

*Electronic Supplementary Information*

for

**Computational Approach to Understand the Role of Metals and Axial Ligands in**

**Artificial Heme Enzymes Catalyzed C-H Insertion**

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## Computational Details

### *Distortion-Interaction Analysis*

To understand the origin of lower barriers in the Ir(Me) system for the first step, we carried out a *distortion-interaction* analysis. The *activation strain* model or *distortion-interaction* model is a robust tool for analyzing the origin of activation barriers. In this model, the strain energy comprises of two terms; the first is the energy required for deformation of the reactants on going from ground state geometry to the TS (transition state) geometry; the second is the and the interaction energy between the deformed reactants in the transition state.(Ref.- F. M. Bickelhaupt and K. N. Houk, *Angew. Chem. Int. Ed.*, 2017, **56**, 10070.)

$$\Delta E_{\text{strain}} = \Delta E_{\text{distortion}} + \Delta E_{\text{interaction}}$$

**Table S1** Single Point Total Electronic Energies (a.u.) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*, LANL2DZ(Fe)//B3LYP/6-31G\*,LANL2DZ(Fe) for Fe(his) System

	CSS	OSS	Triplet	Quintet
<b>Substrate</b>	-761.771745	-761.771745	-761.771745	-761.771745
<b>A</b>	-2185.316306	-2185.317924	-2185.322791	-2185.323771
<b>B</b>	-2947.11358	-2947.114490	-2947.117906	-2947.119302
<b>TS(B-C)</b>	-2947.075407	- <sup>a</sup>	- <sup>a</sup>	- <sup>a</sup>
<b>C</b>	-2947.115093	-2947.117885	-2947.100418	-2947.093364
<b>TS(C-D)</b>	-2837.535702	-2837.532731	-2837.509098	- <sup>a</sup>
<b>D</b>	- <sup>b</sup>	-2837.548337	-2837.548423	-2837.541578 <sup>a</sup>
<b>TS(D-E)</b>	- <sup>b</sup>	- <sup>a</sup>	-2837.531871	- <sup>a</sup>
<b>E</b>	- <sup>b</sup>	-652.18813801	-652.18813801	-652.18813801
<b>TS(E-P)</b>	- <sup>b</sup>	-652.17654247	-652.17654247	-652.17654247
<b>P</b>	-652.2919369	-652.2919369	-652.2919369	-652.2919369

CSS – Closed shell singlet.

OSS – Open shell singlet.

<sup>a</sup>Substrate moves away from Fe(his) system. <sup>b</sup>For CSS, we have concerted hydride transfer mechanism.

**Table S2** Single Point Total Electronic Energies (a.u.) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*, LANL2DZ(Fe)//B3LYP/6-31G\*,LANL2DZ(Fe) for Fe(cys) System

	CSS	OSS	Triplet	Quintet
<b>Substrate</b>	-761.771745	-761.771745	-761.771745	-761.771745
<b>A</b>	-2397.256925	-2397.258367	-2185.322791	-2397.273748
<b>B</b>	-3159.048724	-3159.051186	-3159.056272	-3159.066365
<b>TS(B-C)</b>	-3159.012259	-3159.016936	-3159.019534	-3159.003381 <sup>a</sup>
<b>C</b>	-3159.053811	-3159.061891	-3159.057162	-3159.035085
<b>TS(C-D)</b>	-3049.469844	-3049.475929	-3049.474647	-3049.458500
<b>D</b>	- <sup>b</sup>	-3049.500455	-3049.500604	-3049.492246 <sup>a</sup>
<b>TS(D-E)</b>	- <sup>b</sup>	-3049.494445	-3049.498029	- <sup>a</sup>
<b>E</b>	- <sup>b</sup>	-652.18813801	-652.18813801	-652.18813801
<b>TS(E-P)</b>	- <sup>b</sup>	-652.17654247	-652.17654247	-652.17654247
<b>P</b>	-652.2919369	-652.2919369	-652.2919369	-652.2919369

<sup>a</sup>Substrate moves away from Fe(cys) system. <sup>b</sup>For CSS, we have concerted hydride transfer mechanism.

**Table S3** Single Point Total Electronic Energies (a.u.) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*, LANL2DZ(Ir)//B3LYP/6-31G\*,LANL2DZ(Ir) for Ir Systems

	Ir(Me)	Ir(His)	Ir	Ir(Cl)
<b>Substrate</b>	-761.771745	-761.771745	-761.771745	-761.771745
<b>A</b>	-1980.215866	-2166.450756	-1940.065005	-2400.536386
<b>B</b>	-2742.012524	-2928.274555	-2701.859275	-3162.330682
<b>TS(B-B')</b>	- <sup>a</sup>	- <sup>a</sup>	-2700.874803	-3162.343074
<b>B'</b>	- <sup>a</sup>	-2928.261280	-2701.903215	-3162.343437
<b>TS(B-C)</b>	-2741.981866	-2928.259459	-2701.903009	-3162.338866
<b>C</b>	-2742.011763	-2928.297147	-2701.955117	-3162.384661
<b>TS(C-P)</b>	-2632.424474	-2818.690755	-2592.354467	-3052.774479
<b>P</b>	-652.2919369	-652.2919369	-652.2919369	-652.2919369

<sup>a</sup>Optimization of **B'** and **TS(B-B')** resulted in **B**.

**Table S4** Single Point Total Electronic Energies (a.u.) at the SMD<sub>(diethylether)</sub>/ $\omega$ B97XD/6-311++G\*\*, LANL2DZ(Fe)// $\omega$ B97XD/6-31G\*,LANL2DZ(Fe) for Fe Systems

		CSS	OSS	Triplet	Quintet
<b>Fe(his)</b>	<b>A</b>	-	-	-	-2184.5206
	<b>TS(B-C)</b>	-2945.9869	-	-	-
	<b>TS(C-D)</b>	-2836.4865	-2836.477124	-2836.46982	-
<b>Fe(cys)</b>	<b>A</b>	-	-	-	-2396.5146
	<b>TS(B-C)</b>	-3157.9592	-3157.9599	-3157.9579	-
	<b>TS(C-D)</b>	-3048.4598	-3048.4654	-3048.4604	-

**Table S5** Single Point Total Electronic Energies (a.u.) at the SMD<sub>(diethylether)</sub>/M06/6-311++G\*\*, LANL2DZ(Fe)//M06/6-31G\*,LANL2DZ(Fe) for Fe Systems

		CSS	OSS	Triplet	Quintet
<b>Fe(his)</b>	<b>A</b>	-	-	-	-2183.8072
	<b>TS(B-C)</b>	-2945.0177	-	-2945.0085	-
	<b>TS(C-D)</b>	-2835.5412	-2835.5373	-	-
<b>Fe(cys)</b>	<b>A</b>	-	-	-	-2395.8484
	<b>TS(B-C)</b>	-3157.0519	-3157.0544	-3157.0529	-
	<b>TS(C-D)</b>	-3047.5718	-3047.5782	-3047.5725	-

**Table S6** Single Point Total Electronic Energies (a.u.) at the SMD<sub>(diethylether)</sub>/M06(or  $\omega$ B97XD)/6-311++G\*\*, LANL2DZ(Ir)//M06(or  $\omega$ B97XD)/6-31G\*,LANL2DZ(Ir) for Ir(Me)

	$\omega$ B97XD	M06
<b>A</b>	-1979.4777	-1978.7584
<b>B</b>	-2740.9993	-2740.0398
<b>TS(B-C)</b>	-2740.9593	-2740.0163
<b>C</b>	-2740.9877	-2740.039
<b>TS(C-D)</b>	-2631.4519	-2630.5136

**Table S7** Relative Energies ( $\Delta E$ ) and Free Energies ( $\Delta G$ ) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*,LANL2DZ(Fe)//B3LYP/6-31G\*,LANL2DZ(Fe) for Fe(his) System

	CSS		OSS		Triplet		Quintet	
	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$
<b>A +</b>	6.7	9.8	5.2	7.7	1.8	2.3	0.0	0.0
<b>Substrate</b>								
<b>B</b>	-7.6	10.3	-8.8	7.3	-11.3	2.7	-13.4	-0.3
<b>TS(B-C)</b>	14.2	34.9	-	-	-	-	-	-
<b>C</b>	-11.2	4.5	-13.3	2.7	-3.0	11.3	-0.5	9.9
<b>TS(C-D)</b>	2.2	14.3	2.6	14.0	7.9	18.0	-	-
<b>D</b>	-	-	-5.1	4.9	-5.3	4.0	-3.8	-0.2
<b>TS(D-E)</b>	-	-	-	-	4.2	13.6	-	-
<b>E</b>	-	-	13.7	4.3	13.7	4.3	13.7	4.3
<b>TS(E-P)</b>	-	-	21.1	12.4	21.1	12.4	21.1	12.4
<b>P</b>	-47.9	-56.9	-47.9	-56.9	-47.9	-56.9	-47.9	-56.9

Relative energies and free energies are given in kcal/mol.

**Table S8** Relative Energies ( $\Delta E$ ) and Free Energies ( $\Delta G$ ) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*,LANL2DZ(Fe)//B3LYP/6-31G\*,LANL2DZ(Fe) for Fe(cys) System

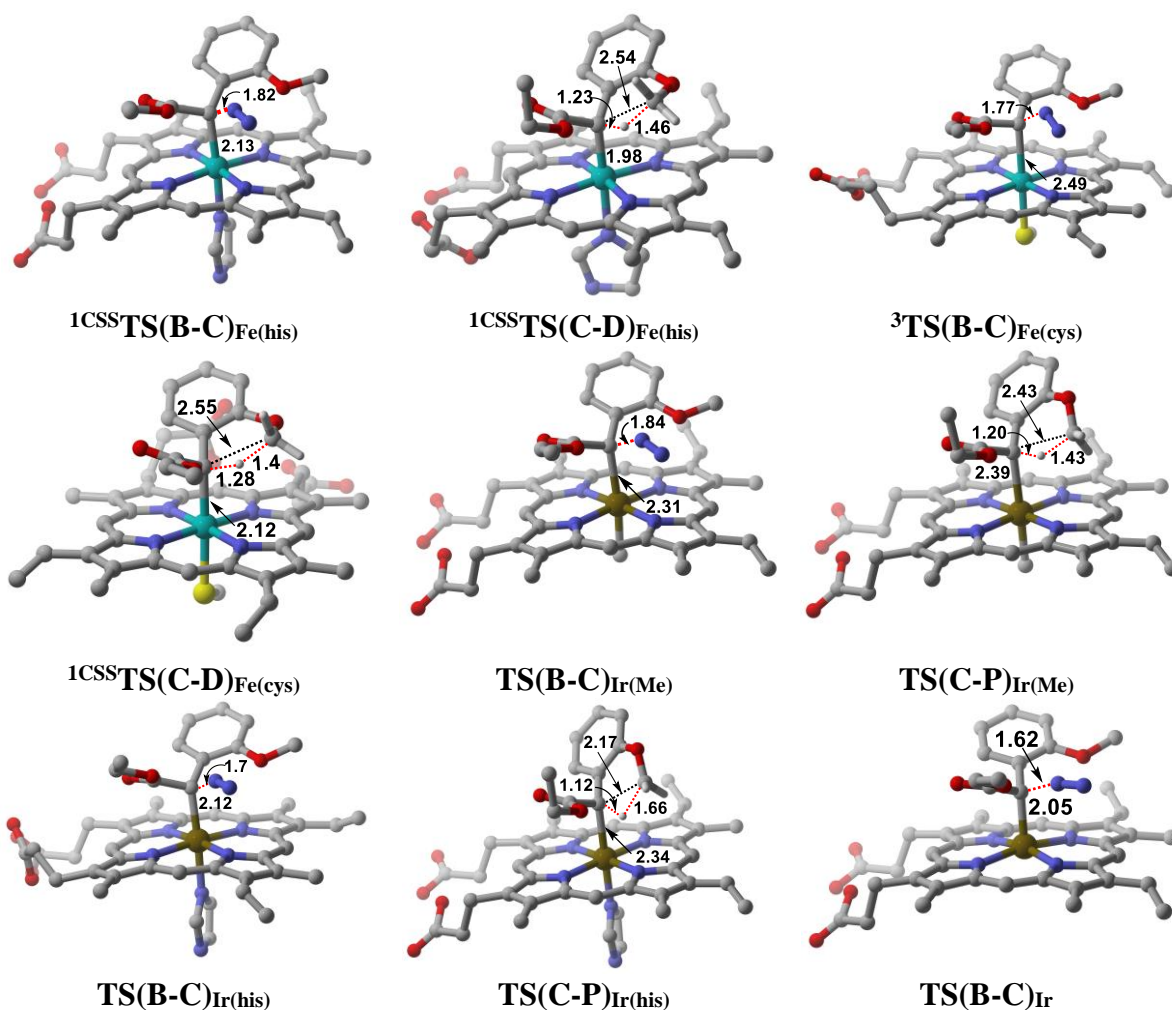
	CSS		OSS		Triplet		Quintet	
	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$
<b>A +</b>	12.4	15.1	11.2	13.5	6.9	8.5	0.0	0.0
<b>Substrate</b>								
<b>B</b>	1.2	17.1	0.0	17.3	-4.4	9.5	-11.7	1.3
<b>TS(B-C)</b>	22.6	44.8	19.3	41.1	17.4	37.7	26.3	42.9
<b>C</b>	-4.4	10.5	-10.7	2.2	-6.9	9.1	5.5	18.5
<b>TS(C-D)</b>	11.4	23.4	6.5	18.6	7.3	20.3	15.4	24.8
<b>D</b>	-	-	-6.9	4.0	-6.9	3.4	-3.8	1.2
<b>TS(D-E)</b>	-	-	-3.8	6.4	-5.8	4.4	-	-
<b>E</b>	-	-	13.7	4.3	13.7	4.3	13.7	4.3
<b>TS(E-P)</b>	-	-	21.1	12.4	21.1	12.4	21.1	12.4
<b>P</b>	-47.9	-56.9	-47.9	-56.9	-47.9	-56.9	-47.9	-56.9

Relative energies and free energies are given in kcal/mol.

