa2

0 1

Fe	-0.10555400	0.25115300	-0.00685600
N	1.84504400	0.79326800	-0.09790700
C	0.83092200	2.86245200	-0.14818400
C	-1.55530000	2.62363000	0.04933900
C	0.68806800	4.24280800	-0.18771800
C	-1.69981400	3.99945000	0.02209900
C	-0.57600600	4.82770900	-0.09715900
H	1.56725200	4.86864300	-0.28291800
H	-2.68967200	4.43532600	0.08260900
H	-0.68735100	5.90230100	-0.12321300
N	-0.29032700	2.03615200	-0.01842700
C	2.02831500	2.11376300	-0.19284700
C	3.38327900	2.77050100	-0.26482700
H	4.08640200	2.10928800	-0.77353400
H	3.30023200	3.67370900	-0.87159300

C	3.93853300	3.13054100	1.12051800
H	4.12965000	2.22893200	1.70239700
H	4.87686700	3.67992500	1.02776800
H	3.22418000	3.74728900	1.66793400
C	2.98756900	-0.04611100	-0.07450300
C	3.49501000	-0.50711100	1.15022600
C	4.58961400	-1.37684700	1.13869000
C	5.16528900	-1.79228700	-0.05393100
C	4.65145100	-1.33035500	-1.26264600
C	3.56693700	-0.45725400	-1.29050800
H	4.98706400	-1.72931500	2.08464100
H	6.01064700	-2.46883300	-0.04447400
H	5.09414900	-1.65098400	-2.19893400
C	2.87263600	-0.10286800	2.46518900
H	2.27353200	-0.92052200	2.87770000
H	3.64668100	0.13088800	3.19862400
H	2.22088400	0.76131900	2.34840500
C	2.99561200	0.02830000	-2.59650900
H	3.10028300	1.11062900	-2.70120900
H	3.49853600	-0.44998500	-3.43688400
H	1.92576100	-0.18512800	-2.65471800
C	-2.58385000	1.64898500	0.12523300
C	-4.04109500	2.03000500	0.18342200
H	-4.60582300	1.23930700	0.67891500
H	-4.14290500	2.92872400	0.79439900
C	-4.63404000	2.28327600	-1.20957100
H	-4.60665300	1.37191500	-1.80590700
H	-5.67230100	2.61000800	-1.13238000
H	-4.06331800	3.05042800	-1.73448500
N	-2.14358900	0.39429700	0.09142000
C	-3.08553000	-0.66490600	0.16360600
C	-3.51868800	-1.09764900	1.43299200
C	-3.51922600	-1.31858500	-0.99988700
C	-4.38455200	-2.18430800	1.51838000
C	-4.38763200	-2.40666400	-0.87341700
C	-4.82038700	-2.84150400	0.37088000
H	-4.71709300	-2.51723200	2.49502800
H	-4.72547600	-2.91169900	-1.77206500
H	-5.49293300	-3.68649400	0.44948300
C	-3.07892600	-0.87416800	-2.37500300
H	-2.35764000	-0.06029600	-2.31537800
H	-2.62695600	-1.70395600	-2.92369900
H	-3.93526200	-0.53382300	-2.96164600
C	-3.04257300	-0.38259900	2.67083400
H	-1.95686200	-0.26082000	2.65779800
H	-3.46516000	0.62337000	2.73481700
H	-3.33270200	-0.93151100	3.56665700
C	-0.11635200	-1.91922700	-0.82812100
H	-1.03419700	-2.34705800	-1.22854000
H	0.05910900	-0.96783300	-1.39203400
C	1.05277900	-2.92919300	-0.82154700
H	2.00251600	-2.39389500	-0.75838800
C	1.10020100	-3.98148900	-1.91197600
H	1.31603700	-3.53077800	-2.88336900
H	1.87822400	-4.71908100	-1.70419200
H	0.14399100	-4.50625600	-1.98374100
C	0.61559600	-3.34126800	0.60088300
H	-0.13781800	-4.13210100	0.52092500
C	-0.14969200	-1.99599900	0.72764000
H	-1.12881700	-2.02956800	1.19606900
H	0.48564400	-1.23681100	1.23572000
C	1.66645600	-3.71771300	1.62618000
H	2.12699600	-4.67398100	1.36791900
H	2.45566000	-2.96569200	1.65963100
H	1.22753800	-3.81424700	2.62201200

Zero-point correction= 0.698449 Hartree

Sum of electronic and thermal Free Energies= -1570.745048 Hartree

Number of imaginary frequencies= 0

1Pa

0 1

C	0.76571200	1.35476600	0.10663100
H	1.29413900	1.55071000	-0.82957500
H	1.17894400	1.99143600	0.88875700
C	0.67982300	-0.16697700	0.37126800
H	0.49724300	-0.34130800	1.43731000
C	1.78966400	-1.07055100	-0.13263800
H	2.72296500	-0.89276200	0.40600900
H	1.52617700	-2.12399400	-0.01152700
H	1.97307900	-0.88809200	-1.19448600
C	-0.67979700	-0.16697000	-0.37119400
H	-0.49709100	-0.34143100	-1.43720900
C	-0.76562700	1.35476500	-0.10670100
H	-1.17889300	1.99154800	-0.88868200
H	-1.29391000	1.55059500	0.82964400
C	-1.78977700	-1.07042300	0.13261900
H	-1.52647700	-2.12389000	0.01133300
H	-1.97311800	-0.88809200	1.19450200

H	-2.72304900	-0.89237100	-0.40598700

Zero-point correction= 0.169486 Hartree

Sum of electronic and thermal Free Energies= -235.677071 Hartree

Number of imaginary frequencies= 0

N_2

0 1

N	0.00000000	0.00000000	0.54839600
N	0.00000000	0.00000000	-0.54839600

Zero-point correction= 0.005821 Hartree

Sum of electronic and thermal Free Energies= -109.526962 Hartree

Number of imaginary frequencies= 0

1TSe

0 1

Fe	-0.11593800	-0.07569700	-0.30207900
N	2.00080800	0.30117900	-0.07931000
C	1.19149600	2.41065200	-0.57903200
C	-1.12353500	2.52726400	-0.08977500
C	1.26068000	3.78202200	-0.72968900
C	-1.08288000	3.92359600	-0.21035300
C	0.09445300	4.55321600	-0.56874900
H	2.20950700	4.26556100	-0.91965000
H	-1.97641400	4.50214800	-0.01197800
H	0.13471100	5.62900700	-0.67069300
N	0.00001900	1.77455400	-0.35797200
C	2.32409300	1.52501000	-0.41655500
C	3.73180700	2.06539700	-0.47862900
H	4.41478000	1.27887100	-0.79357600
H	3.77052700	2.84496500	-1.24082200
C	4.19940600	2.62918500	0.87144900
H	4.28105200	1.83023800	1.60856700
H	5.17933300	3.09686400	0.76753600
H	3.49539100	3.37492900	1.24345000
C	3.04063600	-0.54743000	0.41150000
C	3.09587400	-0.70937900	1.81244800
C	4.05439900	-1.55817300	2.35672200
C	4.95061800	-2.24220400	1.54076800
C	4.89428600	-2.06425900	0.16802200
C	3.94936200	-1.21775600	-0.42056900
H	4.09422100	-1.68261700	3.43261300
H	5.68869700	-2.90421100	1.97579200
H	5.59551900	-2.58337600	-0.47627000
C	2.12827000	0.02836600	2.69995900
H	1.09815000	-0.22043000	2.43708600
H	2.30582600	-0.22068400	3.74602900
H	2.22274100	1.10986700	2.57776700
C	3.97931300	-1.04435000	-1.92052200
H	4.94871900	-0.64936900	-2.23449400
H	3.84200900	-2.00483400	-2.42195900
H	3.20338300	-0.36798200	-2.26895600
C	-2.21921600	1.72697800	0.29365200
C	-3.56435500	2.30979500	0.65254100
H	-4.10029000	1.60477000	1.28981700
H	-3.38425400	3.20094300	1.25964700
C	-4.45059700	2.69093600	-0.54156600
H	-4.80172700	1.80274200	-1.06370500
H	-5.32442400	3.25021100	-0.20258900
H	-3.89991300	3.30835100	-1.25337700
N	-1.90952700	0.42100600	0.34472300
C	-2.98334700	-0.49186500	0.55345000
C	-3.19161000	-1.00186600	1.84506300
C	-3.79313400	-0.88943400	-0.52244000
C	-4.19974300	-1.94409900	2.03950500
C	-4.80303700	-1.82405900	-0.28434600
C	-5.00273100	-2.35894100	0.98126700
H	-4.36019900	-2.34597200	3.03348000
H	-5.43044800	-2.13864600	-1.11125600
H	-5.78499800	-3.08936500	1.14621700
C	-3.57215800	-0.37741900	-1.92640900
H	-4.52975200	-0.18087800	-2.41238100
H	-2.97423500	0.53191600	-1.94192600
H	-3.05010000	-1.12230800	-2.53260000
C	-2.36055500	-0.49900200	2.99544100
H	-1.29882200	-0.53439100	2.75007500
H	-2.59752800	0.54564900	3.21426400
H	-2.54784700	-1.08828000	3.89309900
C	0.38215100	-0.53248600	-2.18767300
H	-0.43557300	-0.46271700	-2.91069400
H	1.21286200	0.07833100	-2.54109800
C	0.69770200	-2.00029500	-1.86403100
H	1.69998000	-2.07235100	-1.43928600
C	0.59824200	-2.96273000	-3.04530900
H	1.34010400	-2.68685600	-3.79782200
H	0.78230800	-3.99860700	-2.75049800
H	-0.38424100	-2.90874700	-3.51883700
C	-0.28510900	-2.26002700	-0.69942800

H	-1.07080200	-0.91802100	-1.04627000
C	0.14016500	-2.03430900	0.60860600
H	-0.53523600	-2.28538000	1.41868900
H	1.19197200	-1.97722900	0.84338500
C	-1.49615400	-3.14000800	-0.94204900
H	-2.04209000	-2.88645400	-1.84970900
H	-1.13513300	-4.16663100	-1.04823500
H	-2.18124100	-3.10203700	-0.09646700