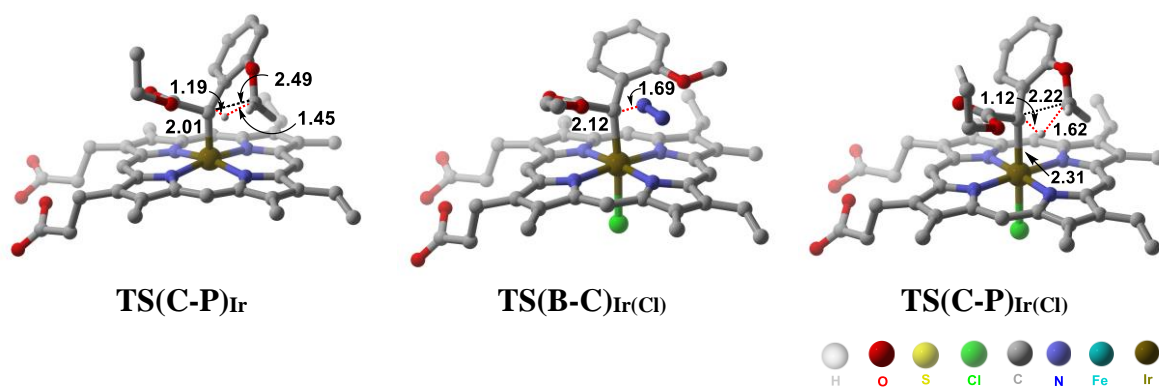
**Table S9** Relative Energies ( $\Delta E$ ) and Free Energies ( $\Delta G$ ) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*,LANL2DZ(Ir)//B3LYP/6-31G\*,LANL2DZ(Ir) for Ir Systems

	Ir(Me)		Ir(His)		Ir		Ir(Cl)	
	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$
A+	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<b>Substrate</b>								
B	-17.5	-5.9	-29.9	-11.1	-12.9	-1.9	-12.7	1.6
TS(B-B')	-	-	-	-	-19.3	-3.9	-20.3	-2.1
B'	-	-	-22.8	-4.8	-40.5	-24.9	-20.6	-2.5
TS(B-C)	2.4	17.9	-22.6	-3.1	-41.1	-25.3	-18.9	-0.3
C	-17.4	-6.5	-47.6	-34.7	-74.7	-63.9	-48.4	-35.0
TS(C-P)	0.3	5.2	-16.5	-8.3	-47.7	-41.6	-15.5	-7.6
P	-47.9	-56.9	-47.9	-56.9	-47.9	-56.9	-47.9	-56.9

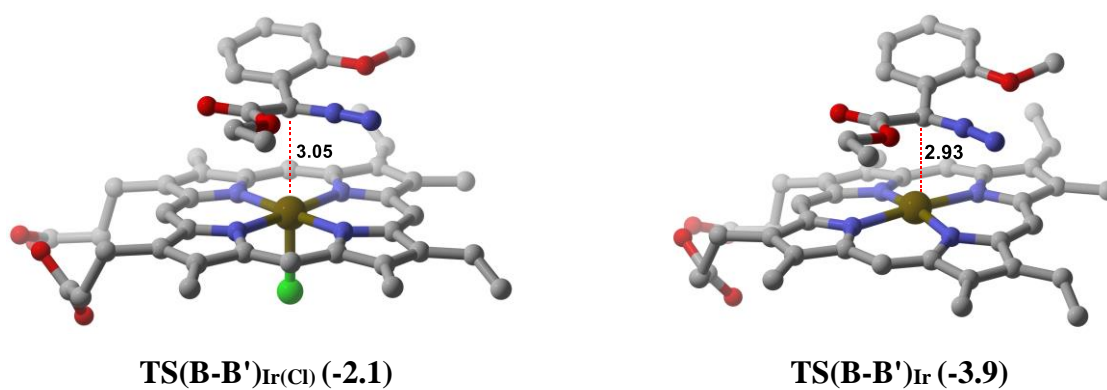
Relative energies and free energies are given in kcal/mol.



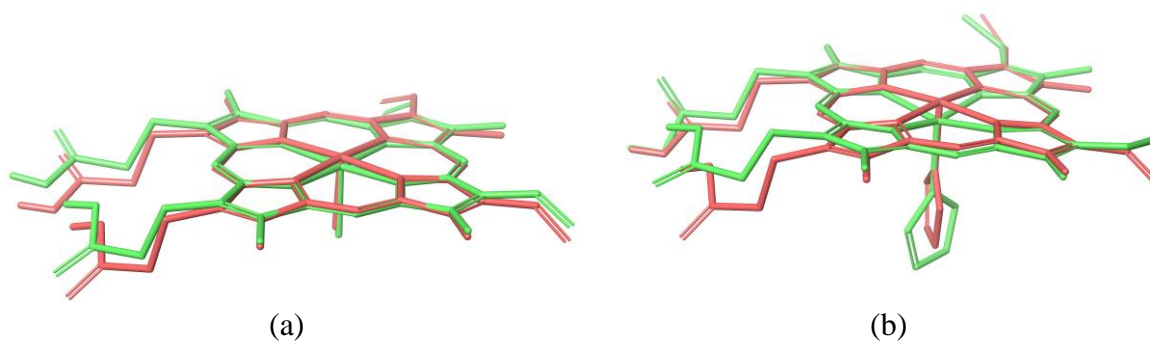




**Fig. S1** Optimized geometries of select TSs.

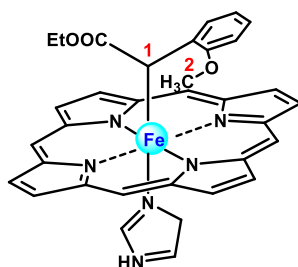


**Fig. S2** Optimized Geometries of **TS(B-B')** for Ir systems and relative free energies (kcal/mol).



**Fig. S3** Overlay of the optimized geometries of ground state metal-porphyrin (in red) with fragment from TS geometry (in green) (a) Ir(Me)-Porphyrin (b) Fe(his)-Porphyrin.

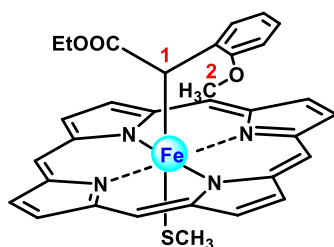
**Table S10** Natural Population Analysis Charges ( $e$ ) and Mulliken Spin Densities for Fe(his) System<sup>a</sup>



			CSS	OSS	Triplet	Quintet	
TS(B-C)	Fe	Charge	0.2005	-	-	-	
		Spin density	0.0	-	-	-	
	C1	Charge	0.0062	-	-	-	
		Spin density	0.0	-	-	-	
	C	Fe	Charge	0.48853	0.19682	0.40730	1.08024
			Spin density	0.0	-0.8	1.4	4.3
C1		Charge	0.11011	0.13903	-0.04245	-0.19697	
		Spin density	0.0	0.6	0.9	-0.4	
TS(C-D)		Fe	Charge	0.24621	0.36735	0.52313	-
			Spin density	0.0	1.04	1.4	-
	C1	Charge	-0.29944	-0.33039	-0.33242	-	
		Spin density	0.0	-0.24	0.3	-	
	C2	Charge	0.0734	-0.05126	-0.13243	-	
		Spin density	0.0	-0.5	0.5	-	

<sup>a</sup>Substituents are not shown on porphyrin for clarity.

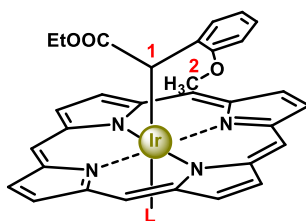
**Table S11** Natural Population Analysis Charges ( $e$ ) and Mulliken Spin Densities for Fe(cys) System<sup>a</sup>



			CSS	OSS	Triplet	Quintet	
<b>TS(B-C)</b>	<b>Fe</b>	<b>Charge</b>	0.04697	0.2675	0.34036	0.53621	
		<b>Spin density</b>	0.0	1.2	1.4	2.5	
	<b>C1</b>	<b>Charge</b>	-0.03485	-0.16371	-0.16183	-0.142406	
		<b>Spin density</b>	0.0	-0.4	0.2	-0.04	
	<b>C</b>	<b>Fe</b>	<b>Charge</b>	-0.07524	0.10987	0.18917	0.68177
			<b>Spin density</b>	0.0	1.0	1.3	3.0
<b>C1</b>		<b>Charge</b>	0.19740	0.00739	-0.06010	-0.18094	
		<b>Spin density</b>	0.0	-0.9	0.8	1.0	
<b>TS(C-D)</b>		<b>Fe</b>	<b>Charge</b>	0.05652	0.27527	0.28554	0.71244
			<b>Spin density</b>	0.0	1.3	1.3	3.98
	<b>C1</b>	<b>Charge</b>	-0.28643	-0.38646	-0.43982	-0.38229	
		<b>Spin density</b>	0.0	-0.6	0.2	0.2	
	<b>C2</b>	<b>Charge</b>	0.04553	-0.13269	-0.09794	-0.12862	
		<b>Spin density</b>	0.0	-0.5	0.7	0.5	

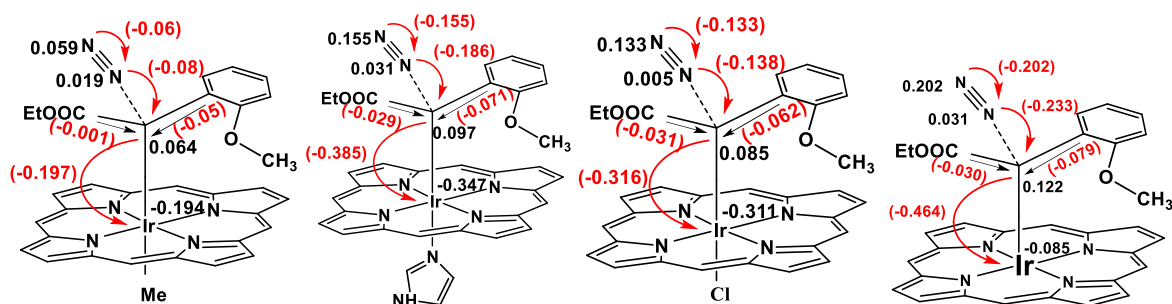
<sup>a</sup>Substituents are not shown on porphyrin for clarity.

**Table S112** Natural Population Analysis Charges ( $e$ ) and Spin Densities for Ir Systems<sup>a</sup>



		Ir(Me)	Ir(His)	Ir	Ir(Cl)
	<b>Ir</b>	0.37453	0.45146	0.64592	0.33191
<b>TS(B-C)</b>	<b>C1</b>	-0.003741	0.00049	0.02027	-0.01664
	<b>Ir</b>	0.33240	0.45944	0.67737	0.34776
<b>C</b>	<b>C1</b>	0.09808	0.20695	0.16789	0.19993
	<b>Ir</b>	0.38572	0.50716	0.67558	0.35345
<b>TS(C-P)</b>	<b>C1</b>	-0.31831	-0.41986	-0.20519	-0.38913
	<b>C2</b>	0.07417	0.14404	0.14308	0.13200

<sup>a</sup>Substituents are not shown on porphyrin due to clarity.



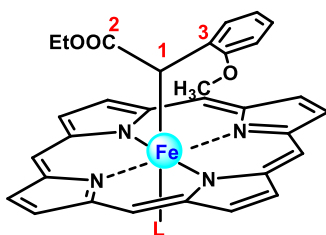
**Fig. S4** Charge transfer ( $e$ ) analysis for Ir Systems (change in charge on going from reactants to TS via **TS(B-C)** is shown in black, and the amount of charge transfer is shown in red).

**Table S13** Comparison of Selected TSs at Different Level of Theories. Relative Free Energies are in kcal/mol

			B3LYP	$\omega$ B97XD	M06
Fe(his)	TS(B-C)	CSS	- <sup>a</sup>	- <sup>a</sup>	0.0
		Triplet	- <sup>a</sup>	- <sup>a</sup>	3.1 <sup>b</sup>
		OSS	0.0	0.0	0.0
	TS(C-D)	CSS	0.3	-3.0	-1.5
		Triplet	4.0	3.6	- <sup>c</sup>
		OSS	0.0	0.0	0.0
Fe(cys)	TS(B-C)	CSS	3.7	1.0	2.4
		Triplet	-3.4	1.0	-0.1
		OSS	0.0	0.0	0.0
	TS(C-D)	CSS	4.8	5.8	6.9
		Triplet	1.7	2.1	2.9

<sup>a</sup>Only CSS is obtained. <sup>b</sup>Relative free energy with respect to CSS. Relative free energies with respect to OSS are given in kcal/mol.

**Table S14** Geometric Parameters at Different Level of Theories and Basis Sets for C Intermediate. Distances are in Å and Angles in °.

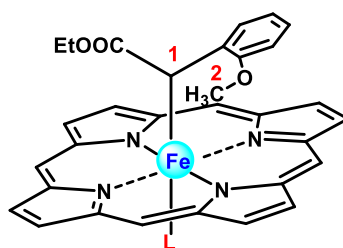


		M-L	M-C1	∠ M-C1-C2	∠ M-C1-C3	∠ C2-C1-C3
Ir(Me)	B3LYP/6-31G*	2.15	2.05	117.11	128.83	110.88
	wB97XD/6-31G*	2.12	2.01	117.21	128.37	111.09
	B3LYP/DEF2SVP	2.15	2.06	117.22	126.46	113.47
Fe(his)	B3LYP/6-31G*	2.22	1.85	118.77	128.73	110.50
	B3LYP/DEF2SVP	2.19	1.86	118.74	128.63	110.59
Fe(cys)	B3LYP/6-31G*	2.41	1.96	121.02	125.62	111.74
	wB97XD/6-31G*	2.36	1.96	119.77	122.01	114.20
	B3LYP/DEF2SVP	2.36	1.98	20.94	124.92	112.33

**Table S15** Relative Free Energies (kcal/mol) for Key Stationary points at Different Level of Theories.

			<b>B3LYP</b>	<b><math>\omega</math>B97XD</b>	<b>M06</b>
<b>Ir(Me)</b>	<b>A+Substrate</b>		0.0	0.0	0.0
	<b>B</b>		-5.9	-8.4	-5.5
	<b>TS(B-C)</b>		17.9	15.9	10.3
	<b>C</b>		-6.5	-5.1	-8.7
	<b>TS(C-P)</b>		5.2	-1.6	5.3
<b>Fe(cys)</b>	<b>A+Substrate</b>	<b>Quintet</b>	0.0	0.0	0.0
	<b>TS(B-C)</b>	<b>Triplet</b>	37.7	47.7	49.4
	<b>C</b>	<b>OSS</b>	2.2	21.7	13.9
	<b>TS(C-D)</b>	<b>OSS</b>	18.6	20.9	29.5
<b>Fe(his)</b>	<b>A+Substrate</b>	<b>Quintet</b>	0.0	0.0	0.0
	<b>TS(B-C)</b>	<b>CSS</b>	34.9	32.9	46.6
	<b>TS(C-D)</b>	<b>OSS</b>	14.0	16.3	29.7

**Table S16** Comparison of TS(C-D) at Different Level of Theories<sup>a</sup>

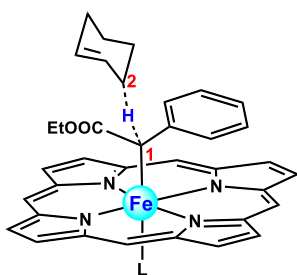


		<b>B3LYP</b>				<b><math>\omega</math>B97XD</b>				<b>Process Involved</b>
		<b>Mulliken Spin</b>				<b>Mulliken Spin</b>				
		$\Delta$ G	<b>densities</b>			$\Delta$ G	<b>densities</b>			
			<b>Fe</b>	<b>C1</b>	<b>C2</b>		<b>Fe</b>	<b>C1</b>	<b>C2</b>	
<b>Fe (his)</b>	<b>OSS</b>	0.0	1.0	-0.3	-0.5	0.0	1.1	-0.3	-0.6	HAT
	<b>CSS</b>	0.3	0.0	0.0	0.0	-3.0	0.0	0.0	0.0	Hydride transfer
	<b>Triplet</b>	4.0	1.4	0.3	0.5	3.6	1.3	0.4	0.5	HAT
<b>Fe (cys)</b>	<b>OSS</b>	0.0	1.3	-0.6	-0.5	0.0	1.2	-0.5	-0.5	HAT
	<b>CSS</b>	4.8	0.0	0.0	0.0	5.8	0.0	0.0	0.0	Hydride transfer
	<b>Triplet</b>	1.7	1.3	0.2	0.7	2.1	1.1	0.4	0.6	HAT
	<b>OSS</b>	0.0	1.2	-0.4	-0.5	0.0	1.3	-0.5	-0.6	HAT

<b>Fe</b>	<b>CSS</b>	5.4	0.0	0.0	0.0	1.2	0.0	0.0	0.0	Hydride transfer
	<b>Triplet</b>	0.8	2.3	-0.2	-0.04	0.3	2.1	-0.1	-0.04	Hydride transfer

<sup>a</sup>Substituents are not shown on porphyrin for clarity. Relative free energies with respect to OSS are given in kcal/mol.