Zero-point correction= 0.695471 Hartree

Sum of electronic and thermal Free Energies= -1570.671599 Hartree

Number of imaginary frequencies= 1

1IMe

0 1

Fe	-0.03649100	0.03712000	-0.12114600
N	2.02943400	0.39783400	-0.09244800
C	1.20437400	2.53477000	-0.41919100
C	-1.17807500	2.59104800	-0.17839700
C	1.22231600	3.91273900	-0.59299800
C	-1.16763400	3.96932800	-0.32219900
C	0.03672900	4.64842300	-0.53305300
H	2.16427200	4.42056500	-0.75801000
H	-2.10026600	4.51858300	-0.27894500
H	0.04919200	5.72253800	-0.65230700
N	0.00804600	1.86172800	-0.18357200
C	2.32763500	1.67577700	-0.34737300
C	3.73477200	2.20733600	-0.48221100
H	4.37919600	1.43244300	-0.89823700
H	3.71868500	3.02302600	-1.20659600
C	4.34093500	2.71157700	0.83546500
H	4.53347200	1.88172400	1.51508700
H	5.28838400	3.21953300	0.64747400
H	3.66189800	3.41240800	1.32413300
C	3.10961300	-0.46097100	0.24804500
C	3.38647300	-0.65577700	1.61816100
C	4.39554000	-1.54399700	1.98348100
C	5.13017700	-2.23066200	1.02122700
C	4.86246300	-2.01899900	-0.32332000
C	3.86062700	-1.13388500	-0.72922000
H	4.60655700	-1.69522600	3.03596500
H	5.90981600	-2.91980400	1.32065100
H	5.43923200	-2.53869800	-1.08094300
C	2.59808000	0.08544600	2.66916900
H	1.54301600	-0.19623700	2.64979100
H	2.99990700	-0.12334700	3.66092300
H	2.62328900	1.16261600	2.49898000
C	3.62920100	-0.89787600	-2.20244000
H	4.49749000	-0.41079400	-2.65327200
H	3.47811800	-1.84374100	-2.72886200
H	2.76220700	-0.26049400	-2.36627800
C	-2.31066200	1.76928700	0.03800700
C	-3.68796800	2.35339000	0.24139400
H	-4.29516300	1.65433200	0.81803000
H	-3.58938500	3.25910300	0.84329000
C	-4.41103500	2.69393300	-1.06969000
H	-4.60560400	1.79344400	-1.64997800
H	-5.36717900	3.17814600	-0.86365000
H	-3.80637900	3.36470100	-1.68142700
N	-2.02710600	0.46601900	0.09855400
C	-3.08151500	-0.42589000	0.42603600
C	-3.28550600	-0.74095800	1.78420300
C	-3.88287500	-1.00576700	-0.56739800
C	-4.26771400	-1.66790200	2.12298100
C	-4.86851900	-1.92102700	-0.18888400
C	-5.05767700	-2.26334000	1.14209100
H	-4.42039400	-1.91592600	3.16734500
H	-5.48562200	-2.37288800	-0.95829600
H	-5.82032900	-2.98080800	1.41828400
C	-3.68373800	-0.70275600	-2.03267600
H	-2.93523800	0.07341400	-2.18127300
H	-3.36473600	-1.59992900	-2.57146900
H	-4.62060000	-0.37865300	-2.49059500
C	-2.47440800	-0.04678800	2.84666800
H	-1.41189600	-0.05325600	2.59681400
H	-2.76508700	1.00454900	2.92666000
H	-2.62735200	-0.51763200	3.81798600
C	0.05943500	-1.38776100	-2.35606000
H	0.68165300	-1.32586200	-3.25088900
H	-0.95943200	-1.62641500	-2.65968600
C	0.61729800	-2.44890800	-1.39558400
H	1.62474900	-2.15703700	-1.09925900
C	0.69326200	-3.80575800	-2.10032700
H	1.38708100	-3.74747600	-2.94151000
H	1.04722500	-4.58073200	-1.41854200
H	-0.28087600	-4.10692700	-2.49111300
C	-0.23578400	-2.48598500	-0.14165300
H	0.04910700	-0.34288300	-1.97924600
C	0.23554300	-2.04342200	1.04239500

H	-0.39028200	-2.09391000	1.92636300
H	1.27682600	-1.78382600	1.16843000
C	-1.56849400	-3.17592800	-0.24625600
H	-2.12100700	-2.88833600	-1.13960300
H	-1.38316700	-4.25245700	-0.31084600
H	-2.19245400	-2.98418200	0.62433600

Zero-point correction= 0.697349 Hartree

Sum of electronic and thermal Free Energies= -1570.748317 Hartree

Number of imaginary frequencies= 0

1Pe

0 1

C	2.36938000	3.62010200	-0.69971100
H	2.63387800	3.51546900	0.35612900
H	3.09365800	4.29697500	-1.15988900
C	0.95806600	4.17960500	-0.85062800
H	0.75001400	4.29555900	-1.92306900
C	0.87553000	5.57308700	-0.20886300
H	1.66015500	6.22145200	-0.60638300
H	-0.08568900	6.05469500	-0.39302700
H	1.01600200	5.49274600	0.87249000
C	0.13213700	2.08126100	0.24743800
H	-0.68357400	1.44508100	0.57819900
H	1.13669900	1.69011600	0.34709900
C	-0.12402100	3.26643200	-0.31035500
C	-1.54360300	3.74280900	-0.48457800
H	-1.76370600	4.60225200	0.15625800
H	-1.71564600	4.05581100	-1.51923400
H	-2.25152000	2.94948100	-0.25070800
H	2.46987400	2.64194600	-1.17049400

Zero-point correction= 0.167722 Hartree

Sum of electronic and thermal Free Energies= -235.683664 Hartree

Number of imaginary frequencies= 0

[Fe2]

-1 1

Fe	-0.00001600	0.22621200	0.42081200
N	2.01576000	0.55327400	0.22844800
C	1.20552800	2.64634600	-0.35140400
C	-1.20553500	2.64635100	-0.35141700
C	1.21112600	3.97924000	-0.73074300
C	-1.21111800	3.97924500	-0.73075900
C	0.00000600	4.65457000	-0.94072200
H	2.14801600	4.51037500	-0.84763600
H	-2.14800100	4.51038500	-0.84768500
H	0.00000700	5.69674100	-1.23302500
N	-0.00000400	1.96067000	-0.21703000
C	2.32347200	1.82580400	-0.05620500
C	3.73926600	2.33759400	-0.05890400
H	3.81146300	3.27875900	-0.60126100
H	4.11487800	2.49704300	0.95603300
C	3.04414200	-0.27149800	0.74008200
C	3.43692400	-0.02125800	2.06342800
C	4.42007700	-0.76483600	2.69647800
C	5.03407800	-1.79844700	2.00102600
C	4.64509300	-2.06351400	0.69281200
C	3.65687100	-1.32875100	0.02393800
H	4.69163700	-0.54591400	3.72273100
H	5.80362900	-2.40226700	2.46747700
H	5.13890800	-2.87584200	0.17879100
C	3.28215400	-1.68467600	-1.42310800
C	-2.32347700	1.82581200	-0.05621200
N	-2.01574600	0.55328000	0.22844800
C	-3.04412500	-0.27150200	0.74008800
C	-3.43690600	-0.02124900	2.06343400
C	-3.65684300	-1.32876500	0.02395600
C	-4.42004700	-0.76483100	2.69649500
H	-2.91161500	0.77034400	2.58435200
C	-4.64505000	-2.06353800	0.69284600
C	-5.03403300	-1.79846200	2.00105700
H	-4.69160900	-0.54589900	3.72274500
H	-5.13885300	-2.87588200	0.17883800
H	-5.80357200	-2.40228900	2.46751800
C	-0.00000900	-1.03009000	1.97772700
H	0.89221400	-1.03036100	2.61167200
H	-0.89210200	-1.03008200	2.61185400
H	-0.00022600	-2.00685100	1.45039600
H	2.91162500	0.77032100	2.58436000
C	4.13933200	-2.83190400	-1.97623400
H	3.99639900	-3.75505800	-1.40997300
H	3.83612200	-3.02435300	-3.00808500
H	5.20341900	-2.58177500	-1.97944800
C	1.81525100	-2.13476600	-1.48873200
H	1.15575900	-1.31464600	-1.21185000
H	1.56794500	-2.45032200	-2.50784100
H	1.63504400	-2.97034700	-0.80838700
C	3.48557400	-0.47981300	-2.35744000
H	2.84083500	0.35016300	-2.07660400

H	4.52784900	-0.14862900	-2.33449100
H	3.24392600	-0.77218200	-3.38401700
C	-3.73927500	2.33758100	-0.05892000
H	-3.81145800	3.27881200	-0.60116500
H	-4.11493800	2.49690200	0.95601700
H	-4.40664500	1.61340400	-0.53148200
H	4.40666400	1.61337000	-0.53135200
C	-3.28215900	-1.68467600	-1.42310400
C	-4.13931900	-2.83192800	-1.97621000
H	-5.20341500	-2.58183700	-1.97939100
H	-3.83613400	-3.02436000	-3.00807200
H	-3.99633400	-3.75507800	-1.40995700
C	-3.48565900	-0.47981100	-2.35741700
H	-4.52794700	-0.14867200	-2.33442700
H	-2.84094000	0.35018900	-2.07660200
H	-3.24403700	-0.77216000	-3.38400700
C	-1.81524600	-2.13471800	-1.48880700
H	-1.15576500	-1.31458600	-1.21193200
H	-1.63497500	-2.97031100	-0.80849400
H	-1.56798500	-2.45023800	-2.50793800

Zero-point correction= 0.617712 Hartree

Sum of electronic and thermal Free Energies= -1453.525307 Hartree

Number of imaginary frequencies= 0

2PC

-1 1

Fe	-0.00516600	0.21460000	-0.73461800
N	-2.03199000	0.51063700	-0.44593900
C	-1.23613400	2.63790200	-0.01607100
C	1.15565200	2.66992800	0.01750900
C	-1.26638000	3.99665700	0.26865000
C	1.14637900	4.02633400	0.30112500
C	-0.07318100	4.70099400	0.45637600
H	-2.21238900	4.51982000	0.33669700
H	2.07551400	4.57563100	0.38849200
H	-0.08972600	5.75998200	0.67888000
N	-0.02768100	1.95083300	-0.06286100
C	-2.35067200	1.78855700	-0.23954300
C	-3.77773200	2.26312700	-0.19523400
H	-3.83450400	3.34407200	-0.08894200
H	-4.30380400	1.97898800	-1.10979700
C	-3.08279900	-0.40889600	-0.64103800
C	-3.45208100	-0.63749100	-1.97966300
C	-4.44593400	-1.53453500	-2.32916800
C	-5.09945900	-2.24088000	-1.32335100
C	-4.73778600	-2.02540300	-0.00259100
C	-3.73691100	-1.11951700	0.39022300
H	-4.70246400	-1.68514600	-3.37133500
H	-5.87926700	-2.95452200	-1.56179600
H	-5.25868400	-2.58800400	0.76308400
C	-3.48181400	-1.01146500	1.91017900
C	2.30253000	1.84704700	-0.17002600
N	2.02870500	0.56732600	-0.40287300
C	3.11965300	-0.31597200	-0.54768000
C	3.64535700	-0.43694600	-1.84652400
C	3.67350600	-1.08731300	0.49896500
C	4.67937600	-1.30493800	-2.14857400
H	3.17516300	0.16562500	-2.61401200
C	4.71174700	-1.96973200	0.15236800
C	5.21530000	-2.09225100	-1.13348800
H	5.05133900	-1.37702500	-3.16393400
H	5.15258800	-2.58279400	0.92941200
H	6.01766400	-2.79154500	-1.33676100
H	-2.90254700	-0.07879400	-2.72825600
C	-4.78928400	-0.58913300	2.60968500
H	-5.59564700	-1.30634500	2.44786900
H	-4.61727700	-0.51061700	3.68703400
H	-5.12439100	0.38440700	2.24661600
C	-3.07264800	-2.39674900	2.44982900
H	-2.13619100	-2.72553300	1.99745400
H	-2.92927900	-2.33875400	3.53258800
H	-3.82991500	-3.15637500	2.24963800
C	-2.39628100	-0.01835400	2.35354500
H	-1.43204700	-0.21583700	1.88844700
H	-2.65735800	1.01410600	2.12283500
H	-2.29219900	-0.10492500	3.44008800
C	3.71268600	2.35742500	-0.04221900
H	3.73402700	3.42271900	0.17447900
H	4.27597900	2.17977900	-0.96157600
H	4.24553200	1.83285400	0.75654000
H	-4.32450000	1.80650300	0.63565800
C	3.30111600	-1.03792900	1.99804000
C	4.55115400	-0.61412600	2.79590200
H	4.89343300	0.37289600	2.47831700
H	4.30512600	-0.56395500	3.86049100
H	5.37814900	-1.31532800	2.67140000
C	2.17232600	-0.07264500	2.38874000
H	2.43301600	0.96895900	2.20111300

H	1.24841900	-0.27594200	1.84989900
H	1.99386500	-0.18772400	3.46295900
C	2.87769700	-2.44095300	2.47563700
H	1.96023100	-2.75744800	1.97865200
H	3.64521200	-3.19312900	2.28696100
H	2.68928200	-2.41451900	3.55272200
C	0.01187200	-1.83893100	-0.21163100
H	0.98632200	-2.09171800	0.19111300
H	-0.83042300	-1.89263900	0.46656000
C	-0.16675000	-1.80636800	-1.57326800
H	-1.17751800	-1.78776300	-1.96373100
C	0.89024600	-2.26166100	-2.54244900
H	0.97083600	-1.58602600	-3.39569000
H	1.86374400	-2.32213000	-2.05637000
H	0.64299600	-3.25872300	-2.92591200
C	-0.03022700	0.70567700	-2.68047300
H	-0.42172300	1.73194600	-2.71108300
H	0.98297700	0.73620400	-3.10449600
H	-0.64160900	0.09882100	-3.36323100

Zero-point correction= 0.703153 Hartree

Sum of electronic and thermal Free Energies= -1571.9793527 Hartree

Number of imaginary frequencies= 0

2TSe1

-1 1

Fe	0.09367800	0.23292900	-0.72424700
N	-1.96636800	0.47427300	-0.57056700
C	-1.26259600	2.64788700	-0.17896400
C	1.12513900	2.76386400	0.00732000
C	-1.35773000	4.00712300	0.08305100
C	1.04841500	4.12016200	0.28244400
C	-0.20137800	4.75243500	0.34660700
H	-2.32342300	4.49765700	0.08523300
H	1.95042000	4.70184900	0.42820700
H	-0.26899200	5.81121000	0.56018700
N	-0.03058300	2.00600400	-0.14231100
C	-2.33199600	1.75358600	-0.44083800
C	-3.76620300	2.20016200	-0.53077600
H	-3.83192400	3.28211900	-0.62322300
H	-4.24635100	1.75112600	-1.40292400
C	-2.99814500	-0.47491700	-0.74659900
C	-3.19849100	-0.91916200	-2.06435400
C	-4.18461200	-1.83135000	-2.39583100
C	-5.00381500	-2.33345100	-1.38953100
C	-4.79372600	-1.92268400	-0.08210000
C	-3.79672000	-1.00678400	0.29390300
H	-4.31182900	-2.14586600	-3.42516300
H	-5.78914900	-3.04546400	-1.61435400
H	-5.43009500	-2.34179100	0.68821200
C	-3.66911200	-0.73971700	1.81296100
C	2.30112100	1.98063600	-0.12421100
N	2.07326900	0.69090800	-0.38397000
C	3.19459600	-0.15542500	-0.51294800
C	3.79361700	-0.20498800	-1.78376200
C	3.70094000	-0.96744700	0.52477000
C	4.85288900	-1.04827000	-2.07057600
H	3.37037600	0.43809700	-2.54550800
C	4.76938600	-1.81901500	0.19622000
C	5.34323300	-1.87584800	-1.06545600
H	5.28032700	-1.06857100	-3.06631300
H	5.16230000	-2.47693000	0.96171600
H	6.16127300	-2.55978600	-1.25813400
H	-2.53761000	-0.50790200	-2.81660800
C	-4.99899800	-0.18058400	2.35545200
H	-5.82769400	-0.87503200	2.20563000
H	-4.90337200	0.00400600	3.42935800
H	-5.25785400	0.76221700	1.87147700
C	-3.39437500	-2.07804700	2.53256900
H	-2.42740700	-2.48486800	2.23574000
H	-3.37600900	-1.90894500	3.61311200
H	-4.15934900	-2.82625300	2.32072400
C	-2.54922000	0.21990000	2.24415000
H	-1.57681400	-0.08564700	1.85902600
H	-2.72025200	1.24486900	1.91677400
H	-2.51336900	0.21819100	3.33834400
C	3.68792900	2.52137500	0.09292400
H	3.66516500	3.57708300	0.35377400
H	4.30637800	2.39820500	-0.79974200
H	4.19278900	1.97825400	0.89862000
H	-4.34891800	1.89398800	0.34227100
C	3.18136600	-1.05684000	1.97405300
C	4.35923700	-0.84585900	2.94615200
H	4.80765500	0.13905200	2.79414200
H	3.99265500	-0.89957600	3.97486400
H	5.14245500	-1.59657800	2.83270400
C	2.09803400	-0.04531700	2.37440600
H	2.43660900	0.98726900	2.27976400
H	1.19650500	-0.15507400	1.77455500

H	1.84906200	-0.22546800	3.42537100
C	2.58723800	-2.46159500	2.18765200
H	1.72650500	-2.60286100	1.53119200
H	3.31776500	-3.24726100	1.98229500
H	2.25534500	-2.56632200	3.22532200
C	-0.57151200	-2.60159600	-0.05781500
H	-0.45592500	-3.66436900	0.17307100
H	-1.40594100	-2.09672300	0.40808100
C	0.26920900	-1.96394000	-0.88168800
H	0.09285900	-0.91811400	-1.82824900
C	1.37410000	-2.77728000	-1.52835300
H	2.35057400	-2.53308600	-1.10606700
H	1.20871100	-3.85325700	-1.40240600
H	1.44209100	-2.56341900	-2.60009500
C	0.12993300	0.11169800	-2.86825300
H	-0.45796100	1.02531300	-2.97008400
H	1.15680300	0.30531100	-3.18329900
H	-0.29076000	-0.63335700	-3.55471200

Zero-point correction= 0.6975601 Hartree

Sum of electronic and thermal Free Energies= -1571.9328357 Hartree

Number of imaginary frequencies= 1

2IMe1

-1 1

Fe	-0.06555100	0.26946900	0.33812400
N	1.96322500	0.65578500	0.21444700
C	1.10850600	2.59272900	-0.72727500
C	-1.28472300	2.44380200	-0.96853400
C	1.12629700	3.83968500	-1.30453600
C	-1.28064300	3.71406400	-1.56707200
C	-0.10070300	4.41518000	-1.73426100
H	2.05227000	4.38493900	-1.43091800
H	-2.21545400	4.15896200	-1.88785600
H	-0.10740500	5.39638000	-2.19143200
N	-0.06140600	1.88967800	-0.55622800
C	2.25078000	1.85051700	-0.25023600
C	3.65483000	2.38942800	-0.29094900
H	3.70496200	3.32448500	-0.84300400
H	4.03300200	2.55892300	0.72034900
C	3.02021500	-0.13441200	0.72816100
C	3.35134900	0.08893800	2.07287400
C	4.33438900	-0.64357900	2.71305500
C	4.99529100	-1.64443400	2.00744600
C	4.66024500	-1.87560100	0.68231900
C	3.68351700	-1.13573800	-0.00643100
H	4.56386800	-0.45310900	3.75455800
H	5.75724800	-2.24877700	2.48524200
H	5.17366400	-2.67337200	0.16062700
C	3.40165700	-1.55039700	-1.46467700
C	-2.36546700	1.60487300	-0.70131100
N	-2.02068600	0.40593700	-0.14744000
C	-3.06197400	-0.42260200	0.31136000
C	-3.85516800	0.06128800	1.36667500
C	-3.34110000	-1.71154500	-0.21455900
C	-4.87966900	-0.68092900	1.93152600
H	-3.61136800	1.04655400	1.74667200
C	-4.37335200	-2.44240900	0.38747600
C	-5.13705200	-1.95499300	1.44263100
H	-5.45793600	-0.27256300	2.75264900
H	-4.60701300	-3.43039700	0.01682400
H	-5.92358600	-2.56695400	1.86837000
H	2.77554300	0.84039300	2.59818200
C	4.72914600	-1.67352700	-2.23846000
H	5.38952700	-2.44079000	-1.83379700
H	4.51669500	-1.93685400	-3.27788700
H	5.26581100	-0.72172600	-2.22947500
C	2.70548400	-2.92289000	-1.43246000
H	1.75861800	-2.85205800	-0.89451100
H	2.50041800	-3.26432100	-2.45174800
H	3.32586300	-3.67129900	-0.93457100
C	2.51725200	-0.59787500	-2.28426400
H	1.51883400	-0.48359300	-1.86573400
H	2.95899000	0.39661000	-2.36966500
H	2.42764500	-1.01232200	-3.29314200
C	-3.78357300	1.94958500	-1.06842300
H	-3.80456700	2.76884400	-1.78629800
H	-4.39028900	2.24023400	-0.20529700
H	-4.27827800	1.08683900	-1.52278800
H	4.32683200	1.66726300	-0.76128600
C	-2.59386700	-2.30077000	-1.42175800
C	-3.22561800	-3.61679600	-1.90182500
H	-4.27749300	-3.48765700	-2.16857800
H	-2.68988700	-3.95419900	-2.79226300
H	-3.14720500	-4.40553400	-1.15010900
C	-2.63139800	-1.32709400	-2.61344100
H	-3.66626800	-1.11956000	-2.90082600
H	-2.13509600	-0.38998300	-2.37098500
H	-2.12460100	-1.78263200	-3.47022700

C	-1.13338800	-2.61185200	-1.06159700
H	-0.58421800	-1.69082700	-0.86615100
H	-1.07380000	-3.24183000	-0.17197400
H	-0.64770600	-3.12530200	-1.89855300
C	0.50599000	-1.65864300	2.30493100
H	0.40316500	-2.28212600	3.19936900
H	1.14070500	-2.07715200	1.52315900
C	-0.09331900	-0.46110200	2.17905900
H	-1.15811600	2.57918600	1.79848200
C	-0.87893400	0.05279100	3.35998100
H	-1.91746800	0.24605400	3.08330000
H	-0.87315300	-0.64362000	4.21100000
H	-0.46761700	1.00899700	3.70031500
C	-1.52036200	3.56237900	2.09956200
H	-1.04097400	4.31260800	1.47140300
H	-2.59992800	3.61189500	1.95304400
H	-1.28564200	3.74496900	3.14892800