**Table S17** Comparison of **TS(C-D)** at Different Level of Theories with Cyclohexene as a Substrate for Intermolecular C-H Insertion<sup>a</sup>



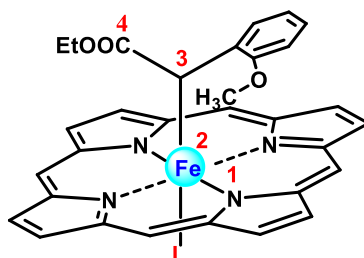
		<b>B3LYP</b>				<b>wB97XD</b>				<b>Process involved</b>
		$\Delta G$	<b>Mulliken Spin densities</b>			$\Delta G$	<b>Mulliken Spin densities</b>			
			<b>Fe</b>	<b>C1</b>	<b>C2</b>		<b>Fe</b>	<b>C1</b>	<b>C2</b>	
<b>Fe(his)</b>	<b>OSS</b>	0.0	-1.1	0.4	0.3	0.0	-1.1	0.4	0.4	HAT
	<b>CSS</b>	1.6	0.0	0.0	0.0	1.4	0.0	0.0	0.0	Hydride transfer
	<b>Triplet</b>	0.7 <sup>b</sup>	2.0	-0.0	0.1	2.9	1.3	0.5	0.3	HAT
<b>Fe</b>	<b>OSS</b>	0.0	1.0	-0.5	-0.3	0.0	1.3	-0.6	-0.3	HAT
	<b>CSS</b>	4.2	0.0	0.0	0.0	5.5	0.0	0.0	0.0	Hydride transfer
	<b>Triplet</b>	11.6 <sup>b</sup>	2.0	0.0	0.1	-0.4	2.1	-0.1	0.1	Hydride transfer

<sup>a</sup>R. L. Khade and Y. Zhang, *Chem. Eur. J.*, 2017, **23**, 17654. <sup>b</sup>Substrate moves away from metal-porphyrin.

Relative Energies with respect to OSS are in kcal/mol.

**Table S18** Energy Gaps for N<sub>2</sub> Expulsion Transition State

	Orbital energy		
	M	C-N*	gap
<sup>1</sup> CSST <b>S(B-C)</b> <sub>Fe(his)</sub>	-0.187 (homo-2)	-0.080(lumo)	0.107
<sup>1</sup> CSST <b>S(B-C)</b> <sub>Fe(cys)</sub>	-0.157(homo-3)	-0.063(lumo)	0.094
<b>TS(B-C)</b> <sub>Ir(Me)</sub>	-0.196(homo-2)	-0.096(lumo)	0.100

**Table S19** Relative Energies( $\Delta E$ ) at the B3LYP/6-31G\*,LANL2DZ(Fe) and Optimized Dihedral Angles for Different Conformations in the Active Site of CYP119<sup>a</sup>

	N1-Fe2-C3-C4		
	Initial	Optimized	$\Delta E$
<sup>1</sup> CSST <b>C</b> <sub>Fe(cys)</sub>	-17.6	-40.5	0.0
<b>conf1</b>	0.0	-24.6	0.1
<b>Conf2</b>	45.2	-26.9	0.1
<b>Conf3</b>	90.4	65.3	2.6
<b>Conf4</b>	127.9	137.1	14.9
<b>Conf5</b>	168.6	169.0	2.1
<b>Conf6</b>	-58.6	-24.6	0.1
<b>Conf7</b>	-135.6	-169.1	0.2

<sup>a</sup>Substituents are not shown on porphyrin for clarity. Relative energies are given in kcal/mol.

As can be seen from Table S19, during optimization Conf6 converges to Conf1. Additionally, <sup>1</sup>CSST**C**<sub>Fe(cys)</sub>, Conf1, Conf2 and Conf7 lie within 0.2 kcal/mol. Such close conformations were also observed by Fasan, Zhang and coworkers in their QM cluster study of cyclopropanation



reaction (A. Tinoco, Y. Wei, J.-P. Bacik, D. M. Carminati, E. J. Moore, N. Ando, Y. Zhang and R. Fasan, *ACS Catal.*, 2019, **9**, 1514-1524). This shows that these conformations are affected by protein environment in a subtle way. However, the energy barriers are not going to be significantly affected by taking an average of these conformations. A thorough molecular dynamics study is currently underway in our laboratory.

**Table S20** Single Point Total Electronic Energies (a.u.) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*, LANL2DZ(Fe/Ir)//B3LYP/6-31G\*,LANL2DZ(Fe/Ir) for Fe(cys) and Ir System

	<b>Fe(cys)</b>	<b>Ir(Me)</b>	<b>(C317G,T213A)- Ir(Me)-CYP119</b>
<b>Substrate</b>	-761.771746	-761.771746	-761.771746
<b>A</b>	-4732.116045	-4753.79759	-4201.65681
<b>B</b>	-	-5515.59190	-4963.44832
<b>TS(B-C)</b>	-5493.831774	-5515.56168	-4963.42169
<b>C</b>	-	-5515.59789	-4963.45357

**Table S21** Relative Energies ( $\Delta E$ ) (kcal/mol) at the SMD<sub>(diethylether)</sub>/B3LYP/6-311++G\*\*,LANL2DZ(Fe/Ir)//B3LYP/6-31G\*,LANL2DZ(Fe/Ir) for Fe-CYP119 and Ir(Me)-CYP119 Systems

	<b>Fe(cys)-CYP119</b>	<b>Ir(Me)-CYP119</b>	<b>(C317G,T213A)- Ir(Me)-CYP119</b>
<b>A+Substrate</b>	0.0	0.0	0.0
<b>B</b>	-	-13.9	-12.2
<b>TS(B-C)</b>	34.4	3.3	2.8
<b>C</b>	-	-20.6	-17.7

## Coordinates of Optimized Geometries

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### Substrate

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Number of imaginary frequencies: 0    Electronic energy:    HF=-761.5076164  
Zero-point correction=                    0.219899 (Hartree/Particle)  
Thermal correction to Energy=            0.235519  
Thermal correction to Enthalpy=         0.236463  
Thermal correction to Gibbs Free Energy= 0.175535  
Sum of electronic and zero-point Energies= -761.287718  
Sum of electronic and thermal Energies= -761.272097  
Sum of electronic and thermal Enthalpies= -761.271153  
Sum of electronic and thermal Free Energies= -761.332082

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### Cartesian Coordinates

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6	-3.566408	-1.563524	0.068343
6	-2.475665	-2.388899	0.328879
6	-1.192049	-1.845874	0.385229
6	-0.970993	-0.478001	0.169944
6	-2.089051	0.346204	-0.110445
6	-3.376139	-0.197003	-0.149316
6	0.399314	0.073797	0.224139
7	0.600111	1.296552	0.674325
7	0.787090	2.348120	1.063158
8	-1.815598	1.666452	-0.335600
6	-2.884152	2.543047	-0.654016
6	1.610795	-0.667264	-0.157992
8	2.727152	0.089233	-0.006375
8	1.625069	-1.816296	-0.559250
1	-0.340075	-2.485100	0.578536
1	-2.616616	-3.452768	0.494958
1	-4.230495	0.436265	-0.358540
1	-4.571786	-1.973758	0.029510
1	-2.429255	3.523581	-0.805283
1	-3.397395	2.232979	-1.573452
1	-3.612987	2.603308	0.164674
6	3.972243	-0.554230	-0.355022
1	4.089794	-1.453499	0.258288
1	3.925968	-0.871539	-1.401754
6	5.084025	0.450092	-0.112979
1	6.050593	0.001191	-0.366746
1	4.945600	1.343342	-0.730572
1	5.111740	0.758126	0.937221

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### 1CSSA<sub>Fe(his)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2184.5514934

Zero-point correction=	0.671040 (Hartree/Particle)
Thermal correction to Energy=	0.716869
Thermal correction to Enthalpy=	0.717813
Thermal correction to Gibbs Free Energy=	0.586983
Sum of electronic and zero-point Energies=	-2183.880453
Sum of electronic and thermal Energies=	-2183.834624
Sum of electronic and thermal Enthalpies=	-2183.833680
Sum of electronic and thermal Free Energies=	-2183.964511

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Cartesian Coordinates  
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6	-1.670072	-3.422859	-0.615443
6	-0.364057	-2.785306	-0.571814
7	-0.485933	-1.425306	-0.409547
6	-1.834649	-1.182355	-0.352140
6	-2.591713	-2.420249	-0.479794
6	0.841265	-3.464779	-0.688662
6	2.107492	-2.884484	-0.695908
7	2.357992	-1.541281	-0.539869
6	3.721546	-1.404596	-0.620941
6	4.354813	-2.697984	-0.866846
6	3.336912	-3.623958	-0.882154
6	4.407725	-0.212563	-0.426914
6	3.836985	1.041019	-0.238618
7	2.484774	1.290626	-0.194761
6	2.364282	2.647144	-0.050478
6	3.675565	3.283366	0.012585
6	4.598533	2.267680	-0.107520
6	1.153956	3.328050	0.041591
6	-0.108395	2.752294	-0.016234
7	-0.354918	1.404682	-0.125208
6	-1.721655	1.281402	-0.133727
6	-2.361716	2.586018	-0.035771
6	-1.351095	3.505353	0.039387
6	-1.446681	4.998525	0.144219
6	-3.844115	2.831420	-0.058568
6	-4.427200	2.840091	-1.482590
6	-5.924917	3.055638	-1.498125
8	-6.639091	3.175983	-0.526270
6	-2.408808	0.076627	-0.218914
6	6.092121	2.374778	-0.164795
6	3.887412	4.722043	0.131673
6	4.936049	5.341266	0.697591
6	3.428024	-5.102247	-1.117412
6	5.774832	-2.979685	-1.071534
6	6.675246	-2.213199	-1.706184
6	-4.090163	-2.530067	-0.444894
6	-4.657574	-2.520224	0.985469
6	-6.167091	-2.623319	1.016671
8	-6.897690	-2.702645	0.053429

6	-1.901710	-4.894022	-0.794752
8	-6.408633	3.100007	-2.765134
8	-6.640084	-2.618541	2.289251
1	1.197027	4.405073	0.161024
1	-3.492481	0.125094	-0.199853
1	0.791684	-4.541730	-0.813832
1	5.488813	-0.269199	-0.427885
1	6.528196	1.611258	-0.817774
1	6.394426	3.355889	-0.545761
1	6.555435	2.254423	0.824650
1	4.467180	-5.443728	-1.120943
1	2.894027	-5.670981	-0.345423
1	2.991082	-5.386264	-2.084235
1	-1.409448	-5.273550	-1.699201
1	-1.509877	-5.476736	0.050014
1	-2.968003	-5.123311	-0.882248
1	-2.485589	5.325612	0.249063
1	-0.893270	5.381250	1.011418
1	-1.034017	5.496708	-0.743162
1	3.101711	5.350548	-0.288032
1	5.000940	6.425565	0.711918
1	5.744707	4.800161	1.178828
1	6.116262	-3.942714	-0.689488
1	7.708874	-2.532951	-1.803765
1	6.411032	-1.268317	-2.171143
1	-4.372898	2.075115	0.532824
1	-4.076363	3.788515	0.420482
1	-3.960246	3.622023	-2.094387
1	-4.212922	1.898078	-2.003214
1	-7.372249	3.230443	-2.680349
1	-4.415179	-3.449376	-0.943081
1	-4.551783	-1.713530	-1.011978
1	-4.246226	-3.348839	1.575941
1	-4.365846	-1.608192	1.521225
1	-7.611390	-2.679800	2.214043
7	1.073261	-0.304003	1.778646
6	1.088651	-1.458187	2.423354
6	1.115374	0.690843	2.735144
7	1.138984	-1.243951	3.762703
1	1.065470	-2.432806	1.961390
6	1.156981	0.121007	3.978481
1	1.113884	1.732692	2.456691
1	1.162359	-1.962004	4.471013
1	1.196915	0.548368	4.967994
26	1.005373	-0.082826	-0.171127

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$1\text{CSS}\mathbf{B}_{\text{Fe}(\text{his})}$

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0694272  
Zero-point correction=                      0.893678 (Hartree/Particle)

Thermal correction to Energy=	0.956372
Thermal correction to Enthalpy=	0.957316
Thermal correction to Gibbs Free Energy=	0.788964
Sum of electronic and zero-point Energies=	-2945.175749
Sum of electronic and thermal Energies=	-2945.113056
Sum of electronic and thermal Enthalpies=	-2945.112111
Sum of electronic and thermal Free Energies=	-2945.280463