Zero-point correction= 0.7007121 Hartree

Sum of electronic and thermal Free Energies= -1571.978926- Hartree

Number of imaginary frequencies= 0

2IMe2

-1 1

Fe	-0.12911800	0.33574600	0.45711900
N	1.91196500	0.65653400	0.34949700
C	1.11836400	2.74115300	-0.28515600
C	-1.28617000	2.72033600	-0.46875100
C	1.18172800	4.04904100	-0.70078800
C	-1.23642500	4.05976100	-0.89914100
C	-0.03167000	4.72354800	-1.01522000
H	2.12755900	4.56642200	-0.79007800
H	-2.15659600	4.58231600	-1.13363000
H	-0.00639800	5.75482900	-1.34386900
N	-0.07425200	2.07298000	-0.17432600
C	2.24020100	1.89160300	0.05157500
C	3.66501600	2.37433000	0.04716500
H	3.74084400	3.38424700	-0.34741600
H	4.07939900	2.36121400	1.05827800
C	2.94277500	-0.23739100	0.73102600
C	3.29059300	-0.21812000	2.09064400
C	4.25935700	-1.05911400	2.60722100
C	4.88996300	-1.96320600	1.75764700
C	4.53651600	-1.99476100	0.41794600
C	3.57028900	-1.14292100	-0.14522000
H	4.50226800	-1.02525400	3.66241600
H	5.64251300	-2.64574600	2.13433700
H	5.02745900	-2.71847200	-0.22089100
C	3.27771600	-1.33631400	-1.64641700
C	-2.38920300	1.88425800	-0.32265500
N	-2.07805200	0.59740200	0.02926300
C	-3.13717500	-0.26328200	0.35866300
C	-3.96808000	0.10127400	1.43482700
C	-3.40527700	-1.48373900	-0.31858800
C	-5.01700200	-0.69041000	1.87235600
H	-3.73574300	1.03284900	1.93635200
C	-4.46412400	-2.26755300	0.15666000
C	-5.26566400	-1.89690200	1.23099800
H	-5.62201700	-0.37274900	2.71420200
H	-4.69031000	-3.20354700	-0.33430400
H	-6.07218000	-2.54472200	1.55378200
H	2.74040400	0.46469800	2.72485100
C	4.59663800	-1.27913800	-2.44153600
H	5.30406200	-2.05409800	-2.14503200
H	4.38407000	-1.41156800	-3.50580800
H	5.08009000	-0.30836900	-2.30808500
C	2.63880200	-2.72605400	-1.82325300
H	1.70874600	-2.78577300	-1.25573800
H	2.41377600	-2.90349100	-2.87923000
H	3.30182200	-3.52033600	-1.47455600
C	2.33744000	-0.31024300	-2.29621900
H	1.35046900	-0.29247200	-1.83661500
H	2.74132700	0.70233900	-2.25142800
H	2.22695600	-0.58136700	-3.35073900
C	-3.79108800	2.30676900	-0.67353100
H	-3.77931800	3.23864500	-1.23798100
H	-4.43682200	2.44767200	0.19786700
H	-4.26861900	1.54211200	-1.29356300
H	4.29003600	1.71203900	-0.55736100
C	-2.60888900	-1.95091900	-1.54729100
C	-3.26689000	-3.15983900	-2.23211400
H	-4.29676600	-2.94418800	-2.52713300
H	-2.69851600	-3.40037000	-3.13374800
H	-3.26203600	-4.04622900	-1.59385800
C	-2.51645800	-0.83853400	-2.60778100
H	-3.51856000	-0.53674900	-2.92620200
H	-1.99071600	0.03170100	-2.22183900
H	-1.98026500	-1.21797500	-3.48368500
C	-1.19621600	-2.39131900	-1.13487700

H	-0.61909600	-1.54247500	-0.76607000
H	-1.23610400	-3.14474300	-0.34587100
H	-0.66925400	-2.80444700	-2.00155600
C	0.35905700	-1.70668700	2.44330000
H	0.24908600	-2.25935500	3.38213500
H	0.93516900	-2.21670900	1.67086300
C	-0.16773700	-0.48481000	2.25381900
C	-0.90184100	0.15428000	3.40744000
H	-1.94410100	0.33900500	3.13833300
H	-0.88525700	-0.45872100	4.32056200
H	-0.46523900	1.13141700	3.63969200

Zero-point correction= 0.652898 Hartree

Sum of electronic and thermal Free Energies= -1531.469091 Hartree

Number of imaginary frequencies= 0

2IMe3

-1 1

Fe	-0.09616000	0.28902700	0.75304500
N	2.03512200	0.60621000	0.37227200
C	1.13900500	2.63108000	-0.35615600
C	-1.24684600	2.64935800	-0.36805000
C	1.19006100	3.93773800	-0.78722700
C	-1.21969800	3.98040000	-0.81749900
C	-0.02241300	4.62381800	-1.05582100
H	2.13397700	4.44939900	-0.91310500
H	-2.14977800	4.51546300	-0.96673000
H	-0.00533900	5.64822300	-1.40453000
N	-0.04085900	1.94055600	-0.22628900
C	2.29576000	1.82276900	-0.05119500
C	3.69866100	2.30668400	-0.31625700
H	3.72727900	3.37988000	-0.47967800
H	4.35247600	2.06046900	0.52102800
C	3.16193200	-0.24422700	0.51915900
C	3.73980400	-0.29021700	1.79466100
C	4.84199900	-1.07830400	2.07670700
C	5.39183500	-1.84995500	1.05911600
C	4.82169100	-1.80835300	-0.20462300
C	3.70430000	-1.02138700	-0.52742600
H	5.26073500	-1.09266600	3.07593300
H	6.25043400	-2.48400800	1.24496300
H	5.25729500	-2.42868800	-0.97816200
C	3.17742200	-1.15675800	-1.97413600
C	-2.36872700	1.86922400	-0.08452500
N	-2.08920000	0.59054900	0.28710800
C	-3.20860300	-0.26039800	0.39868800
C	-3.91205700	-0.24521100	1.61124100
C	-3.65036900	-1.10763000	-0.65155100
C	-5.01355500	-1.05485200	1.84343500
H	-3.54822700	0.43048100	2.37733700
C	-4.76793600	-1.91111200	-0.38476100
C	-5.44315200	-1.90212300	0.83179000
H	-5.52345400	-1.02460900	2.79957800
H	-5.13523000	-2.57786000	-1.15172300
H	-6.29782200	-2.55239300	0.97764500
H	3.28343800	0.32387600	2.55946100
C	4.30899200	-0.80944600	-2.96101500
H	5.17188700	-1.46924000	-2.85705800
H	3.93608800	-0.90343300	-3.98453700
H	4.64950700	0.21855000	-2.81732900
C	2.74692700	-2.62012600	-2.20324300
H	1.90570500	-2.86758400	-1.55407200
H	2.43486100	-2.74585000	-3.24424100
H	3.55783200	-3.32343100	-2.00461200
C	1.96759900	-0.28892300	-2.34734500
H	1.11890600	-0.46737600	-1.68933100
H	2.18865800	0.77900400	-2.32849800
H	1.67462600	-0.54984900	-3.36919500
C	-3.78068800	2.36083200	-0.26216700
H	-3.79892000	3.37025600	-0.66834500
H	-4.32558800	2.36401100	0.68612000
H	-4.34357100	1.71038700	-0.93703900
H	4.11477600	1.81125400	-1.19806600
C	-2.92668200	-1.26067600	-2.00636900
C	-3.84095700	-1.91638300	-3.05676900
H	-4.77451400	-1.36092700	-3.18171000
H	-3.31783200	-1.92620400	-4.01546800
H	-4.07959200	-2.95302600	-2.81178400
C	-2.43993400	0.06683100	-2.61758500
H	-3.25579000	0.78844200	-2.70733200
H	-1.63670200	0.50946300	-2.03393800
H	-2.06267800	-0.13773200	-3.62453700
C	-1.70797000	-2.17615700	-1.80815500
H	-1.01786000	-1.75823800	-1.07507900
H	-2.01942800	-3.16263600	-1.45321600
H	-1.17900300	-2.29886300	-2.75992000
C	0.94390700	-2.58119600	1.00267900
H	0.88940400	-3.65172500	1.23224600
H	1.90632000	-2.24527500	0.64469300

C	-0.10998900	-1.76137600	1.17932300
C	-1.33113900	-2.49139200	1.72593600
H	-2.16570300	-2.47177100	1.02255300
H	-1.11434100	-3.54402100	1.95581100
H	-1.71330000	-2.02847500	2.64225500
C	-0.36107500	0.35219300	3.03401200
H	-1.37800100	-0.02093500	3.04509200
C	-0.13861700	1.59004900	2.52393600
H	0.84163000	2.05169600	2.59996700
H	-0.94616000	2.21489300	2.16468200
C	0.63399700	-0.40368100	3.87060000
H	0.28481900	-0.44290200	4.90799500
H	0.77143400	-1.41931100	3.50157000
H	1.60054500	0.10079800	3.86305300

Zero-point correction= 0.738666 Hartree

Sum of electronic and thermal Free Energies= -1649.3627387 Hartree

Number of imaginary frequencies= 0

2TSe2

-1 1

Fe	0.08117300	0.22769300	-0.72021400
N	-2.05750100	0.62898100	-0.39488700
C	-1.11875400	2.73922700	-0.09421700
C	1.26354900	2.73210400	-0.16478900
C	-1.15664600	4.10757200	0.05426600
C	1.25288200	4.13130600	-0.00405900
C	0.06895300	4.82159300	0.13411000
H	-2.09368100	4.64538500	0.07870400
H	2.18832100	4.67775800	-0.00773700
H	0.06798300	5.89729400	0.25652900
N	0.04789300	2.02466800	-0.10419400
C	-2.29346900	1.90833800	-0.22394900
C	-3.69209200	2.45591400	-0.09222800
H	-4.21874300	1.96189100	0.72904600
H	-3.69267400	3.52523700	0.09383900
C	-3.19474500	-0.21080700	-0.44358200
C	-3.75943000	-0.41468300	-1.71218400
C	-4.82584500	-1.27519200	-1.91089500
C	-5.35147100	-1.95581000	-0.81766500
C	-4.80399400	-1.74490900	0.43981900
C	-3.72960000	-0.87342800	0.68121700
H	-5.23145100	-1.42050100	-2.90509100
H	-6.17585500	-2.64808200	-0.93934200
H	-5.22218800	-2.29548400	1.27332700
C	-3.22302000	-0.79356800	2.13772100
C	2.37220400	1.90867600	-0.31648600
N	2.08630700	0.57219900	-0.38424400
C	3.20535100	-0.27888900	-0.36693500
C	3.87053900	-0.50615000	-1.58150400
C	3.67704000	-0.92020400	0.81140900
C	4.96304700	-1.35482500	-1.68409900
H	3.47662000	0.00741100	-2.45164500
C	4.78605600	-1.76559800	0.67475500
C	5.42468600	-1.99340400	-0.54124900
H	5.44266800	-1.51564800	-2.64305500
H	5.17581600	-2.27499100	1.54469300
H	6.27483400	-2.66421500	-0.58489500
H	-3.30356400	0.11428200	-2.54079200
C	-4.41102800	-0.48468900	3.07055300
H	-5.17904900	-1.25899200	3.04997200
H	-4.04906900	-0.40323700	4.09881600
H	-4.87762200	0.46482700	2.79710900
C	-2.62361900	-2.16081400	2.51727600
H	-1.74402800	-2.36437900	1.90441500
H	-2.32271800	-2.15016900	3.56916300
H	-3.34102000	-2.97183400	2.37349900
C	-2.14789900	0.26248500	2.43612000
H	-1.24716000	0.12325500	1.84121100
H	-2.50470300	1.27979100	2.26752500
H	-1.88389700	0.17407200	3.49461000
C	3.78793600	2.41884900	-0.30068300
H	3.81893400	3.48994000	-0.11016200
H	4.29704100	2.22918800	-1.25059300
H	4.38194400	1.91951000	0.47048500
H	-4.26974100	2.25514200	-0.99711700
C	2.98147200	-0.79085600	2.18152500
C	3.83693200	-1.39219600	3.30865100
H	4.81895300	-0.91517000	3.36867000
H	3.32217300	-1.23108600	4.25852600
H	3.97571300	-2.46920200	3.19260400
C	2.69007200	0.66811700	2.57835700
H	3.60244800	1.27001300	2.55276800
H	1.94565600	1.12074400	1.92829400
H	2.30908300	0.68026500	3.60452600
C	1.65299000	-1.56543700	2.15052300
H	0.99929300	-1.17887100	1.36868300
H	1.82751800	-2.62782300	1.96013700
H	1.14373000	-1.46225100	3.11490000

C	-0.98483800	-2.56968300	-0.63462600
H	-0.98896500	-3.58446500	-0.23138300
H	-1.95058900	-2.09815500	-0.72345300
C	0.16078700	-1.98895800	-1.02300300
C	1.38089600	-2.88756700	-1.00203000
H	2.24473900	-2.43855900	-0.52187000
H	1.15517800	-3.83042900	-0.49281600
H	1.68685100	-3.13426100	-2.02549500
C	0.29979000	-0.92006500	-2.67923400
H	1.35181100	-1.16932600	-2.78190700
C	0.03901900	0.48257900	-2.71831500
H	-0.92967300	0.81168300	-3.08711100
H	0.86314400	1.16517100	-2.89405100
C	-0.60865400	-1.81328100	-3.51473200
H	-0.46983400	-1.55364300	-4.56952200
H	-0.40504600	-2.87555800	-3.37366200
H	-1.65114700	-1.63195800	-3.25054100

Zero-point correction= 0.73835 Hartree

Sum of electronic and thermal Free Energies= -1648.5995709 Hartree

Number of imaginary frequencies= 1

2IMe4

-1 1

Fe	0.00262900	0.29748200	-0.46718100
N	-2.18334400	0.55178600	-0.31310400
C	-1.40766200	2.75498100	-0.38114500
C	0.97707700	2.92246900	-0.23961200
C	-1.56385400	4.11984700	-0.43381500
C	0.84375500	4.33478800	-0.27455500
C	-0.38948700	4.92985100	-0.36188500
H	-2.53692900	4.57617200	-0.54788800
H	1.73154100	4.95592700	-0.25425400
H	-0.47424400	6.00920600	-0.39554500
N	-0.20060300	2.15314600	-0.23614500
C	-2.51467300	1.80774200	-0.44375400
C	-3.93413400	2.27330600	-0.65159400
H	-4.08316800	3.25975300	-0.21830500
H	-4.16779300	2.32684100	-1.71833100
C	-3.20288500	-0.42762900	-0.41330700
C	-3.62576900	-0.75853000	-1.70680100
C	-4.56809200	-1.75035500	-1.93549100
C	-5.10806100	-2.42854400	-0.85216200
C	-4.70100200	-2.09530900	0.43566700
C	-3.75182700	-1.10121100	0.70524300
H	-4.86745900	-1.99026200	-2.94868000
H	-5.84146300	-3.21248600	-0.99810800
H	-5.14667700	-2.63621700	1.25775200
C	-3.37878800	-0.76322600	2.15880100
C	2.13144300	2.16647400	-0.16996700
N	1.93465800	0.79834500	-0.06357500
C	3.09586600	0.01386800	-0.14724500
C	3.78411400	-0.00190900	-1.37659500
C	3.62501300	-0.75305200	0.92882900
C	4.92813700	-0.75496300	-1.58840700
H	3.35655300	0.59760100	-2.17249500
C	4.77679800	-1.51199900	0.68119800
C	5.42840000	-1.52974500	-0.54819700
H	5.41430600	-0.74529400	-2.55766700
H	5.19798700	-2.10873900	1.47828300
H	6.31591000	-2.13707700	-0.68199700
H	-3.17140200	-0.22130600	-2.52908200
C	-4.11731100	-1.66302400	3.16047500
H	-3.87744200	-2.71784500	3.00933200
H	-3.79983300	-1.39004400	4.16906000
H	-5.20142100	-1.53565000	3.10533700
C	-1.87441600	-0.95368400	2.39979400
H	-1.28564500	-0.28615500	1.77224700
H	-1.64176600	-0.73535700	3.44670100
H	-1.57472300	-1.98212700	2.18723900
C	-3.76323100	0.68914500	2.49452700
H	-3.17165400	1.40267700	1.92452100
H	-4.82423300	0.86435400	2.29684400
H	-3.57795700	0.87438400	3.55645400
C	3.50377200	2.77783700	-0.07191000
H	3.43867700	3.84943800	0.11393500
H	4.10662300	2.62956200	-0.97358900
H	4.06767700	2.32810400	0.75111200
H	-4.63845100	1.57896200	-0.19563900
C	2.99872400	-0.75644000	2.33230300
C	3.86503800	-1.50845400	3.35391600
H	4.86558200	-1.07578800	3.43396700
H	3.38602900	-1.43682700	4.33355000
H	3.95946700	-2.56926600	3.10991000
C	2.82499700	0.67725600	2.86504300
H	3.79537300	1.17821500	2.92809500
H	2.16488500	1.25732600	2.22419600
H	2.39828800	0.63732200	3.87266300
C	1.63341700	-1.45517800	2.29214200

H	0.96772800	-0.93792700	1.60479900
H	1.74298300	-2.48997500	1.95671700
H	1.18279300	-1.45628500	3.29070100
C	-0.31645300	-2.39151500	-0.58302600
H	-0.34205100	-3.04581600	0.28171000
H	-1.21747300	-1.84322500	-0.82367300
C	0.76569900	-2.34037700	-1.37361900
C	1.96527700	-3.21286400	-1.11854900
H	2.86225800	-2.60559000	-0.98642300
H	1.82907900	-3.84192200	-0.23710100
H	2.13817100	-3.86287000	-1.98242800
C	0.82959900	-1.44173100	-2.59760400
H	1.87864200	-1.14090400	-2.68377800
C	-0.02779100	-0.18452400	-2.41670500
H	-1.04146400	-0.39500300	-2.79248900
H	0.37200700	0.62219100	-3.04420500
C	0.47782500	-2.25784600	-3.85580300
H	1.10678800	-3.14555800	-3.98432900
H	-0.56442000	-2.58271100	-3.79649500
H	0.58790700	-1.63000000	-4.74330500

Zero-point correction= 0.74002 Hartree

Sum of electronic and thermal Free Energies= -1649.3984357 Hartree

Number of imaginary frequencies= 0

2IMe5

-1 1

Fe	-0.02803000	0.45120000	-0.16610100
N	-2.11673100	0.63739700	-0.16180200
C	-1.48652000	2.85478700	0.08328000
C	0.89782200	3.07016500	0.29850400
C	-1.64177500	4.22148700	0.18721900
C	0.75494200	4.45235900	0.41152400
C	-0.50665500	5.03923800	0.37295900
H	-2.62247100	4.67236700	0.10414000
H	1.63316800	5.08008600	0.50541300
H	-0.61492200	6.11298400	0.45436700
N	-0.24039700	2.26067500	0.19471200
C	-2.52452900	1.90016100	-0.15170200
C	-3.95627100	2.30065600	-0.39285400
H	-4.15392200	3.29622200	-0.00059100
H	-4.19076200	2.29948100	-1.46124000
C	-3.06317500	-0.36092700	-0.49354400
C	-3.35528400	-0.50852600	-1.85606200
C	-4.21883100	-1.48974500	-2.31938100
C	-4.81317400	-2.34753800	-1.40412000
C	-4.53598600	-2.20121700	-0.04873900
C	-3.66856900	-1.22246800	0.45380900
H	-4.41177300	-1.58757100	-3.38101300
H	-5.48551700	-3.13049900	-1.73388300
H	-5.01709000	-2.88393700	0.63671600
C	-3.41874000	-1.11945700	1.96792100
C	2.09348200	2.33275800	0.25335900
N	1.92269400	0.99516500	0.18264200
C	3.04168000	0.20094800	-0.13183400
C	3.59514900	0.36243600	-1.41366200
C	3.57225100	-0.79490600	0.72737700
C	4.62095700	-0.44223000	-1.88367800
H	3.14037800	1.11180400	-2.05103900
C	4.60233500	-1.59737600	0.21921600
C	5.12318500	-1.44362700	-1.06181800
H	5.00343900	-0.30451300	-2.88848700
H	5.02246500	-2.37483000	0.84180000
H	5.91305000	-2.10075200	-1.40553600
H	-2.84906400	0.16042000	-2.54148100
C	-3.86985200	0.24993100	2.50526000
H	-4.92734500	0.42252800	2.28618300
H	-3.73874600	0.27281400	3.59130900
H	-3.27977600	1.05856900	2.07816300
C	-4.19937600	-2.18656300	2.74876300
H	-3.89944500	-3.19658500	2.46057000
H	-3.98228100	-2.06431200	3.81216500
H	-5.27951200	-2.08622700	2.61430200
C	-1.92997300	-1.31775600	2.29036700
H	-1.55954800	-2.25799400	1.87665700
H	-1.33675400	-0.50476400	1.87631100
H	-1.78952000	-1.32931000	3.37633900
C	3.45763000	2.96732200	0.32480300
H	3.94974400	3.01055700	-0.65097600
H	4.11082700	2.38635000	0.98068400
H	3.39424600	3.98110900	0.71734300
H	-4.63976600	1.59725600	0.08446400
C	3.07414000	-1.00072400	2.16526400
C	3.20046600	0.30876600	2.96312200
H	2.58017800	1.08998800	2.52782600
H	2.87392600	0.14066500	3.99422100
H	4.24096900	0.64557700	2.98431700
C	1.60788300	-1.45757600	2.17521300
H	0.96725700	-0.67021400	1.78363200

H	1.46528500	-2.35365100	1.56776800
H	1.29459700	-1.67627200	3.20186300
C	3.88806400	-2.06753900	2.91109400
H	3.78063500	-3.05354200	2.45227700
H	4.95016700	-1.81369300	2.95844800
H	3.51218000	-2.13644600	3.93461800
C	0.25486000	-0.64633200	-1.87046300
H	-0.68532900	-0.86462000	-2.40068000
H	0.80830700	0.03961500	-2.52986600
C	1.08242800	-1.94302900	-1.83106100
H	2.04872800	-1.73125500	-1.36206500
C	1.40112300	-2.44214700	-3.25680500
H	1.93768700	-1.66102100	-3.80005600
H	2.01932900	-3.34559200	-3.27096400
H	0.46883300	-2.65236600	-3.78859700
C	-0.80471300	-3.14725000	-0.68997400
H	-1.19511700	-3.99315400	-0.13090000
H	-1.49906700	-2.36333700	-0.95789700
C	0.48287000	-3.08512100	-1.03439100
H	-0.48768900	3.86921900	-2.58431600
C	1.43602800	-4.19617700	-0.65921000
H	1.78587100	-4.73515000	-1.54435300
H	2.32485900	-3.78489800	-0.17035900
H	0.96380000	-4.91611900	0.01217200
C	-0.04503700	2.97628200	-3.02380600
H	1.00894800	2.93651000	-2.74911100
H	-0.14851800	2.99645600	-4.10954200
H	-0.52812800	2.09378300	-2.60705000