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Cartesian Coordinates  
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6	3.068830	2.086458	2.183004
6	2.474433	0.839226	1.746199
7	1.190617	1.035054	1.297180
6	0.943544	2.376992	1.449246
6	2.123230	3.061924	1.973285
6	3.136928	-0.382602	1.765734
6	2.661358	-1.580885	1.246924
7	1.427340	-1.745559	0.676162
6	1.386273	-3.051534	0.247506
6	2.624621	-3.739735	0.551358
6	3.424742	-2.825153	1.201701
6	0.291961	-3.645999	-0.375982
6	-0.923710	-3.032098	-0.647761
7	-1.232824	-1.729776	-0.335325
6	-2.530770	-1.551619	-0.744993
6	-3.062750	-2.775324	-1.332019
6	-2.054546	-3.698519	-1.276948
7	-1.485414	1.027178	0.344083
6	-2.756082	0.837992	-0.139921
6	-3.515997	2.077908	-0.088567
6	-2.679486	3.023458	0.446112
6	-1.417422	2.351436	0.703786
6	-3.244986	-0.363441	-0.641278
6	-0.288430	2.979753	1.220216
8	5.632254	-0.750668	-1.355332
6	5.120257	0.505861	-1.280659
8	5.627140	1.403217	-0.627017
6	3.904120	0.639160	-2.090609
7	3.539585	-0.458724	-2.727932
7	3.249246	-1.412057	-3.271769
6	3.147855	1.894265	-2.288405
6	3.800002	3.133215	-2.202640
6	3.114141	4.329514	-2.411982
6	1.757799	4.304447	-2.727047
6	1.081623	3.085759	-2.814785
6	1.761410	1.886324	-2.585236
8	1.161704	0.659950	-2.626961
6	-0.187311	0.567776	-3.074364
1	-0.371332	4.032567	1.462066
1	-4.267634	-0.372636	-0.998376

1	0.391948	-4.686439	-0.665709
1	4.133774	-0.383172	2.191073
1	4.853473	3.148903	-1.955014
1	3.646022	5.273316	-2.336004
1	0.022776	3.074121	-3.044308
1	1.215210	5.229135	-2.905544
1	-0.426863	-0.495846	-3.066716
1	-0.868550	1.089682	-2.394519
1	-0.290584	0.968372	-4.091385
6	6.870561	-0.990057	-0.652382
1	6.845112	-2.056359	-0.416508
1	6.867481	-0.413926	0.276093
6	8.072069	-0.630753	-1.514838
1	8.086228	0.442558	-1.726012
1	8.999171	-0.890193	-0.990200
1	8.048587	-1.177944	-2.463054
6	4.483393	2.249940	2.649565
1	4.657223	3.251031	3.055521
1	4.742542	1.524283	3.430941
1	5.181839	2.104959	1.815346
6	2.948675	-5.152708	0.171606
1	4.020092	-5.263423	-0.027365
1	2.692739	-5.868326	0.966092
1	2.409603	-5.462569	-0.729563
6	2.293198	4.493386	2.216408
6	1.798933	5.504640	1.485677
1	2.923408	4.747840	3.069716
1	1.997616	6.537575	1.758069
1	1.224229	5.338591	0.579627
6	4.774769	-2.978959	1.727882
6	5.383781	-4.116651	2.104526
1	5.343971	-2.056578	1.834405
1	6.404345	-4.101419	2.476594
1	4.891931	-5.083403	2.083134
6	-2.950961	4.474449	0.713800
1	-3.938942	4.772996	0.349360
1	-2.916024	4.705298	1.786938
1	-2.210849	5.121924	0.226848
6	-4.937173	2.250361	-0.547587
1	-5.122775	3.301155	-0.797595
1	-5.116294	1.672753	-1.461646
6	-4.468003	-2.932717	-1.845497
1	-4.519761	-3.786780	-2.528999
1	-4.740445	-2.054216	-2.438123
6	-5.521467	-3.131142	-0.713102
1	-5.064430	-2.864965	0.249423
1	-5.835718	-4.174455	-0.631559
6	-5.980149	1.806278	0.520487
1	-5.841872	0.746599	0.745050
1	-5.838773	2.389054	1.434746

6	-6.780167	-2.285087	-0.806350
8	-7.891906	-2.660666	-0.504907
8	-6.504628	-1.019500	-1.195686
1	-7.296311	-0.439645	-1.081455
6	-7.387031	2.002667	0.011304
8	-8.037043	1.202066	-0.642953
8	-7.881140	3.220785	0.310457
1	-8.769611	3.267330	-0.093279
6	-2.057038	-5.122682	-1.747439
1	-1.919962	-5.827164	-0.916117
1	-3.000272	-5.379433	-2.239141
1	-1.248976	-5.314127	-2.465040
7	-0.721723	-0.860959	2.408858
6	-1.017206	-0.004397	3.371632
6	-0.943939	-2.126099	2.914728
7	-1.424530	-0.671902	4.481187
1	-0.946376	1.069470	3.296526
6	-1.382664	-2.025902	4.207032
1	-0.768769	-3.004558	2.314292
1	-1.699706	-0.246198	5.353511
1	-1.659555	-2.771093	4.936051
26	-0.066669	-0.387448	0.620305

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**<sup>1</sup>CCS<sup>S</sup>TS(B-C)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2946.0186418  
Zero-point correction=                    0.890263 (Hartree/Particle)  
Thermal correction to Energy=            0.952599  
Thermal correction to Enthalpy=         0.953543  
Thermal correction to Gibbs Free Energy= 0.789974  
Sum of electronic and zero-point Energies= -2945.128379  
Sum of electronic and thermal Energies= -2945.066043  
Sum of electronic and thermal Enthalpies= -2945.065099  
Sum of electronic and thermal Free Energies= -2945.228668

.....  
Cartesian Coordinates

.....  

6	3.122529	-3.742782	-0.686685
6	1.914788	-3.022221	-0.332748
7	2.062798	-1.674259	-0.565136
6	3.315610	-1.517390	-1.094486
6	4.001029	-2.804411	-1.184413
6	0.734371	-3.630835	0.096131
6	-0.490732	-2.994901	0.281682
7	-0.696563	-1.644931	0.169078
6	-2.045960	-1.453531	0.301077
6	-2.723352	-2.726550	0.520995
6	-1.748873	-3.689585	0.523213
6	-2.689752	-0.220056	0.255376
6	-2.084444	1.018525	0.062006

7	-0.750871	1.214524	-0.168240
6	-0.589155	2.559764	-0.363263
6	-1.858941	3.255707	-0.209336
6	-2.795205	2.292428	0.056279
6	0.603778	3.181226	-0.722638
6	1.813050	2.539821	-0.986130
7	2.005278	1.188485	-0.911943
6	3.250467	0.945954	-1.426095
6	3.884633	2.183163	-1.839675
6	3.006890	3.195714	-1.524312
6	3.854204	-0.305921	-1.518095
1	0.574304	4.252883	-0.876496
1	4.841613	-0.335883	-1.966433
1	0.751136	-4.709265	0.215452
1	-3.764027	-0.222675	0.396756
6	1.066264	0.188968	1.777337
6	1.461030	1.560634	2.258786
6	0.484820	2.421316	2.794294
6	2.778152	2.080945	2.141836
6	0.778310	3.728237	3.182980
1	-0.528768	2.058190	2.883173
6	3.077488	3.381968	2.560005
6	2.078502	4.209233	3.072523
1	-0.013784	4.357005	3.579542
1	4.089709	3.757645	2.474542
1	2.327438	5.220401	3.383904
6	0.025882	-0.470264	2.664775
8	-1.062760	0.027218	2.876684
8	0.387922	-1.665286	3.171051
8	3.728201	1.239917	1.649345
6	5.074217	1.677435	1.563613
1	5.628499	0.836034	1.144408
1	5.166646	2.541886	0.895903
1	5.479642	1.929041	2.552557
7	3.201616	-1.679310	2.050670
7	2.492271	-0.844509	2.228820
6	-4.265157	2.480312	0.308246
1	-4.602742	1.795137	1.095311
1	-4.455926	3.493785	0.676129
6	-5.145082	2.260411	-0.952306
1	-5.060855	1.233291	-1.310710
1	-4.802246	2.933184	-1.746633
6	-6.587855	2.609456	-0.666376
8	-6.998871	3.693315	-0.323118
8	-7.443344	1.546135	-0.816490
1	-8.333976	1.887550	-0.604527
6	-4.213692	-2.883919	0.641345
1	-4.617028	-2.078839	1.262322
1	-4.455962	-3.818861	1.158377
6	-4.934713	-2.872391	-0.741067



1	-4.273790	-2.397638	-1.477984
1	-5.140445	-3.884213	-1.098177
6	-6.231822	-2.090166	-0.801623
8	-7.251129	-2.447189	-1.349969
8	-6.100010	-0.874153	-0.215602
1	-6.890741	-0.330114	-0.414552
6	-1.897565	-5.173345	0.691332
1	-2.925442	-5.444138	0.952660
1	-1.640397	-5.718566	-0.226998
1	-1.244534	-5.561699	1.483495
6	-2.041038	4.740013	-0.322130
1	-1.803607	5.104881	-1.330343
1	-3.071144	5.037189	-0.102604
1	-1.385155	5.278377	0.373965
6	3.342261	-5.212789	-0.492853
1	2.785278	-5.591903	0.370891
1	3.028482	-5.803838	-1.365402
1	4.403817	-5.425400	-0.327018
6	5.251707	2.293352	-2.447522
1	6.037856	1.964485	-1.753913
1	5.344378	1.673222	-3.348271
1	5.482803	3.324714	-2.729653
6	5.364548	-2.977083	-1.672292
6	5.896134	-4.076645	-2.231554
1	6.014868	-2.108760	-1.565049
1	6.937688	-4.095954	-2.539745
1	5.318415	-4.975968	-2.420019
6	3.238267	4.627480	-1.706242
6	2.813986	5.622195	-0.910621
1	3.852759	4.896801	-2.566483
1	3.050591	6.657703	-1.139657
1	2.248804	5.437113	-0.002067
6	-0.623531	-2.359627	3.938859
1	-0.973320	-1.700054	4.738947
1	-1.468986	-2.576542	3.280505
6	0.015335	-3.625687	4.479263
1	0.865720	-3.392032	5.128371
1	-0.719015	-4.190898	5.063987
1	0.370061	-4.259954	3.660547
7	0.135859	-0.458919	-2.277852
6	-0.011274	-1.613800	-2.900526
6	-0.128665	0.524341	-3.209527
7	-0.361623	-1.414996	-4.197740
1	0.125193	-2.587205	-2.456109
6	-0.440093	-0.051307	-4.411677
1	-0.074442	1.568798	-2.947428
1	-0.524893	-2.139058	-4.881116
1	-0.701365	0.368236	-5.370618
26	0.686053	-0.215412	-0.282273

1CSSC<sub>Fe(his)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0612815  
Zero-point correction=                    0.889470 (Hartree/Particle)  
Thermal correction to Energy=            0.953959  
Thermal correction to Enthalpy=           0.954903  
Thermal correction to Gibbs Free Energy=    0.781196  
Sum of electronic and zero-point Energies=    -2945.171811  
Sum of electronic and thermal Energies=    -2945.107322  
Sum of electronic and thermal Enthalpies=    -2945.106378  
Sum of electronic and thermal Free Energies=   -2945.280086  
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Cartesian Coordinates

-----  
6    3.259159 -3.128148 -1.278785  
6    2.018641 -2.576872 -0.770459  
7    1.997552 -1.212624 -0.915943  
6    3.171397 -0.872404 -1.526741  
6    3.976331 -2.064044 -1.784968  
6    0.950827 -3.349069 -0.312868  
6    -0.321729 -2.873062 -0.017798  
7    -0.677471 -1.549861 -0.015660  
6    -2.028282 -1.518119 0.199913  
6    -2.553058 -2.870394 0.345505  
6    -1.482704 -3.717075 0.226980  
6    -2.794385 -0.361384 0.304042  
6    -2.316977 0.942659 0.231037  
7    -1.022407 1.295575 -0.031026  
6    -0.978393 2.664656 0.003377  
6    -2.293983 3.206235 0.308796  
6    -3.131621 2.131399 0.445182  
6    0.142355 3.441735 -0.273097  
6    1.380438 2.961201 -0.694916  
7    1.678084 1.638082 -0.858857  
6    2.887753 1.590585 -1.498552  
6    3.393091 2.928189 -1.737619  
6    2.475032 3.795127 -1.190581  
6    3.562721 0.424326 -1.844824  
1    0.018306 4.517184 -0.238720  
1    4.500026 0.544365 -2.377038  
1    1.098768 -4.423026 -0.273892  
1    -3.853290 -0.487578 0.493898  
6    0.941717 0.212682 1.436543  
6    1.799319 1.207204 2.118997  
6    1.188155 2.194036 2.917028  
6    3.212817 1.221898 2.007757  
6    1.929234 3.217474 3.506345  
1    0.111094 2.162219 3.036904  
6    3.955365 2.241766 2.613640  
6    3.312791 3.242289 3.345669

1	1.425936	3.982003	4.091214
1	5.035235	2.256875	2.526452
1	3.906313	4.029373	3.803357
6	0.088069	-0.495127	2.448975
8	-0.942921	-0.042156	2.909921
8	0.634107	-1.663465	2.835838
8	3.774645	0.170862	1.355000
6	5.185178	0.131692	1.219917
1	5.401805	-0.777062	0.657647
1	5.558780	1.000703	0.663043
1	5.679471	0.084629	2.198948
7	3.893217	-3.493598	2.333758
7	4.198830	-2.639605	2.964989
6	-4.598306	2.140443	0.774193
1	-4.832094	1.329495	1.474449
1	-4.861276	3.074451	1.281357
6	-5.516251	2.001199	-0.471434
1	-5.357868	1.040171	-0.963628
1	-5.275678	2.799979	-1.181504
6	-6.967679	2.171148	-0.084953
8	-7.467107	3.177360	0.361513
8	-7.714404	1.033371	-0.266023
1	-8.620010	1.258554	0.023483
6	-4.009341	-3.196495	0.528490
1	-4.447369	-2.509121	1.258523
1	-4.121986	-4.201089	0.949998
6	-4.819694	-3.114270	-0.801682
1	-4.253350	-2.508972	-1.521388
1	-4.960979	-4.100421	-1.249975
6	-6.181004	-2.454529	-0.702738
8	-7.203958	-2.856740	-1.211344
8	-6.111690	-1.286776	-0.016168
1	-6.960712	-0.805173	-0.105334
6	-1.461215	-5.216251	0.283183
1	-2.438867	-5.619346	0.565401
1	-1.193687	-5.658589	-0.685983
1	-0.730170	-5.586156	1.013494
6	-2.610154	4.667220	0.432693
1	-2.488704	5.193285	-0.523678
1	-3.640573	4.828305	0.763806
1	-1.950008	5.163869	1.154847
6	3.651015	-4.573793	-1.222047
1	3.226695	-5.069986	-0.343135
1	3.317596	-5.133944	-2.107588
1	4.740056	-4.676353	-1.169612
6	4.698387	3.254444	-2.399956
1	5.556021	2.931781	-1.793702
1	4.792319	2.760965	-3.375562
1	4.806937	4.331034	-2.560950
6	5.289500	-2.047066	-2.419891

6	5.881884	-3.045066	-3.096846
1	5.842066	-1.111660	-2.332185
1	6.877522	-2.919283	-3.512772
1	5.398080	-3.999207	-3.279140
6	2.583754	5.251253	-1.132773
6	2.159996	6.048584	-0.139879
1	3.096367	5.718834	-1.974544
1	2.296289	7.125270	-0.191134
1	1.698045	5.654607	0.760610
6	-0.127010	-2.415348	3.811987
1	-0.331312	-1.772330	4.673520
1	-1.085869	-2.692182	3.362878
6	0.691190	-3.634698	4.193123
1	1.644511	-3.342253	4.644449
1	0.137120	-4.239898	4.919610
1	0.901373	-4.252603	3.314336
7	-0.128184	-0.002014	-2.425130
6	-0.199125	-1.079051	-3.182436
6	-0.540540	1.053290	-3.210858
7	-0.642093	-0.762750	-4.428255
1	0.058563	-2.080400	-2.872582
6	-0.864873	0.601688	-4.462363
1	-0.572483	2.058060	-2.818987
1	-0.775234	-1.410049	-5.190907
1	-1.220698	1.105261	-5.347797
26	0.541388	0.046168	-0.323976

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**<sup>1</sup>ICSS<sup>†</sup>TS(C-P)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2836.5129554  
Zero-point correction=                    0.878137 (Hartree/Particle)  
Thermal correction to Energy=            0.937272  
Thermal correction to Enthalpy=         0.938216  
Thermal correction to Gibbs Free Energy= 0.781514  
Sum of electronic and zero-point Energies= -2835.634818  
Sum of electronic and thermal Energies= -2835.575684  
Sum of electronic and thermal Enthalpies= -2835.574740  
Sum of electronic and thermal Free Energies= -2835.731442

.....  
Cartesian Coordinates

.....  

6	3.499470	-3.311954	-0.973347
6	2.213434	-2.758579	-0.605657
7	2.227494	-1.385863	-0.689714
6	3.483671	-1.048276	-1.117369
6	4.301859	-2.241519	-1.304881
6	1.112719	-3.524930	-0.245498
6	-0.142148	-3.037562	0.097778
7	-0.489211	-1.713973	0.152508
6	-1.812765	-1.682176	0.505925

6	-2.321792	-3.032604	0.694737
6	-1.273886	-3.878665	0.437794
6	-2.579381	-0.525063	0.597171
6	-2.151319	0.763594	0.290977
7	-0.872376	1.109763	-0.060972
6	-0.892580	2.457300	-0.305200
6	-2.225638	2.991286	-0.112193
6	-3.014920	1.933716	0.257388
6	0.200250	3.232914	-0.675686
6	1.490246	2.768174	-0.884612
7	1.855896	1.449403	-0.839961
6	3.165333	1.404784	-1.240514
6	3.660331	2.735065	-1.534168
6	2.622732	3.600287	-1.283599
6	3.922492	0.245882	-1.375954
1	0.029004	4.291680	-0.824362
1	4.938460	0.364623	-1.734763
1	1.238219	-4.601993	-0.246099
1	-3.616027	-0.642792	0.890173
6	-4.503078	1.946356	0.457918
1	-4.822000	1.131650	1.116958
1	-4.811141	2.878995	0.945137
6	-5.252235	1.830079	-0.903660
1	-5.002224	0.877719	-1.382165
1	-4.940441	2.648411	-1.556950
6	-6.743444	1.942654	-0.720980
8	-7.413509	2.945021	-0.781257
8	-7.313605	0.729431	-0.412484
1	-8.264479	0.892882	-0.263127
6	-3.728883	-3.426697	1.043494
1	-4.182874	-2.714038	1.740652
1	-3.706536	-4.387541	1.569286
6	-4.670256	-3.597945	-0.188253
1	-4.142698	-4.103969	-0.999918
1	-5.531516	-4.206091	0.110209
6	-5.196583	-2.277670	-0.705304
8	-4.832460	-1.707962	-1.718188
8	-6.128979	-1.778047	0.130082
1	-6.456611	-0.917437	-0.214846
6	-1.250272	-5.378685	0.465259
1	-2.179957	-5.788562	0.871977
1	-1.118779	-5.804141	-0.538737
1	-0.427473	-5.759666	1.083118
6	-2.615001	4.427353	-0.301876
1	-2.499662	4.748414	-1.345444
1	-3.657769	4.601723	-0.019027
1	-1.993077	5.094550	0.307939
6	3.859054	-4.766487	-0.943842
1	3.316142	-5.300425	-0.156706
1	3.632180	-5.270603	-1.893894

1	4.930664	-4.895079	-0.758859
6	5.059703	3.060651	-1.960972
1	5.783761	2.835785	-1.166595
1	5.361213	2.484568	-2.845097
1	5.165446	4.121935	-2.203792
6	5.698709	-2.223089	-1.726457
6	6.354957	-3.185119	-2.395192
1	6.259041	-1.325434	-1.464972
1	7.407134	-3.072771	-2.640817
1	5.871275	-4.094334	-2.737834
6	2.660696	5.058435	-1.393233
6	2.059878	5.938354	-0.577862
1	3.273170	5.453008	-2.205016
1	2.157709	7.007822	-0.743062
1	1.488171	5.625241	0.290760
6	1.234999	0.130780	1.640945
6	1.289575	1.500408	2.254008
6	0.670252	-0.884820	2.587449
6	0.157692	2.179377	2.735497
6	2.528385	2.163050	2.394839
8	-0.359716	-0.761302	3.225463
8	1.463768	-1.986980	2.682532
6	0.250313	3.457936	3.286684
1	-0.801523	1.680838	2.678645
6	2.634607	3.444950	2.928986
8	3.704338	1.563849	1.965819
6	1.486814	4.101494	3.371129
1	-0.647532	3.948756	3.652996
1	3.617528	3.899928	3.002268
6	3.735693	0.198441	2.107153
1	1.564522	5.098159	3.797517
1	3.644119	-0.174128	3.130244
1	4.497807	-0.254474	1.480717
1	2.431496	-0.166923	1.543174
7	0.046383	-0.353177	-2.347787
6	-1.145976	-0.757464	-2.749630
6	0.775126	-0.093613	-3.489978
7	-1.213191	-0.767294	-4.105636
1	-1.973801	-1.040493	-2.117121
6	0.008364	-0.346224	-4.596079
1	1.795210	0.252647	-3.433167
1	-2.022082	-1.033987	-4.647464
1	0.211308	-0.269726	-5.652961
6	0.991498	-3.048802	3.537081
1	-0.094507	-3.122615	3.443046
1	1.452122	-3.952037	3.127562
6	1.403082	-2.824151	4.985836
1	0.924568	-1.924679	5.382996
1	1.096836	-3.678883	5.601023
1	2.489922	-2.714101	5.069790

26 0.707744 -0.118995 -0.259019

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1OSSA<sub>Fe(his)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2184.5545156  
Zero-point correction=                    0.670254 (Hartree/Particle)  
Thermal correction to Energy=            0.716454  
Thermal correction to Enthalpy=         0.717398  
Thermal correction to Gibbs Free Energy= 0.585380  
Sum of electronic and zero-point Energies= -2183.884261  
Sum of electronic and thermal Energies= -2183.838062  
Sum of electronic and thermal Enthalpies= -2183.837117  
Sum of electronic and thermal Free Energies= -2183.969135

.....  
Cartesian Coordinates

.....  
6    -1.672326 -3.421637 -0.645799  
6    -0.366107 -2.784963 -0.602863  
7    -0.489279 -1.427074 -0.430552  
6    -1.836367 -1.181733 -0.369314  
6    -2.593604 -2.419283 -0.500267  
6    0.839810 -3.463375 -0.725421  
6    2.107013 -2.883461 -0.726233  
7    2.358678 -1.542599 -0.560051  
6    3.720970 -1.402347 -0.635110  
6    4.355357 -2.694391 -0.885062  
6    3.337410 -3.621035 -0.911466  
6    4.405018 -0.208769 -0.435121  
6    3.834832 1.046244 -0.246603  
7    2.484239 1.299228 -0.205838  
6    2.362242 2.655057 -0.062770  
6    3.673788 3.289734 0.003954  
6    4.596578 2.272604 -0.112907  
6    1.150794 3.335756 0.027678  
6    -0.112167 2.759721 -0.028189  
7    -0.359270 1.412879 -0.136573  
6    -1.724310 1.285201 -0.142957  
6    -2.365563 2.589108 -0.041804  
6    -1.355835 3.510581 0.031442  
6    -1.454203 5.003548 0.136954  
6    -3.848219 2.832453 -0.062058  
6    -4.430720 2.842453 -1.486270  
6    -5.928196 3.059422 -1.502779  
8    -6.641934 3.186769 -0.531512  
6    -2.409726 0.078223 -0.230070  
6    6.090399 2.378883 -0.163356  
6    3.887136 4.728216 0.122860  
6    4.935850 5.346742 0.689351  
6    3.431165 -5.097669 -1.156062  
6    5.776490 -2.975842 -1.082954

6	6.680468	-2.207623	-1.710304
6	-4.091520	-2.531232	-0.454029
6	-4.644352	-2.530213	0.981974
6	-6.153487	-2.632687	1.028639
8	-6.894020	-2.711197	0.072940
6	-1.905791	-4.891865	-0.830784
8	-6.411875	3.097013	-2.769983
8	-6.613067	-2.628674	2.306099
1	1.193411	4.412698	0.147623
1	-3.493491	0.125909	-0.209063
1	0.790504	-4.539432	-0.857698
1	5.486062	-0.265332	-0.432446
1	6.529037	1.612598	-0.811279
1	6.395387	3.358568	-0.545933
1	6.548196	2.261802	0.829028
1	4.470585	-5.438450	-1.155163
1	2.892453	-5.672191	-0.391737
1	3.001196	-5.375407	-2.127814
1	-1.422050	-5.266713	-1.741767
1	-1.506470	-5.479073	0.007275
1	-2.972918	-5.120566	-0.909591
1	-2.491821	5.327777	0.262186
1	-0.885036	5.388714	0.992675
1	-1.060705	5.502016	-0.758969
1	3.102560	5.357323	-0.297962
1	5.001622	6.430987	0.703066
1	5.743525	4.805446	1.171978
1	6.115521	-3.940210	-0.702171
1	7.714500	-2.527481	-1.803120
1	6.419366	-1.261172	-2.173880
1	-4.374912	2.073672	0.527970
1	-4.081907	3.788203	0.418834
1	-3.962606	3.624667	-2.096870
1	-4.215983	1.900807	-2.007182
1	-7.375236	3.229846	-2.686070
1	-4.419631	-3.448074	-0.954705
1	-4.559266	-1.711885	-1.011866
1	-4.227291	-3.363096	1.562416
1	-4.345766	-1.621994	1.520345
1	-7.585099	-2.690222	2.241299
7	1.073237	-0.317081	1.879402
6	1.090648	-1.471989	2.518644
6	1.116057	0.670036	2.841788
7	1.142620	-1.268666	3.860220
1	1.067520	-2.445395	2.052481
6	1.159879	0.096065	4.083719
1	1.113260	1.713801	2.568151
1	1.167661	-1.989847	4.565761
1	1.200636	0.516330	5.076431
26	1.003321	-0.080089	-0.182213



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**1OSSB<sub>Fe(his)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0722852  
Zero-point correction=                    0.892586 (Hartree/Particle)  
Thermal correction to Energy=            0.955826  
Thermal correction to Enthalpy=           0.956770  
Thermal correction to Gibbs Free Energy=   0.785090  
Sum of electronic and zero-point Energies=   -2945.179699  
Sum of electronic and thermal Energies=   -2945.116460  
Sum of electronic and thermal Enthalpies=   -2945.115515  
Sum of electronic and thermal Free Energies=   -2945.287195

.....  
Cartesian Coordinates  
.....

6	3.045589	2.004454	2.230148
6	2.440090	0.771386	1.769242
7	1.160419	0.990495	1.321529
6	0.927797	2.332437	1.489699
6	2.111685	2.994532	2.032329
6	3.090735	-0.457821	1.767100
6	2.603900	-1.646915	1.234882
7	1.367504	-1.798086	0.668026
6	1.312046	-3.099084	0.227456
6	2.543984	-3.801260	0.523846
6	3.355793	-2.897555	1.176137
6	0.212907	-3.673666	-0.407302
6	-0.991652	-3.039951	-0.685637
7	-1.285211	-1.736064	-0.366744
6	-2.573237	-1.530969	-0.791659
6	-3.117160	-2.741277	-1.394825
6	-2.125401	-3.682584	-1.333268
7	-1.507298	1.027650	0.340387
6	-2.772394	0.858376	-0.162536
6	-3.518162	2.106475	-0.102059
6	-2.677344	3.034979	0.456464
6	-1.426081	2.345434	0.718852
6	-3.269885	-0.331575	-0.684825
6	-0.295232	2.953128	1.256126
8	5.735965	-0.752116	-1.377729
6	5.230492	0.504112	-1.263244
8	5.713637	1.363572	-0.544021
6	4.051899	0.687882	-2.117095
7	3.708767	-0.370566	-2.828269
7	3.433230	-1.288453	-3.437144
6	3.302285	1.953367	-2.267841
6	3.954305	3.184151	-2.104545
6	3.271931	4.391312	-2.254638
6	1.919658	4.385121	-2.587592
6	1.243920	3.174363	-2.754590