Zero-point correction= 0.7858149 Hartree

Sum of electronic and thermal Free Energies= -1689.9066304 Hartree

Number of imaginary frequencies= 0

2TSe3

-1 1

Fe	-0.18119500	0.59062400	-0.53176100
N	-2.24374600	0.61549900	-0.35134700
C	-1.76359300	2.87917900	-0.21159300
C	0.60069800	3.26133100	-0.11940100
C	-2.00928600	4.23831200	-0.16474300
C	0.37487900	4.63505700	-0.05761000
C	-0.92747900	5.13280300	-0.03920500
H	-3.01816000	4.62147600	-0.25519700
H	1.20945000	5.32619100	-0.05825900
H	-1.10432200	6.19975600	0.00324900
N	-0.48099100	2.38139800	-0.06065200
C	-2.74029100	1.84789400	-0.38425200
C	-4.20179200	2.13172000	-0.60856000
H	-4.47063800	3.12406900	-0.25109800
H	-4.44897500	2.07049200	-1.67256400
C	-3.10805100	-0.48392500	-0.56255800
C	-3.38989200	-0.79917000	-1.89814400
C	-4.16550700	-1.89401400	-2.24720700
C	-4.67590200	-2.70244500	-1.24100300
C	-4.40715100	-2.39215700	0.08791100
C	-3.63172900	-1.29156100	0.47801800
H	-4.35682000	-2.11554900	-3.29063400
H	-5.27793500	-3.57139100	-1.47880400
H	-4.82389300	-3.04036500	0.84498800
C	-3.41075300	-1.00304800	1.97588600
C	1.84008500	2.59532800	-0.21832900
N	1.75230000	1.24881000	-0.23274400
C	2.94989400	0.51610900	-0.37928300
C	3.47569100	0.41707300	-1.67613600
C	3.60514900	-0.15798200	0.68592800
C	4.59974000	-0.34159700	-1.96685400
H	2.94384700	0.94285500	-2.45936200
C	4.74265300	-0.90838600	0.35938100
C	5.23840700	-1.01719900	-0.93648000
H	4.96226400	-0.40927800	-2.98611100
H	5.26806600	-1.43921300	1.14049000
H	6.11521300	-1.62423500	-1.12854600
H	-2.94897200	-0.16207100	-2.65506700
C	-3.98901400	0.36927400	2.36388600
H	-5.04850600	0.43276000	2.10113600
H	-3.89848000	0.50337100	3.44595200
H	-3.44972000	1.18111900	1.87967000
C	-4.10640300	-2.04429800	2.86559000
H	-3.72217800	-3.05075400	2.68613300
H	-3.90746400	-1.79366400	3.90994500
H	-5.19004500	-2.04844300	2.72266800
C	-1.91830200	-1.02758500	2.33710800
H	-1.48154500	-2.00525600	2.12153400
H	-1.37326500	-0.26799600	1.77881000
H	-1.80136100	-0.82434600	3.40661500
C	3.16250400	3.31267600	-0.24883900
H	3.63892000	3.23344900	-1.23028400
H	3.85864900	2.87644300	0.47154800
H	3.04302700	4.36854000	-0.01290600

H	-4.82392200	1.39756000	-0.09608200
C	3.10151300	-0.13198400	2.13975100
C	2.96175400	1.30653000	2.66691100
H	2.21712100	1.86709900	2.10605700
H	2.64783600	1.27321500	3.71466800
H	3.92071000	1.83029000	2.61852100
C	1.73878000	-0.83455200	2.23236600
H	1.00649700	-0.31146600	1.62089100
H	1.80322600	-1.86986200	1.88705300
H	1.39365100	-0.83391300	3.27177900
C	4.05801000	-0.86420900	3.09273900
H	4.13831100	-1.92667200	2.85156900
H	5.05852900	-0.42351300	3.08733500
H	3.66057500	-0.78631500	4.10727400
C	-0.01819700	-1.62695300	-0.74336900
H	-0.23884900	-1.68603900	0.32282000
H	-0.86104900	-2.12610100	-1.24349700
C	1.26544300	-2.40691400	-1.02822900
H	2.12030600	-1.83012300	-0.66201800
C	1.47023100	-2.57648700	-2.54408800
H	1.52362200	-1.59763100	-3.02244500
H	2.39075700	-3.11488400	-2.78273800
H	0.62649500	-3.12632500	-2.97118100
C	0.31205300	-4.41988300	0.15066900
H	0.43125600	-5.39041800	0.62171800
H	-0.68557700	-4.00176100	0.10178400
C	1.36252700	-3.76476500	-0.34688400
H	-0.82841400	1.41701500	-2.68703200
C	2.75401300	-4.33927300	-0.23929800
H	3.20869500	-4.47013500	-1.22482300
H	3.39977700	-3.64666300	0.30947100
H	2.75309800	-5.30392200	0.27137200
C	-0.18439000	0.53506900	-2.69150100
H	-0.04923200	-0.47861000	-1.73650000
H	0.80171400	0.82205300	-3.05982300
H	-0.61191100	-0.18679900	-3.39656100

Zero-point correction= 0.784449 Hartree

Sum of electronic and thermal Free Energies= -1689.8680316 Hartree

Number of imaginary frequencies= 1

2IMe6

-1 1

Fe	-0.05647600	-0.64156500	-0.77656200
N	1.90958800	-1.15667200	-0.49954700
C	0.93131900	-3.25318000	-0.45085800
C	-1.46827400	-3.06337700	-0.52048700
C	0.83186900	-4.63086500	-0.35806700
C	-1.58203200	-4.44486900	-0.43147400
C	-0.43443900	-5.23947400	-0.33809400
H	1.72245700	-5.24498300	-0.30356100
H	-2.55858000	-4.91405700	-0.43049400
H	-0.52052700	-6.31581200	-0.26220600
N	-0.21044400	-2.46658600	-0.49851900
C	2.12140200	-2.47246300	-0.47203300
C	3.50300800	-3.06536000	-0.44190500
H	3.46655200	-4.15227200	-0.42108500
H	4.07749700	-2.75605900	-1.31922000
C	3.03271000	-0.30239200	-0.53321100
C	3.50921100	0.03060400	-1.81456800
C	4.59623300	0.86643300	-2.00390900
C	5.23279300	1.40784200	-0.89038500
C	4.76023300	1.09538500	0.37504300
C	3.66467600	0.24506700	0.60606000
H	4.93433300	1.10124000	-3.00633800
H	6.08124500	2.07234400	-1.00286200
H	5.26727600	1.53087500	1.22772900
C	3.30393100	-0.00393400	2.08704200
C	-2.51044600	-2.10890200	-0.58971900
N	-2.09060800	-0.83540100	-0.59327100
C	-3.06917300	0.17919100	-0.61042000
C	-3.39251500	0.69895100	-1.87714400
C	-3.70627300	0.70720500	0.53730100
C	-4.33537700	1.69758000	-2.04891500
H	-2.85691300	0.27643800	-2.71730000
C	-4.66224600	1.71655400	0.32407900
C	-4.98578200	2.21128200	-0.93048700
H	-4.55753700	2.07162900	-3.04152100
H	-5.16922800	2.14139900	1.18197100
H	-5.72896200	2.99367400	-1.02921900
H	2.96888100	-0.39133900	-2.65264400
C	4.51332300	-0.64916300	2.79144500
H	5.40032900	-0.01449000	2.75085300
H	4.27079500	-0.82817700	3.84290300
H	4.76112100	-1.60759500	2.33107800
C	3.00525200	1.34393200	2.77417300
H	2.12161200	1.81223700	2.33793600
H	2.81009700	1.17332000	3.83682600
H	3.83810100	2.04477300	2.69430100

C	2.09072200	-0.90828600	2.34553300
H	1.18960000	-0.53179200	1.86304300
H	2.24341400	-1.92717500	1.99059800
H	1.92539000	-0.94408800	3.42739400
C	-3.96836800	-2.47569200	-0.62794000
H	-4.10016100	-3.55164600	-0.72361700
H	-4.46474600	-1.99241100	-1.47360400
H	-4.49366200	-2.14499000	0.27384800
H	4.06188400	-2.72228600	0.43395100
C	-3.45149500	0.32417800	2.01243700
C	-4.77284600	-0.13453300	2.65923400
H	-5.16630300	-1.01677500	2.15061100
H	-4.59299300	-0.39692500	3.70576400
H	-5.53984100	0.64119200	2.63407400
C	-2.42055700	-0.78633600	2.26385500
H	-2.72874000	-1.74700700	1.85225000
H	-1.44696700	-0.55391100	1.83491100
H	-2.31202900	-0.89947200	3.34750400
C	-2.95079100	1.57574900	2.76240400
H	-2.00059400	1.91889400	2.34947600
H	-3.66187200	2.40164700	2.70424500
H	-2.79814500	1.33329200	3.81819500
C	2.36938000	3.62010200	-0.69971100
H	2.63387800	3.51546900	0.35612900
H	3.09365800	4.29697500	-1.15988900
C	0.95806600	4.17960500	-0.85062800
H	0.75001400	4.29555900	-1.92306900
C	0.87553000	5.57308700	-0.20886300
H	1.66015500	6.22145200	-0.60638300
H	-0.08568900	6.05469500	-0.39302700
H	1.01600200	5.49274600	0.87249000
C	0.13213700	2.08126100	0.24743800
H	-0.68357400	1.44508100	0.57819900
H	1.13669900	1.69011600	0.34709900
C	-0.12402100	3.26643200	-0.31035500
H	0.18675700	-0.38249800	-3.36270700
C	-1.54360300	3.74280900	-0.48457800
H	-1.76370600	4.60225200	0.15625800
H	-1.71564600	4.05581100	-1.51923400
H	-2.25152000	2.94948100	-0.25070800
C	0.11790900	0.33919700	-2.53625200
H	2.46987400	2.64194600	-1.17049400
H	-0.72940300	1.00393500	-2.75237700
H	1.01954600	0.96687500	-2.58434900

Zero-point correction= 0.7854922 Hartree

Sum of electronic and thermal Free Energies= -1689.8965627 Hartree

Number of imaginary frequencies= 0

2PCa

0 1

Fe	0.00223500	0.27050700	-0.76569200
N	-2.04573300	0.44594600	-0.50714600
C	-1.34899200	2.59756800	-0.05334300
C	1.02819600	2.69346200	0.17620800
C	-1.43674800	3.95632800	0.21707600
C	0.95408200	4.05096800	0.45783400
C	-0.28453500	4.69395900	0.49486200
H	-2.40238000	4.44507500	0.21782400
H	1.85849600	4.61662700	0.63884100
H	-0.34835700	5.75004500	0.71547800
N	-0.12296200	1.94377100	-0.02632700
C	-2.42648800	1.69785700	-0.30125700
C	-3.86791300	2.12386400	-0.23585000
H	-3.97036400	3.17952600	-0.47972000
H	-4.46711100	1.54567200	-0.93863900
C	-3.04969000	-0.56427300	-0.48379300
C	-3.49983000	-1.01661500	-1.73334000
C	-4.44128600	-2.02263700	-1.86370000
C	-4.95417800	-2.60822700	-0.71208900
C	-4.51980700	-2.16020800	0.52510000
C	-3.57171200	-1.13565400	0.69973800
H	-4.76765000	-2.34109300	-2.84583400
H	-5.68817200	-3.40184900	-0.77217600
H	-4.94261300	-2.62808400	1.40430600
C	-3.25500200	-0.77972000	2.17395800
C	2.20762200	1.89875400	0.05881300
N	1.97847900	0.63488900	-0.25307800
C	3.09284100	-0.23877600	-0.39076300
C	3.63728300	-0.31481500	-1.68304700
C	3.62703200	-1.03394800	0.64608500
C	4.65273700	-1.19795300	-2.00593000
H	3.22415700	0.34819200	-2.43416400
C	4.64681600	-1.92930500	0.27669400
C	5.15060600	-2.03283000	-1.01085900
H	5.04415300	-1.23664800	-3.01470400
H	5.07592000	-2.56740200	1.03842800
H	5.93523900	-2.74665700	-1.22752400
H	-3.08324400	-0.53841600	-2.60748200