6	1.920606	1.962800	-2.586282
8	1.325641	0.741205	-2.711951
6	-0.041412	0.676215	-3.103824
1	-0.368368	4.003381	1.511539
1	-4.288104	-0.321953	-1.054574
1	0.299966	-4.712985	-0.704923
1	4.088595	-0.473231	2.189687
1	5.004209	3.184283	-1.841161
1	3.802633	5.328850	-2.117781
1	0.188559	3.177374	-2.999824
1	1.379638	5.319098	-2.719569
1	-0.283283	-0.386055	-3.152223
1	-0.690755	1.156133	-2.363872
1	-0.190368	1.137087	-4.089258
6	6.933297	-1.041676	-0.624595
1	6.883311	-2.117474	-0.441111
1	6.888904	-0.509791	0.328920
6	8.182019	-0.659172	-1.406211
1	8.219579	0.422655	-1.564526
1	9.077666	-0.956198	-0.847947
1	8.201142	-1.160346	-2.379601
6	4.457794	2.143608	2.711501
1	4.641203	3.137584	3.130493
1	4.699210	1.405625	3.487001
1	5.162534	1.998683	1.882682
6	2.853975	-5.215079	0.135575
1	3.922744	-5.332909	-0.073619
1	2.600066	-5.931549	0.929888
1	2.304266	-5.517861	-0.761514
6	2.295401	4.419103	2.304723
6	1.817500	5.449885	1.590723
1	2.921436	4.649897	3.167750
1	2.024624	6.475033	1.885252
1	1.248067	5.307760	0.677388
6	4.708115	-3.066039	1.692297
6	5.309628	-4.211066	2.058200
1	5.285980	-2.149107	1.799548
1	6.332749	-4.206799	2.423472
1	4.809197	-5.173338	2.034954
6	-2.936084	4.484547	0.743659
1	-3.918793	4.798538	0.378087
1	-2.905231	4.698882	1.820277
1	-2.186544	5.131468	0.270575
6	-4.932552	2.302243	-0.572515
1	-5.103291	3.358557	-0.809336
1	-5.109631	1.739908	-1.496396
6	-4.518721	-2.872561	-1.925516
1	-4.575341	-3.717571	-2.619748
1	-4.773101	-1.983236	-2.509580
6	-5.586012	-3.069300	-0.805975

1	-5.134899	-2.821834	0.164338
1	-5.916315	-4.108767	-0.739954
6	-5.990034	1.855242	0.479835
1	-5.865819	0.790927	0.690263
1	-5.849799	2.422814	1.403748
6	-6.831570	-2.203773	-0.899416
8	-7.949185	-2.564328	-0.601286
8	-6.536839	-0.941071	-1.283593
1	-7.320170	-0.350220	-1.167301
6	-7.389860	2.075697	-0.038861
8	-8.042012	1.293886	-0.713397
8	-7.873812	3.293544	0.277318
1	-8.757884	3.356888	-0.133742
6	-2.147152	-5.103139	-1.814316
1	-2.028115	-5.815822	-0.987279
1	-3.090675	-5.340754	-2.315024
1	-1.336915	-5.302646	-2.527324
7	-0.826939	-0.930204	2.501772
6	-1.065284	-0.084719	3.487144
6	-1.119802	-2.190135	2.980126
7	-1.503699	-0.751372	4.585900
1	-0.932878	0.985560	3.438578
6	-1.543523	-2.099271	4.278655
1	-1.001036	-3.062265	2.355881
1	-1.747844	-0.332802	5.471206
1	-1.859283	-2.843470	4.993019
26	-0.113045	-0.416651	0.622631

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**10SSC<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0635899  
Zero-point correction=                    0.888944 (Hartree/Particle)  
Thermal correction to Energy=            0.953584  
Thermal correction to Enthalpy=         0.954529  
Thermal correction to Gibbs Free Energy= 0.781092  
Sum of electronic and zero-point Energies= -2945.174646  
Sum of electronic and thermal Energies= -2945.110005  
Sum of electronic and thermal Enthalpies= -2945.109061  
Sum of electronic and thermal Free Energies= -2945.282498

.....  
Cartesian Coordinates

.....

6	3.253985	-3.110596	-1.292685
6	2.008538	-2.561472	-0.798280
7	1.991105	-1.195150	-0.935940
6	3.177506	-0.853194	-1.523433
6	3.981800	-2.043774	-1.778531
6	0.937957	-3.335583	-0.353495
6	-0.333411	-2.859004	-0.056976
7	-0.688996	-1.535972	-0.054527

6	-2.037948	-1.504133	0.174959
6	-2.561432	-2.855849	0.325519
6	-1.492197	-3.702478	0.197425
6	-2.800935	-0.347427	0.290611
6	-2.319273	0.954896	0.220486
7	-1.025215	1.305943	-0.051043
6	-0.977672	2.675185	-0.005041
6	-2.288583	3.217177	0.312986
6	-3.128165	2.143157	0.449437
6	0.143414	3.453496	-0.273860
6	1.382979	2.974114	-0.688558
7	1.678183	1.651661	-0.862961
6	2.900259	1.607458	-1.478856
6	3.413661	2.945584	-1.694785
6	2.488082	3.809378	-1.156579
6	3.579374	0.443836	-1.822950
1	0.021533	4.528661	-0.229002
1	4.528110	0.565526	-2.333614
1	1.085687	-4.409437	-0.316159
1	-3.857830	-0.471480	0.491999
6	0.953561	0.194636	1.440948
6	1.818318	1.189797	2.117852
6	1.216515	2.198808	2.892347
6	3.233011	1.168354	2.041989
6	1.970328	3.198579	3.507782
1	0.136153	2.194272	2.986136
6	3.989080	2.168230	2.664628
6	3.357432	3.185256	3.384085
1	1.473364	3.974975	4.082802
1	5.070887	2.154588	2.602993
1	3.961150	3.954636	3.858395
6	0.095647	-0.518969	2.438522
8	-0.930707	-0.063777	2.910289
8	0.618467	-1.706439	2.811158
8	3.784565	0.107709	1.388512
6	5.195031	0.041055	1.279578
1	5.405622	-0.867609	0.714246
1	5.597960	0.906613	0.736961
1	5.672350	-0.023536	2.266270
7	3.842065	-3.569283	2.294140
7	4.147375	-2.734698	2.950929
6	-4.591508	2.153652	0.792423
1	-4.817723	1.344987	1.497829
1	-4.849961	3.089052	1.298993
6	-5.520432	2.010163	-0.444147
1	-5.364040	1.049087	-0.936730
1	-5.288393	2.808341	-1.158000
6	-6.968968	2.177560	-0.045214
8	-7.462780	3.177899	0.420027
8	-7.719767	1.044955	-0.240937

1	-8.623617	1.267732	0.055962
6	-4.015107	-3.182662	0.526211
1	-4.446162	-2.490455	1.255527
1	-4.120722	-4.183930	0.957199
6	-4.840953	-3.113675	-0.795079
1	-4.280830	-2.521649	-1.530598
1	-4.993048	-4.104815	-1.228615
6	-6.197957	-2.445757	-0.688789
8	-7.226253	-2.844711	-1.189012
8	-6.117911	-1.275934	-0.007287
1	-6.965837	-0.791100	-0.090352
6	-1.468629	-5.201263	0.260243
1	-2.446765	-5.604371	0.540496
1	-1.196282	-5.647808	-0.705574
1	-0.740077	-5.565689	0.995751
6	-2.600183	4.677906	0.450575
1	-2.477364	5.211640	-0.501255
1	-3.629773	4.839051	0.783854
1	-1.938090	5.165419	1.177025
6	3.641274	-4.557692	-1.243787
1	3.212633	-5.058061	-0.369519
1	3.308762	-5.110373	-2.134304
1	4.729765	-4.663778	-1.188706
6	4.733239	3.274181	-2.326703
1	5.576252	2.941240	-1.705933
1	4.845780	2.791706	-3.305843
1	4.848742	4.352142	-2.472674
6	5.304788	-2.026836	-2.393610
6	5.894999	-3.018368	-3.081414
1	5.865723	-1.099326	-2.279746
1	6.897585	-2.896557	-3.481456
1	5.402436	-3.963033	-3.288174
6	2.598600	5.264878	-1.080948
6	2.166036	6.049754	-0.082106
1	3.119953	5.741606	-1.912106
1	2.304371	7.126783	-0.118118
1	1.696248	5.644453	0.809242
6	-0.155047	-2.449198	3.781901
1	-0.330340	-1.815651	4.657005
1	-1.127957	-2.688716	3.341228
6	0.627538	-3.700401	4.134807
1	1.594313	-3.445823	4.580394
1	0.062421	-4.300650	4.856958
1	0.809814	-4.309706	3.243640
7	-0.131273	0.028401	-2.467092
6	-0.240739	-1.050535	-3.216975
6	-0.490412	1.094700	-3.263837
7	-0.657554	-0.724731	-4.469106
1	-0.029329	-2.059543	-2.897046
6	-0.821807	0.647633	-4.515096

1	-0.484075	2.102688	-2.878969
1	-0.811144	-1.371373	-5.228569
1	-1.147902	1.159055	-5.407430
26	0.531360	0.060234	-0.352565

-----  
<sup>10</sup>SS<sup>TS(C-D)</sup>Fe(his)  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2836.5129554  
 Zero-point correction=                    0.878137 (Hartree/Particle)  
 Thermal correction to Energy=            0.937272  
 Thermal correction to Enthalpy=         0.938216  
 Thermal correction to Gibbs Free Energy= 0.781514  
 Sum of electronic and zero-point Energies= -2835.634818  
 Sum of electronic and thermal Energies= -2835.575684  
 Sum of electronic and thermal Enthalpies= -2835.574740  
 Sum of electronic and thermal Free Energies= -2835.731442

.....  
 Cartesian Coordinates  
 .....

6	3.499470	-3.311954	-0.973347
6	2.213434	-2.758579	-0.605657
7	2.227494	-1.385863	-0.689714
6	3.483671	-1.048276	-1.117369
6	4.301859	-2.241519	-1.304881
6	1.112719	-3.524930	-0.245498
6	-0.142148	-3.037562	0.097778
7	-0.489211	-1.713973	0.152508
6	-1.812765	-1.682176	0.505925
6	-2.321792	-3.032604	0.694737
6	-1.273886	-3.878665	0.437794
6	-2.579381	-0.525063	0.597171
6	-2.151319	0.763594	0.290977
7	-0.872376	1.109763	-0.060972
6	-0.892580	2.457300	-0.305200
6	-2.225638	2.991286	-0.112193
6	-3.014920	1.933716	0.257388
6	0.200250	3.232914	-0.675686
6	1.490246	2.768174	-0.884612
7	1.855896	1.449403	-0.839961
6	3.165333	1.404784	-1.240514
6	3.660331	2.735065	-1.534168
6	2.622732	3.600287	-1.283599
6	3.922492	0.245882	-1.375954
1	0.029004	4.291680	-0.824362
1	4.938460	0.364623	-1.734763
1	1.238219	-4.601993	-0.246099
1	-3.616027	-0.642792	0.890173
6	-4.503078	1.946356	0.457918
1	-4.822000	1.131650	1.116958
1	-4.811141	2.878995	0.945137

6	-5.252235	1.830079	-0.903660
1	-5.002224	0.877719	-1.382165
1	-4.940441	2.648411	-1.556950
6	-6.743444	1.942654	-0.720980
8	-7.413509	2.945021	-0.781257
8	-7.313605	0.729431	-0.412484
1	-8.264479	0.892882	-0.263127
6	-3.728883	-3.426697	1.043494
1	-4.182874	-2.714038	1.740652
1	-3.706536	-4.387541	1.569286
6	-4.670256	-3.597945	-0.188253
1	-4.142698	-4.103969	-0.999918
1	-5.531516	-4.206091	0.110209
6	-5.196583	-2.277670	-0.705304
8	-4.832460	-1.707962	-1.718188
8	-6.128979	-1.778047	0.130082
1	-6.456611	-0.917437	-0.214846
6	-1.250272	-5.378685	0.465259
1	-2.179957	-5.788562	0.871977
1	-1.118779	-5.804141	-0.538737
1	-0.427473	-5.759666	1.083118
6	-2.615001	4.427353	-0.301876
1	-2.499662	4.748414	-1.345444
1	-3.657769	4.601723	-0.019027
1	-1.993077	5.094550	0.307939
6	3.859054	-4.766487	-0.943842
1	3.316142	-5.300425	-0.156706
1	3.632180	-5.270603	-1.893894
1	4.930664	-4.895079	-0.758859
6	5.059703	3.060651	-1.960972
1	5.783761	2.835785	-1.166595
1	5.361213	2.484568	-2.845097
1	5.165446	4.121935	-2.203792
6	5.698709	-2.223089	-1.726457
6	6.354957	-3.185119	-2.395192
1	6.259041	-1.325434	-1.464972
1	7.407134	-3.072771	-2.640817
1	5.871275	-4.094334	-2.737834
6	2.660696	5.058435	-1.393233
6	2.059878	5.938354	-0.577862
1	3.273170	5.453008	-2.205016
1	2.157709	7.007822	-0.743062
1	1.488171	5.625241	0.290760
6	1.234999	0.130780	1.640945
6	1.289575	1.500408	2.254008
6	0.670252	-0.884820	2.587449
6	0.157692	2.179377	2.735497
6	2.528385	2.163050	2.394839
8	-0.359716	-0.761302	3.225463
8	1.463768	-1.986980	2.682532

6	0.250313	3.457936	3.286684
1	-0.801523	1.680838	2.678645
6	2.634607	3.444950	2.928986
8	3.704338	1.563849	1.965819
6	1.486814	4.101494	3.371129
1	-0.647532	3.948756	3.652996
1	3.617528	3.899928	3.002268
6	3.735693	0.198441	2.107153
1	1.564522	5.098159	3.797517
1	3.644119	-0.174128	3.130244
1	4.497807	-0.254474	1.480717
1	2.431496	-0.166923	1.543174
7	0.046383	-0.353177	-2.347787
6	-1.145976	-0.757464	-2.749630
6	0.775126	-0.093613	-3.489978
7	-1.213191	-0.767294	-4.105636
1	-1.973801	-1.040493	-2.117121
6	0.008364	-0.346224	-4.596079
1	1.795210	0.252647	-3.433167
1	-2.022082	-1.033987	-4.647464
1	0.211308	-0.269726	-5.652961
6	0.991498	-3.048802	3.537081
1	-0.094507	-3.122615	3.443046
1	1.452122	-3.952037	3.127562
6	1.403082	-2.824151	4.985836
1	0.924568	-1.924679	5.382996
1	1.096836	-3.678883	5.601023
1	2.489922	-2.714101	5.069790
26	0.707744	-0.118995	-0.259019

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**IOSSD<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2836.531508  
Zero-point correction=                    0.881503 (Hartree/Particle)  
Thermal correction to Energy=            0.941880  
Thermal correction to Enthalpy=         0.942824  
Thermal correction to Gibbs Free Energy= 0.782612  
Sum of electronic and zero-point Energies= -2835.650005  
Sum of electronic and thermal Energies= -2835.589628  
Sum of electronic and thermal Enthalpies= -2835.588684  
Sum of electronic and thermal Free Energies= -2835.748896

.....  
Cartesian Coordinates

.....  