C	-4.56444200	-0.34838500	2.86649600
H	-5.30451800	-1.14873300	2.89023600
H	-4.34961100	-0.05914300	3.89828800
H	-5.01193400	0.50779500	2.35852200
C	-2.72527100	-2.03474200	2.89860100
H	-1.76428600	-2.35299000	2.49213800
H	-2.58435700	-1.80518400	3.95760300
H	-3.41441500	-2.87610200	2.82741400
C	-2.23661800	0.34443400	2.42396400
H	-1.28667500	0.19377000	1.91457400
H	-2.61676300	1.32072400	2.12559400
H	-2.04864800	0.38605200	3.50002500
C	3.59290800	2.44663300	0.26365200
H	3.57079400	3.44190900	0.69997000
H	4.13018800	2.49355800	-0.68672900
H	4.16905700	1.79394800	0.91999300
H	-4.28668800	1.96414200	0.76081500
C	3.28539900	-0.99092400	2.15452700
C	4.56110300	-0.57349000	2.91600300
H	4.90876300	0.40809800	2.58803000
H	4.34437300	-0.51752700	3.98576100
H	5.37553800	-1.28441500	2.77226600
C	2.17912200	-0.01301500	2.58181500
H	2.46958800	1.02621500	2.42824900
H	1.23828000	-0.17413100	2.06001600
H	2.01093700	-0.15055100	3.65319500
C	2.87926800	-2.39329100	2.65053500
H	1.94994500	-2.73001800	2.19040900
H	3.64535000	-3.14179000	2.44782200
H	2.72537400	-2.35885300	3.73171900
C	0.22414300	1.37193400	-2.59462600
H	-0.69292800	1.93372000	-2.74602100
H	1.09746700	1.94836400	-2.31937000
C	0.31358400	0.07931400	-3.02353500
H	1.28717700	-0.39465300	-3.04026200
C	-0.74252300	-0.53098300	-3.90936600
H	-0.36158700	-0.57679700	-4.93379700
H	-1.03045100	-1.54224300	-3.62388200
H	-1.63211300	0.09899500	-3.92186800
C	0.03751400	-1.70337100	0.14984500
H	1.00071400	-1.80504700	0.63005700
H	-0.82733700	-1.56203600	0.78043900
C	-0.09228000	-2.03862000	-1.16478000
H	-1.09588300	-2.11611700	-1.56960100
C	1.00450500	-2.74454700	-1.92040000
H	0.99686900	-2.52505200	-2.98840200
H	1.98681700	-2.49459700	-1.51896300
H	0.86164400	-3.82421600	-1.81581000

Zero-point correction= 0.754667 Hartree

Sum of electronic and thermal Free Energies= -1649.272312 Hartree

Number of imaginary frequencies= 0

2TSa1

0 1

Fe	-0.01408900	0.18084200	-0.71421300
N	-2.05331200	0.48305600	-0.51480100
C	-1.26076500	2.64075000	-0.53172600
C	1.10424500	2.69693800	-0.47798800
C	-1.30812700	4.02683300	-0.55225200
C	1.08626300	4.08422000	-0.49519000
C	-0.12775600	4.76925700	-0.52570000
H	-2.26882400	4.52479700	-0.59012200
H	2.02288100	4.62739200	-0.48905700
H	-0.15322800	5.84962900	-0.53785500
N	-0.06209500	1.95966100	-0.46941200
C	-2.38396000	1.74966900	-0.53071700
C	-3.79220700	2.27981800	-0.50003300
H	-3.97478400	2.90014500	-1.37986700
H	-4.51697800	1.46961100	-0.49244500
C	-3.08308200	-0.49407600	-0.39772500
C	-3.54858700	-1.01822200	-1.61083800
C	-4.49167300	-2.02972200	-1.65989500
C	-4.99048700	-2.53241800	-0.46301100
C	-4.56011900	-1.98621700	0.73606100
C	-3.61405100	-0.94917500	0.82660800
H	-4.83062600	-2.41538900	-2.61319000
H	-5.72164600	-3.33084000	-0.45997400
H	-4.99024400	-2.37458400	1.64997900
C	-3.34926500	-0.40426900	2.25009900
C	2.26877900	1.86114400	-0.45501900
N	2.00214400	0.57921700	-0.46526600
C	3.08213700	-0.34695800	-0.40777400
C	3.56790000	-0.77428700	-1.65255600
C	3.63633700	-0.85143900	0.78589900
C	4.55134000	-1.74196500	-1.76082900
H	3.13932900	-0.31832600	-2.53695100
C	4.62398600	-1.84139800	0.63381300
C	5.07200600	-2.29684400	-0.59663100

H	4.90197800	-2.05772400	-2.73523300
H	5.07149000	-2.26652600	1.52269100
H	5.83353700	-3.06496300	-0.64252200
H	-3.14624400	-0.58698800	-2.51830000
C	-4.68241400	0.14851500	2.79528400
H	-5.45112600	-0.62177800	2.86612100
H	-4.52374100	0.56172300	3.79460200
H	-5.05913100	0.94591600	2.15081800
C	-2.88416900	-1.55010000	3.17121000
H	-1.91614900	-1.94112100	2.85591700
H	-2.78248800	-1.17102300	4.19091300
H	-3.59254600	-2.37820100	3.19374400
C	-2.32104400	0.73189000	2.38432800
H	-1.35714600	0.49708700	1.93683900
H	-2.68342300	1.66074900	1.94426000
H	-2.17455500	0.91851800	3.45136500
C	3.64847300	2.45922800	-0.39007100
H	3.74009900	3.11820500	0.47598300
H	3.84054700	3.05620700	-1.28408900
H	4.40956200	1.68595600	-0.32284800
H	-3.95268000	2.90164500	0.38353000
C	3.34918200	-0.40276600	2.23692500
C	4.65610600	0.17743100	2.81579200
H	4.99322000	1.03020500	2.22222600
H	4.48089800	0.52036500	3.83865100
H	5.46041300	-0.55877200	2.83896200
C	2.27126000	0.67707800	2.42779600
H	2.59033900	1.64087200	2.03055400
H	1.31904500	0.41827400	1.96900500
H	2.11984600	0.80609500	3.50264100
C	2.93738600	-1.61933600	3.08964100
H	1.99719200	-2.04725100	2.74030100
H	3.69121300	-2.40674500	3.07984100
H	2.80249200	-1.30132700	4.12619500
C	0.05741700	0.23170400	-2.64875800
H	-0.87797000	0.54811500	-3.10717100
H	0.91024600	0.83371900	-2.95233100
C	0.26023600	-1.20116100	-2.49787700
H	1.30449700	-1.48674000	-2.55930800
C	-0.61870700	-2.09694300	-3.35624900
H	-0.33034900	-1.97610900	-4.40345400
H	-0.53128700	-3.15344400	-3.10069100
H	-1.66636500	-1.81882800	-3.26412800
C	-0.04240400	-1.36546200	0.51432200
H	0.85870400	-1.48199700	1.10489800
H	-0.95827800	-1.37548600	1.08815200
C	-0.06327400	-2.09612100	-0.74095400
H	-1.05782400	-2.45072500	-1.00044000
C	1.00740100	-3.17351600	-0.85827800
H	1.10721000	-3.58722100	-1.86295100
H	1.97789600	-2.77901500	-0.55537100
H	0.75396300	-3.99203200	-0.18023500

Zero-point correction= 0.757093 Hartree

Sum of electronic and thermal Free Energies= -1649.251409 Hartree

Number of imaginary frequencies= 1

2IMa1

0 1

Fe	-0.04946000	0.28517800	0.25257900
N	1.98816900	0.70788400	0.04388600
C	1.06555800	2.82132600	-0.28239500
C	-1.27005400	2.77628800	-0.28606600
C	1.07324000	4.20647700	-0.41816000
C	-1.33118800	4.16057800	-0.41870200
C	-0.14249100	4.88219700	-0.49169100
H	2.00835700	4.74880300	-0.45417600
H	-2.28611400	4.66719600	-0.45473200
H	-0.16305300	5.95877800	-0.59417300
N	-0.08940000	2.13006300	-0.22658800
C	2.24875300	1.95796900	-0.14116200
C	3.62043300	2.56383700	-0.23472500
H	3.82916200	3.16900800	0.65077700
H	4.38167400	1.79212900	-0.31329800
C	3.06290500	-0.20187300	0.28357800
C	3.57847600	-0.17349300	1.58546800
C	4.57280400	-1.04945700	1.98604700
C	5.05810800	-1.97689600	1.07117500
C	4.55535300	-1.98846500	-0.22108000
C	3.56121300	-1.10483900	-0.67118600
H	4.94985600	-1.01580600	3.00008200
H	5.82364500	-2.68656500	1.35802500
H	4.94989900	-2.72090300	-0.91277500
C	3.12392400	-1.24106300	-2.14053600
C	-2.41825300	1.86376600	-0.16075800
N	-2.10366300	0.62165600	-0.00133300
C	-3.11621200	-0.35980200	0.19243400
C	-3.73482800	-0.37394500	1.44339400
C	-3.42806100	-1.32031600	-0.78941600