6	3.410286	-3.461844	-0.871298
6	2.127400	-2.871265	-0.553583
7	2.177513	-1.503135	-0.653816
6	3.454108	-1.200503	-1.040418
6	4.250046	-2.414609	-1.181117
6	0.998116	-3.600846	-0.205859



6	-0.238381	-3.067410	0.129371
7	-0.547049	-1.730588	0.164384
6	-1.863496	-1.654658	0.539461
6	-2.406381	-2.985566	0.759004
6	-1.388911	-3.866956	0.497723
6	-2.599201	-0.477865	0.622341
6	-2.141769	0.791879	0.283638
7	-0.860092	1.093656	-0.095568
6	-0.849909	2.436565	-0.373699
6	-2.163542	3.010325	-0.172081
6	-2.973755	1.983156	0.236267
6	0.254280	3.170602	-0.785751
6	1.529030	2.663014	-0.989886
7	1.861299	1.336955	-0.901698
6	3.179958	1.249477	-1.267366
6	3.707076	2.556546	-1.599317
6	2.683753	3.453000	-1.400215
6	3.922676	0.075945	-1.327366
1	0.110828	4.228877	-0.963044
1	4.952348	0.164907	-1.653746
1	1.089386	-4.681019	-0.189861
1	-3.633293	-0.563542	0.934097
6	-4.457019	2.041303	0.463323
1	-4.786067	1.247797	1.142796
1	-4.729198	2.990840	0.939067
6	-5.233852	1.922096	-0.882233
1	-5.020011	0.954352	-1.347257
1	-4.911299	2.719036	-1.556389
6	-6.717833	2.080519	-0.675158
8	-7.360848	3.099620	-0.746778
8	-7.315009	0.890898	-0.328691
1	-8.258241	1.083608	-0.166232
6	-3.816934	-3.332775	1.141917
1	-4.236888	-2.593795	1.832731
1	-3.810559	-4.282808	1.687150
6	-4.785342	-3.502025	-0.068776
1	-4.287262	-4.037914	-0.879910
1	-5.656771	-4.080535	0.257571
6	-5.285363	-2.177853	-0.602090
8	-4.924394	-1.637804	-1.632106
8	-6.188375	-1.637392	0.240052
1	-6.499829	-0.775156	-0.115618
6	-1.408252	-5.366213	0.553579
1	-2.350784	-5.741334	0.963828
1	-1.284969	-5.813843	-0.441638
1	-0.599284	-5.757908	1.182761
6	-2.516624	4.452136	-0.386786
1	-2.401153	4.750201	-1.437082
1	-3.552120	4.659140	-0.099522
1	-1.872534	5.113057	0.206506

6	3.731481	-4.924315	-0.811687
1	3.153877	-5.432428	-0.032167
1	3.517946	-5.436724	-1.760375
1	4.793828	-5.076597	-0.594593
6	5.122805	2.845140	-1.997428
1	5.806135	2.738846	-1.144088
1	5.474157	2.165260	-2.782983
1	5.230791	3.868074	-2.370101
6	5.662719	-2.433281	-1.546525
6	6.315864	-3.412566	-2.192285
1	6.236338	-1.552814	-1.257332
1	7.379869	-3.331812	-2.395778
1	5.818646	-4.306209	-2.556179
6	2.758192	4.905254	-1.562275
6	2.179550	5.829691	-0.781171
1	3.381982	5.253683	-2.386603
1	2.304941	6.889364	-0.985986
1	1.599997	5.563983	0.097987
6	1.377035	0.104480	1.700918
6	1.296461	1.496307	2.232286
6	0.765186	-0.925666	2.589756
6	0.120444	2.054883	2.762895
6	2.454235	2.308212	2.275219
8	-0.271987	-0.835977	3.224646
8	1.555854	-2.037829	2.649088
6	0.085091	3.350392	3.278577
1	-0.770159	1.440714	2.781064
6	2.427270	3.614984	2.768013
8	3.624609	1.748264	1.798993
6	1.235819	4.139157	3.270351
1	-0.844901	3.742556	3.681889
1	3.330133	4.215684	2.737665
6	4.826552	2.218371	2.229689
1	1.215262	5.155359	3.656027
1	5.655113	1.680953	1.783879
1	4.888560	2.580264	3.253676
1	2.405369	-0.172075	1.490098
7	0.012221	-0.469588	-2.413731
6	-1.197670	-0.831589	-2.801441
6	0.751524	-0.283531	-3.562704
7	-1.266413	-0.885503	-4.156843
1	-2.036030	-1.056175	-2.158609
6	-0.027003	-0.538567	-4.660382
1	1.786789	0.017559	-3.516259
1	-2.086275	-1.133726	-4.691076
1	0.177863	-0.507835	-5.719261
6	1.080888	-3.119714	3.470726
1	-0.006415	-3.186505	3.381572
1	1.535197	-4.014568	3.035400
6	1.499139	-2.940096	4.924431

1	1.024625	-2.051016	5.348863
1	1.193482	-3.811762	5.516100
1	2.586268	-2.832987	5.005312
26	0.675719	-0.184084	-0.289946

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**1CSS<sub>E</sub>Fe**

---

Number of imaginary frequencies: 0    Electronic energy:    HF=-651.9553325  
Zero-point correction=                    0.207676 (Hartree/Particle)  
Thermal correction to Energy=            0.221445  
Thermal correction to Enthalpy=         0.222389  
Thermal correction to Gibbs Free Energy= 0.166289  
Sum of electronic and zero-point Energies= -651.747657  
Sum of electronic and thermal Energies= -651.733888  
Sum of electronic and thermal Enthalpies= -651.732943  
Sum of electronic and thermal Free Energies= -651.789043

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Cartesian Coordinates

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6	-3.528469	-1.325185	0.000119
6	-2.387087	-2.183676	0.000062
6	-1.117480	-1.680153	-0.000027
6	-0.859341	-0.253335	-0.000055
6	-2.050342	0.574638	-0.000006
6	-3.357671	0.036552	0.000088
6	0.415431	0.293045	-0.000082
8	-1.833043	1.903262	-0.000026
6	-2.669390	2.901262	-0.000071
6	1.659966	-0.455194	-0.000087
8	2.722865	0.408345	0.000062
8	1.820905	-1.671314	-0.000194
1	-0.252739	-2.331048	-0.000084
1	-2.536151	-3.260094	0.000090
1	-4.221318	0.693095	0.000117
1	-4.528337	-1.748525	0.000179
1	-3.739762	2.743925	-0.000005
1	0.526567	1.370425	-0.000054
1	-2.205518	3.876203	-0.000082
6	4.021362	-0.205723	0.000050
6	5.053516	0.908655	0.000117
1	4.117227	-0.849372	-0.881659
1	4.117205	-0.849459	0.881698
1	6.063883	0.484435	0.000122
1	4.945098	1.541413	-0.887068
1	4.945060	1.541338	0.887352

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**1CSS<sub>TS</sub>(E-P)**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-651.9391778  
 Zero-point correction=                    0.207457 (Hartree/Particle)  
 Thermal correction to Energy=            0.220196  
 Thermal correction to Enthalpy=         0.221140  
 Thermal correction to Gibbs Free Energy= 0.167651  
 Sum of electronic and zero-point Energies= -651.731721  
 Sum of electronic and thermal Energies= -651.718982  
 Sum of electronic and thermal Enthalpies= -651.718037  
 Sum of electronic and thermal Free Energies= -651.771526

.....  
 Cartesian Coordinates

.....

6	0.331932	0.402218	-0.422274
6	-0.930294	-0.230365	-0.292904
6	1.600963	-0.283052	-0.297738
6	-1.174110	-1.620969	-0.090404
6	-2.088495	0.589893	-0.236565
8	1.788626	-1.468523	-0.039416
8	2.636270	0.592627	-0.507543
6	-2.449782	-2.085435	0.190801
1	-0.332291	-2.297850	-0.157569
6	-3.352733	0.154488	0.120688
8	-1.841089	1.963649	-0.445509
6	-3.547555	-1.215355	0.305601
1	-2.602541	-3.153110	0.325736
1	-4.171304	0.865501	0.186763
6	-1.573836	2.628344	0.649540
1	-4.541713	-1.599956	0.509751
1	-1.595259	2.121709	1.607903
1	-1.505285	3.704826	0.541555
1	0.384563	1.442116	-0.707273
6	3.962257	0.044677	-0.408140
1	3.967775	-0.961616	-0.835608
1	4.579651	0.703174	-1.026189
6	4.454748	0.021362	1.033777
1	3.842025	-0.657170	1.633808
1	5.493853	-0.327259	1.070899
1	4.411503	1.022774	1.475689

-----  
**P**

Number of imaginary frequencies: 0    Electronic energy:    HF=-652.0616192  
 Zero-point correction=                    0.212779 (Hartree/Particle)  
 Thermal correction to Energy=            0.225119  
 Thermal correction to Enthalpy=         0.226063  
 Thermal correction to Gibbs Free Energy= 0.172469  
 Sum of electronic and zero-point Energies= -651.848841  
 Sum of electronic and thermal Energies= -651.836500  
 Sum of electronic and thermal Enthalpies= -651.835556

Sum of electronic and thermal Free Energies= -651.889150

.....  
Cartesian Coordinates

.....  
6 -0.209046 0.398183 0.615283  
6 1.135619 -0.216018 0.277875  
6 1.590284 -1.529259 0.264452  
6 2.015515 0.834789 0.005646  
6 2.938650 -1.769338 -0.033218  
1 0.905900 -2.346468 0.464826  
6 3.357965 0.620081 -0.285049  
6 3.806950 -0.705762 -0.298654  
1 3.310714 -2.789473 -0.057016  
1 4.020330 1.453088 -0.496463  
1 4.850395 -0.907995 -0.525825  
6 -1.422796 -0.315479 0.039424  
8 -1.516291 -1.515785 -0.099548  
8 -2.410391 0.560504 -0.247461  
8 1.425709 2.068656 0.066943  
6 -0.002402 1.858454 0.131704  
1 -0.421663 2.002179 -0.870449  
1 -0.358908 0.383393 1.707255  
1 -0.423075 2.608987 0.802606  
6 -3.649774 0.003915 -0.756991  
1 -4.094441 0.821619 -1.329024  
1 -3.409984 -0.823021 -1.429455  
6 -4.559462 -0.448652 0.375036  
1 -5.515792 -0.793994 -0.034254  
1 -4.104563 -1.275777 0.927105  
1 -4.760138 0.374975 1.068175

-----  
<sup>3</sup>A<sub>Fe(his)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2184.5622635  
Zero-point correction=                    0.669628 (Hartree/Particle)  
Thermal correction to Energy=            0.716265  
Thermal correction to Enthalpy=         0.717209  
Thermal correction to Gibbs Free Energy= 0.581510  
Sum of electronic and zero-point Energies= -2183.892636  
Sum of electronic and thermal Energies= -2183.845999  
Sum of electronic and thermal Enthalpies= -2183.845054  
Sum of electronic and thermal Free Energies= -2183.980754

.....  
Cartesian Coordinates

.....  
6 -1.666460 -3.419655 -0.685534  
6 -0.362761 -2.780745 -0.650462  
7 -0.489212 -1.423129 -0.472202  
6 -1.836094 -1.180493 -0.402081  
6 -2.589423 -2.419589 -0.530109

6	0.842658	-3.456464	-0.782063
6	2.107392	-2.872922	-0.777673
7	2.356052	-1.532044	-0.605129
6	3.717818	-1.387174	-0.673991
6	4.355094	-2.676516	-0.924735
6	3.339444	-3.606084	-0.959328
6	4.399341	-0.193443	-0.467503
6	3.825620	1.059151	-0.274637
7	2.475036	1.311420	-0.239883
6	2.349948	2.666799	-0.089873
6	3.659077	3.301432	-0.011377
6	4.583838	2.285207	-0.128624
6	1.138149	3.345858	-0.000859
6	-0.121870	2.765571	-0.055289
7	-0.366224	1.417867	-0.169219
6	-1.730251	1.284884	-0.168517
6	-2.373821	2.585873	-0.055750
6	-1.366633	3.510901	0.016312
6	-1.469684	5.002708	0.133700
6	-3.857209	2.824946	-0.062591
6	-4.450016	2.844836	-1.482464
6	-5.947713	3.061235	-1.485884
8	-6.652901	3.187315	-0.508283
6	-2.413307	0.076898	-0.257479
6	6.077709	2.394128	-0.165221
6	3.870409	4.739321	0.118862
6	4.916195	5.354829	0.693809
6	3.438655	-5.082036	-1.206084
6	5.778286	-2.953725	-1.114690
6	6.680695	-2.183676	-1.741816
6	-4.086324	-2.536880	-0.469585
6	-4.624154	-2.545208	0.972094
6	-6.132522	-2.651710	1.032759
8	-6.882061	-2.723194	0.083503
6	-1.897801	-4.890321	-0.869994
8	-6.442043	3.100020	-2.748831
8	-6.579410	-2.660063	2.314489
1	1.178140	4.422091	0.124163
1	-3.496866	0.121154	-0.230554
1	0.795619	-4.531840	-0.918821
1	5.480290	-0.248402	-0.460227
1	6.524273	1.627398	-0.806959
1	6.384148	3.373748	-0.546794
1	6.525327	2.280360	0.832088
1	4.479486	-5.418387	-1.206233
1	2.902887	-5.659557	-0.442027
1	3.009357	-5.360120	-2.177978
1	-1.417169	-5.264064	-1.783013
1	-1.494286	-5.476694	-0.033458
1	-2.964826	-5.120707	-0.944696

1	-2.507557	5.321717	0.269453
1	-0.895597	5.383373	0.988036
1	-1.085300	5.509437	-0.761512
1	3.087000	5.370576	-0.300759
1	4.980453	6.439010	0.715510
1	5.722542	4.811290	1.176036
1	6.119575	-3.915049	-0.728478
1	7.716645	-2.498664	-1.829672
1	6.416225	-1.240413	-2.210020
1	-4.376874	2.059814	0.525314
1	-4.089868	3.776066	0.427723
1	-3.987178	3.632233	-2.090476
1	-4.238353	1.907451	-2.012129
1	-7.404639	3.233071	-2.656825
1	-4.415992	-3.452294	-0.971789
1	-4.562432	-1.716370	-1.018408
1	-4.199049	-3.379937	1.543881
1	-4.322353	-1.639090	1.512187
1	-7.551924	-2.723006	2.258951
7	1.091736	-0.343743	2.086029
6	1.116532	-1.501846	2.714073
6	1.146537	0.626088	3.063955
7	1.184690	-1.321497	4.061279
1	1.088340	-2.472417	2.240159
6	1.204978	0.040371	4.301233
1	1.141210	1.674940	2.806345
1	1.217857	-2.050853	4.758321
1	1.257536	0.447161	5.299362
26	0.997544	-0.069734	-0.246744

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**<sup>3</sup>B<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0801418  
Zero-point correction=                    0.892028 (Hartree/Particle)  
Thermal correction to Energy=            0.955730  
Thermal correction to Enthalpy=         0.956674  
Thermal correction to Gibbs Free Energy= 0.781132  
Sum of electronic and zero-point Energies= -2945.188114  
Sum of electronic and thermal Energies= -2945.124412  
Sum of electronic and thermal Enthalpies= -2945.123468  
Sum of electronic and thermal Free Energies= -2945.299010

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Cartesian Coordinates

.....