C	-4.66508300	-1.35097200	1.76778500
H	-3.44296000	0.38065500	2.16383800
C	-4.37152200	-2.28847000	-0.42706200
C	-4.97885900	-2.31864600	0.82424100
H	-5.12651000	-1.35720200	2.74692300
H	-4.64398700	-3.05373400	-1.13825900
H	-5.69341600	-3.09905900	1.05314500
H	3.15027000	0.53703500	2.28211100
C	4.36659500	-1.27621200	-3.05143300
H	5.00420300	-2.13897800	-2.86246100
H	4.04626800	-1.32888300	-4.09470400
H	4.96655300	-0.37265000	-2.92098800
C	2.34531100	-2.55855400	-2.29322900
H	1.45359600	-2.54575700	-1.66582600
H	2.04217300	-2.69447000	-3.33538900
H	2.95558000	-3.41430400	-1.99904900
C	2.24031700	-0.10411500	-2.66878900
H	1.29836400	-0.02727400	-2.13002100
H	2.75036200	0.86094100	-2.61881100
H	2.01318600	-0.30845800	-3.71815900
C	-3.81389800	2.41589900	-0.23490700
H	-3.90914800	3.07228700	-1.10182800
H	-4.03385300	3.00443500	0.65898100
H	-4.54499900	1.61548300	-0.31146400
H	3.67925000	3.21519100	-1.10869200
C	-2.84183900	-1.29051600	-2.20940100
C	-3.22740100	-2.54671800	-3.00428100
H	-4.30646100	-2.62286400	-3.15075600
H	-2.76657000	-2.49126100	-3.99219800
H	-2.87127800	-3.45540000	-2.51471100
C	-3.40625100	-0.07651500	-2.96809200
H	-4.49730900	-0.11664700	-3.00233200
H	-3.10728400	0.86110900	-2.49909300
H	-3.02782400	-0.07392800	-3.99385200
C	-1.30407400	-1.21841700	-2.20199700
H	-0.95673200	-0.22329000	-1.91166900
H	-0.87900600	-1.95353600	-1.51834300
H	-0.92408200	-1.40753000	-3.20974500
C	-0.12485600	0.93032200	2.15486700
H	0.85240400	1.35987100	2.42895400
H	-0.87213400	1.72469900	2.31499500
C	-0.42118900	-0.28273300	3.03938800
H	-1.48569900	-0.53560100	2.93378400
C	-0.14168000	0.00152300	4.51834800
H	-0.65078200	0.91413900	4.84085100
H	-0.46627700	-0.81394700	5.16931100
H	0.93287800	0.14872600	4.67229600
C	0.00647100	-1.59444900	0.98764500
H	-0.98396600	-2.07722200	0.91272100
H	0.71746400	-2.29001700	0.51120900
C	0.35331900	-1.48250900	2.48067400
H	1.42273500	-1.24610900	2.57583700
C	0.08771700	-2.77643100	3.25527600
H	0.43321200	-2.73378700	4.29242900
H	-0.98679200	-2.98924700	3.26258500
H	0.58881700	-3.61658400	2.76832200

Zero-point correction= 0.754605 Hartree

Sum of electronic and thermal Free Energies= -1649.276998 Hartree

Number of imaginary frequencies= 0

2TSa2

0 1

Fe	-0.00152600	0.37300400	0.21972600
N	1.96647700	0.67394300	-0.17368800
C	1.10270600	2.76260800	-0.63557800
C	-1.29141300	2.71666700	-0.52992000
C	1.06897900	4.11940700	-0.92795000
C	-1.33706100	4.07246300	-0.81974000
C	-0.15375900	4.78505500	-1.03293300
H	1.99296200	4.66678900	-1.06241000
H	-2.28924700	4.58415600	-0.87023500
H	-0.18452800	5.84149100	-1.25904200
N	-0.07783400	2.04523400	-0.47538100
C	2.24965300	1.93193000	-0.48444400
C	3.65255500	2.42441800	-0.71001100
H	4.17552600	2.60151700	0.23247400
H	4.22734400	1.67692500	-1.25933200
C	3.04076900	-0.23095500	0.04524500
C	3.73988100	-0.07452100	1.25316900
C	4.73500500	-0.95262400	1.64620200
C	5.04147300	-2.02663900	0.81756600
C	4.37651200	-2.16517900	-0.39150000
C	3.38618300	-1.27348400	-0.83798300
H	5.24977500	-0.80950500	2.58810800
H	5.79817300	-2.74666100	1.10243200
H	4.64274800	-3.00370000	-1.02050600
C	2.77986400	-1.53835100	-2.23020000
C	-2.38813200	1.84934300	-0.25150400

N	-2.04254100	0.59137100	-0.00930900
C	-3.07273900	-0.30724000	0.39052000
C	-3.51084800	-0.18821300	1.71569900
C	-3.61578900	-1.30612100	-0.44951900
C	-4.47625200	-1.03065900	2.24690500
H	-3.05548600	0.58578400	2.32395800
C	-4.59051400	-2.13792100	0.11870300
C	-5.02028300	-2.01636800	1.43556600
H	-4.79329800	-0.91733000	3.27611100
H	-5.03934100	-2.91313200	-0.48418300
H	-5.77570400	-2.69140500	1.81760600
H	3.45239500	0.75451700	1.89011900
C	3.90334400	-1.88760600	-3.22816600
H	4.41061900	-2.82238600	-2.99160900
H	3.47210700	-1.99829900	-4.22532300
H	4.64948500	-1.09096900	-3.26370700
C	1.82426800	-2.73787200	-2.12448300
H	1.00456500	-2.51742800	-1.43911300
H	1.39700700	-2.96636500	-3.10486900
H	2.34619000	-3.62494400	-1.75907100
C	2.02038600	-0.35568200	-2.85185200
H	1.12676600	-0.08253600	-2.29532500
H	2.65557700	0.52996000	-2.92556600
H	1.72242100	-0.63956600	-3.86454100
C	-3.81382600	2.32939800	-0.23714900
H	-3.92357000	3.23936000	-0.82310600
H	-4.15129800	2.53257500	0.78195000
H	-4.47542900	1.56860000	-0.65032800
H	3.65236400	3.34896400	-1.28284400
C	-3.19982900	-1.49710400	-1.91795000
C	-3.97850700	-2.63826800	-2.58823500
H	-5.05349200	-2.44564900	-2.60116400
H	-3.64367600	-2.72502000	-3.62353000
H	-3.79710500	-3.59774000	-2.09939100
C	-3.46927100	-0.22513600	-2.74058900
H	-4.52378800	0.05545400	-2.68211200
H	-2.85784300	0.60982700	-2.40419700
H	-3.22860600	-0.41716400	-3.78944600
C	-1.70818300	-1.85251200	-2.00732900
H	-1.09132900	-1.02242900	-1.66453600
H	-1.48619800	-2.73548800	-1.40240700
H	-1.43884900	-2.06874600	-3.04509800
C	0.11392800	0.98086700	2.22039500
H	1.03254300	1.53732400	2.03248600
H	-0.73741300	1.66011000	2.25368800
C	0.27460300	0.07675700	3.45858400
H	-0.71561800	-0.11756400	3.88952000
C	1.19173800	0.63810600	4.53575200
H	0.81497400	1.59029900	4.91596600
H	1.28009800	-0.05184300	5.37817900
H	2.19248500	0.80774600	4.13003900
C	-0.13024000	-0.98366200	1.54458800
H	-1.17146700	-1.22523000	1.75618300
H	0.18193800	-1.47303500	0.56561100
C	0.73879400	-1.20521100	2.76487000
H	1.79237500	-1.10051900	2.49467200
C	0.50671000	-2.51077900	3.51143600
H	1.08036500	-2.53559800	4.44066700
H	-0.55201000	-2.62226500	3.76103000
H	0.80724600	-3.37031600	2.90896500

Zero-point correction= 0.755343 Hartree

Sum of electronic and thermal Free Energies= -1649.246172 Hartree

Number of imaginary frequencies= 1

2IMa2

0 1

Fe	0.08383400	0.46549200	-0.54086600
N	-1.84364900	1.03073700	-0.34983300
C	-0.82737700	3.08598300	-0.56172200
C	1.56444200	2.80570500	-0.70211000
C	-0.67322600	4.45941200	-0.67494800
C	1.71859300	4.17742300	-0.82391000
C	0.60104400	5.01900100	-0.80404700
H	-1.54384000	5.10279800	-0.67261700
H	2.70771300	4.60223600	-0.93731900
H	0.72195200	6.08940000	-0.89212100
N	0.29245600	2.24977700	-0.55547100
C	-2.02925200	2.34602300	-0.44535400
C	-3.39420700	2.97208000	-0.40465900
H	-3.94001300	2.79627900	-1.33492100
H	-3.98891300	2.53517200	0.40064600
C	-2.97583700	0.17935000	-0.26698600
C	-3.61230400	-0.11659900	-1.48304600
C	-4.64226900	-1.03892100	-1.57008500
C	-5.04571400	-1.70014400	-0.41451000
C	-4.44214300	-1.38546300	0.79441800
C	-3.42014400	-0.42896200	0.92534300
H	-5.10693500	-1.25149600	-2.52507600

H	-5.82989400	-2.44591500	-0.44881400
H	-4.78374900	-1.90534700	1.68009700
C	-2.90963400	-0.16103300	2.35546800
C	2.57823200	1.81429100	-0.67731000
N	2.12702400	0.57723900	-0.46786200
C	3.06361900	-0.49358800	-0.45603700
C	3.49789200	-0.95044400	-1.70727900
C	3.52811000	-1.12393200	0.72568400
C	4.34243900	-2.04309100	-1.84216400
H	3.14598100	-0.41399200	-2.58158800
C	4.37110900	-2.23051500	0.55127600
C	4.77029300	-2.69822800	-0.69662000
H	4.65651700	-2.37293900	-2.82459500
H	4.74526600	-2.75025900	1.42035900
H	5.42290600	-3.55970800	-0.76266400
H	-3.24524600	0.39074700	-2.36858100
C	-4.11783000	0.12657200	3.27084200
H	-4.80383100	-0.71656700	3.34783900
H	-3.76061200	0.35391900	4.27787900
H	-4.67810400	0.98921900	2.90360100
C	-2.18528400	-1.41675700	2.87136300
H	-1.29820900	-1.62760100	2.27103000
H	-1.86415200	-1.26222100	3.90485700
H	-2.83201900	-2.29589900	2.84151800
C	-1.96162400	1.03585000	2.51852300
H	-1.03574000	0.92415100	1.95884900
H	-2.43170900	1.96856700	2.20264800
H	-1.71719200	1.12718300	3.58034600
C	4.03322500	2.13113400	-0.88586800
H	4.24414600	3.17166600	-0.64828000
H	4.32397300	1.95103400	-1.92438700
H	4.66225000	1.49827000	-0.26118600
H	-3.32917200	4.04529700	-0.24178600
C	3.20967600	-0.62601700	2.14988600
C	3.89869000	-1.48498700	3.22062200
H	4.98627800	-1.46503900	3.12399600
H	3.64495400	-1.08129600	4.20254900
H	3.55966200	-2.52287400	3.19173700
C	3.71355500	0.81527000	2.34207700
H	4.78168900	0.88440300	2.12236400
H	3.17225500	1.51911800	1.71232100
H	3.56228400	1.11273800	3.38313600
C	1.70344300	-0.66568200	2.44549100
H	1.16203300	0.01386100	1.78930400
H	1.31180300	-1.67912900	2.32593100
H	1.52705700	-0.35344600	3.47874400
C	0.09375400	-1.42574100	-1.92975100
H	-0.51529400	-0.53049700	-2.18489800
H	1.08949400	-1.32456600	-2.34745800
C	-0.68883400	-2.71911500	-2.28327500
H	0.04891200	-3.50792200	-2.46414200
C	-1.71300200	-2.69172900	-3.40043600
H	-1.23586900	-2.51490400	-4.36682800
H	-2.24566600	-3.64392400	-3.45559100
H	-2.44732800	-1.90497500	-3.22513800
C	-0.00106200	-1.86000100	-0.43597600
H	0.90806600	-2.38203700	-0.13553300
H	-0.23975400	-1.13585300	0.37864600
C	-1.15979200	-2.81131300	-0.81448000
H	-2.11451000	-2.29278900	-0.70364300
C	-1.21096700	-4.17433900	-0.15150900
H	-1.97507200	-4.80128300	-0.61626100
H	-0.24858100	-4.68419100	-0.24427100
H	-1.44998500	-4.08542200	0.91052100

Zero-point correction= 0.757372 Hartree

Sum of electronic and thermal Free Energies= -1649.282946 Hartree

Number of imaginary frequencies= 0