6	2.586313	2.422149	1.824005
6	2.027070	1.135769	1.470235
7	0.742567	1.271659	1.002808
6	0.464287	2.616086	1.047970
6	1.619731	3.361294	1.538690
6	2.723382	-0.062721	1.577069

6	2.271152	-1.313344	1.174051
7	1.036413	-1.567150	0.640440
6	1.020647	-2.911400	0.350022
6	2.275509	-3.535312	0.712684
6	3.061532	-2.536957	1.248116
6	-0.061880	-3.589054	-0.204893
6	-1.286229	-3.026196	-0.539433
7	-1.616769	-1.702412	-0.370267
6	-2.908162	-1.580944	-0.815009
6	-3.418609	-2.867112	-1.269940
6	-2.402216	-3.768899	-1.101687
7	-1.917032	1.118162	0.021730
6	-3.171524	0.857243	-0.465723
6	-3.954035	2.080797	-0.540118
6	-3.147164	3.088657	-0.077326
6	-1.878312	2.470771	0.261176
6	-3.635418	-0.396220	-0.851106
6	-0.775619	3.168569	0.742466
8	6.714793	-1.390726	-1.025400
6	6.160410	-0.179386	-0.761605
8	6.408142	0.479849	0.236216
6	5.236437	0.231429	-1.820453
7	5.026225	-0.647379	-2.780873
7	4.833879	-1.401925	-3.608078
6	4.576682	1.552463	-1.887764
6	5.278147	2.707552	-1.517112
6	4.675448	3.964177	-1.562786
6	3.357579	4.079636	-2.000418
6	2.637597	2.946033	-2.381934
6	3.234813	1.682533	-2.320053
8	2.603954	0.523432	-2.659049
6	1.225831	0.568720	-3.008870
1	-0.893086	4.233424	0.899694
1	-4.651336	-0.455606	-1.221876
1	0.056008	-4.652324	-0.382809
1	3.727060	-0.001710	1.980394
1	6.301380	2.606944	-1.173797
1	5.235967	4.844404	-1.262329
1	1.609719	3.048055	-2.709184
1	2.876272	5.052665	-2.038988
1	0.928837	-0.467446	-3.176337
1	0.622919	0.991582	-2.196804
1	1.067226	1.148550	-3.927834
6	7.681742	-1.888988	-0.075071
1	7.605313	-2.975889	-0.155195
1	7.385586	-1.580930	0.929770
6	9.081916	-1.395487	-0.409862
1	9.140503	-0.307854	-0.306427
1	9.810061	-1.845146	0.275407
1	9.357935	-1.668824	-1.433618



6	3.978932	2.636157	2.336594
1	4.198061	3.699409	2.468121
1	4.132052	2.140755	3.304770
1	4.724459	2.227521	1.643689
6	2.626566	-4.974948	0.488363
1	3.704662	-5.089625	0.334038
1	2.352944	-5.609372	1.343438
1	2.118066	-5.382169	-0.391973
6	1.759137	4.806859	1.702820
6	1.214818	5.779511	0.954319
1	2.415129	5.113660	2.518085
1	1.402243	6.825414	1.180560
1	0.597180	5.572966	0.085799
6	4.421745	-2.601143	1.770259
6	5.029007	-3.668935	2.314326
1	4.990502	-1.673668	1.717691
1	6.054121	-3.603624	2.668277
1	4.529425	-4.622331	2.452935
6	-3.454194	4.550970	0.056866
1	-4.446712	4.791263	-0.336771
1	-3.431350	4.877881	1.104919
1	-2.727378	5.169784	-0.484592
6	-5.370397	2.182920	-1.033574
1	-5.566433	3.199649	-1.392512
1	-5.527152	1.512528	-1.886015
6	-4.815383	-3.096923	-1.778762
1	-4.848588	-4.019674	-2.367410
1	-5.090881	-2.290340	-2.464407
6	-5.878887	-3.186503	-0.642135
1	-5.436858	-2.812568	0.291127
1	-6.181534	-4.219034	-0.451922
6	-6.421104	1.834400	0.061701
1	-6.271387	0.805268	0.394693
1	-6.299875	2.508469	0.913932
6	-7.146765	-2.372099	-0.838313
8	-8.255548	-2.725272	-0.501178
8	-6.884090	-1.156104	-1.368568
1	-7.683414	-0.576982	-1.323343
6	-7.823319	1.957817	-0.482297
8	-8.451984	1.087088	-1.063761
8	-8.339338	3.191132	-0.309629
1	-9.222664	3.184111	-0.727065
6	-2.386941	-5.236287	-1.412187
1	-2.249027	-5.843243	-0.507476
1	-3.324202	-5.555171	-1.878144
1	-1.572403	-5.497286	-2.099970
7	-1.245781	-0.604820	2.630378
6	-1.413276	0.336297	3.537441
6	-1.559042	-1.796102	3.248730
7	-1.824361	-0.197866	4.719637

1	-1.248830	1.392768	3.381903
6	-1.921958	-1.566904	4.549966
1	-1.497585	-2.731957	2.713023
1	-2.015073	0.313540	5.568808
1	-2.229941	-2.224293	5.348423
26	-0.481436	-0.242627	0.442354

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<sup>3</sup>C<sub>Fe(his)</sub>  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0448528  
 Zero-point correction=                    0.887889 (Hartree/Particle)  
 Thermal correction to Energy=            0.952949  
 Thermal correction to Enthalpy=         0.953894  
 Thermal correction to Gibbs Free Energy= 0.777381  
 Sum of electronic and zero-point Energies= -2945.156964  
 Sum of electronic and thermal Energies= -2945.091903  
 Sum of electronic and thermal Enthalpies= -2945.090959  
 Sum of electronic and thermal Free Energies= -2945.267472

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 Cartesian Coordinates  
 .....

6	3.300078	-3.225152	-1.099304
6	2.034987	-2.647929	-0.686652
7	2.031499	-1.290326	-0.876004
6	3.240470	-0.980148	-1.427092
6	4.054018	-2.182882	-1.594547
6	0.932162	-3.388502	-0.272009
6	-0.339173	-2.877221	-0.043193
7	-0.681592	-1.547494	-0.087629
6	-2.033079	-1.491142	0.141685
6	-2.570930	-2.828788	0.315068
6	-1.509471	-3.693005	0.217350
6	-2.785134	-0.326581	0.250127
6	-2.287662	0.967641	0.175078
7	-0.988767	1.293275	-0.100310
6	-0.928527	2.661472	-0.089416
6	-2.231070	3.229809	0.222916
6	-3.082959	2.170562	0.384386
6	0.200581	3.411508	-0.390244
6	1.426270	2.891308	-0.792068
7	1.700593	1.555467	-0.935006
6	2.945079	1.474979	-1.511915
6	3.476657	2.796425	-1.751012
6	2.551422	3.689098	-1.254592
6	3.642479	0.301863	-1.780306
1	0.106561	4.489988	-0.369880
1	4.608863	0.409581	-2.259770
1	1.055344	-4.462600	-0.188123
1	-3.842793	-0.440149	0.452356
6	1.002576	0.143380	1.526901

6	1.735160	1.275068	2.125014
6	1.057867	2.288718	2.830673
6	3.151692	1.367234	2.056767
6	1.729990	3.370379	3.402467
1	-0.019514	2.207619	2.920330
6	3.826700	2.453597	2.623398
6	3.115273	3.456854	3.287616
1	1.171393	4.135080	3.936063
1	4.907002	2.520111	2.565126
1	3.655940	4.292708	3.724564
6	0.049462	-0.499956	2.469054
8	-0.979380	-0.011423	2.908132
8	0.478582	-1.729263	2.859661
8	3.791929	0.325504	1.450043
6	5.204731	0.339693	1.396614
1	5.492658	-0.584667	0.892831
1	5.581472	1.196681	0.821048
1	5.647883	0.360080	2.401512
7	3.721444	-3.217820	2.516052
7	3.824520	-2.356457	3.200569
6	-4.544505	2.203863	0.732868
1	-4.776879	1.407115	1.449648
1	-4.788986	3.148703	1.228665
6	-5.479834	2.056358	-0.498187
1	-5.335043	1.088956	-0.981908
1	-5.243693	2.845112	-1.221239
6	-6.925327	2.241569	-0.095372
8	-7.405840	3.248976	0.368255
8	-7.689275	1.117299	-0.286737
1	-8.589935	1.350466	0.011945
6	-4.028732	-3.136153	0.517166
1	-4.453308	-2.427399	1.234004
1	-4.145326	-4.128398	0.965353
6	-4.851297	-3.081203	-0.806645
1	-4.284022	-2.509396	-1.552587
1	-5.014599	-4.078054	-1.222518
6	-6.200822	-2.396200	-0.712375
8	-7.232797	-2.790939	-1.207921
8	-6.108269	-1.217537	-0.047690
1	-6.951920	-0.725931	-0.134776
6	-1.508979	-5.189584	0.323417
1	-2.498994	-5.570502	0.591903
1	-1.221128	-5.666323	-0.622960
1	-0.803629	-5.541930	1.086592
6	-2.519011	4.697303	0.334857
1	-2.386542	5.213092	-0.625515
1	-3.546026	4.880606	0.664537
1	-1.849066	5.184815	1.053996
6	3.676008	-4.669202	-0.962522
1	3.198915	-5.124615	-0.088725

1	3.387703	-5.263389	-1.841639
1	4.759414	-4.775233	-0.844252
6	4.815923	3.096461	-2.355665
1	5.638410	2.774228	-1.702889
1	4.950569	2.587079	-3.318033
1	4.943398	4.169273	-2.526485
6	5.404716	-2.191065	-2.145294
6	6.027129	-3.212446	-2.756775
1	5.958847	-1.257671	-2.047024
1	7.048065	-3.107923	-3.112773
1	5.545222	-4.167272	-2.941040
6	2.684449	5.145490	-1.209564
6	2.290307	5.946923	-0.208718
1	3.187118	5.601886	-2.063288
1	2.439892	7.021798	-0.262265
1	1.843863	5.556103	0.701117
6	-0.367906	-2.411768	3.807043
1	-0.523469	-1.767839	4.678869
1	-1.346105	-2.586768	3.346889
6	0.317382	-3.713795	4.182397
1	1.290067	-3.524435	4.647394
1	-0.302354	-4.271936	4.893632
1	0.477975	-4.338476	3.297365
7	-0.061265	-0.095265	-2.561788
6	0.183818	-1.096768	-3.384016
6	-0.739528	0.855183	-3.295049
7	-0.311419	-0.832567	-4.621289
1	0.704672	-2.005956	-3.125534
6	-0.904844	0.416003	-4.581424
1	-1.054956	1.783311	-2.844078
1	-0.248107	-1.439128	-5.425675
1	-1.372292	0.859179	-5.447063
26	0.541584	0.012471	-0.407740

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<sup>3</sup>TS(C-D)<sub>Fe(his)</sub>  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2836.5033584  
 Zero-point correction=                    0.877330 (Hartree/Particle)  
 Thermal correction to Energy=            0.936870  
 Thermal correction to Enthalpy=         0.937815  
 Thermal correction to Gibbs Free Energy= 0.778643  
 Sum of electronic and zero-point Energies= -2835.626029  
 Sum of electronic and thermal Energies= -2835.566488  
 Sum of electronic and thermal Enthalpies= -2835.565544  
 Sum of electronic and thermal Free Energies= -2835.724715

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 Cartesian Coordinates  
 .....

6	3.555051	-3.276348	-0.903234
6	2.261795	-2.724414	-0.550933

7	2.263683	-1.357944	-0.668588
6	3.514375	-1.020201	-1.106582
6	4.345944	-2.207672	-1.263593
6	1.164452	-3.492896	-0.184354
6	-0.101295	-3.016908	0.133171
7	-0.480394	-1.698968	0.157797
6	-1.808389	-1.690802	0.505310
6	-2.288106	-3.045253	0.709117
6	-1.218929	-3.873127	0.475887
6	-2.597162	-0.549319	0.587720
6	-2.178396	0.740452	0.282276
7	-0.898404	1.087004	-0.067771
6	-0.919829	2.434836	-0.307663
6	-2.254501	2.966549	-0.113624
6	-3.043314	1.907159	0.251183
6	0.167936	3.213529	-0.683089
6	1.459481	2.757064	-0.904176
7	1.841820	1.443181	-0.868847
6	3.153862	1.417213	-1.273478
6	3.626204	2.751586	-1.569701
6	2.578206	3.602328	-1.309265
6	3.931745	0.272589	-1.398865
1	-0.007678	4.271958	-0.827686
1	4.944801	0.403327	-1.761312
1	1.302061	-4.568016	-0.158291
1	-3.632319	-0.680827	0.879019
6	-4.531349	1.912371	0.451999
1	-4.843401	1.101598	1.119396
1	-4.846243	2.847070	0.930287
6	-5.280477	1.776906	-0.907610
1	-5.015073	0.827724	-1.383798
1	-4.983688	2.598377	-1.564242
6	-6.772962	1.865107	-0.720239
8	-7.453933	2.861452	-0.745957
8	-7.328234	0.635628	-0.452133
1	-8.280405	0.782980	-0.294071
6	-3.691310	-3.462034	1.047394
1	-4.162975	-2.754620	1.738036
1	-3.657553	-4.420213	1.577026
6	-4.617847	-3.652530	-0.192731
1	-4.075045	-4.154200	-0.997061
1	-5.472522	-4.272419	0.100288
6	-5.159447	-2.342605	-0.721270
8	-4.794321	-1.771848	-1.733229
8	-6.107269	-1.853622	0.102742
1	-6.445167	-0.999721	-0.249042
6	-1.165063	-5.371445	0.531945
1	-2.096526	-5.793258	0.921457
1	-0.997734	-5.811244	-0.460269
1	-0.351462	-5.722714	1.178688

6	-2.643154	4.403648	-0.293255
1	-2.509775	4.736935	-1.330672
1	-3.690823	4.573024	-0.026317
1	-2.032073	5.062675	0.336054
6	3.928434	-4.725695	-0.833415
1	3.396354	-5.240688	-0.026503
1	3.699497	-5.259786	-1.766442
1	5.002500	-4.838112	-0.652717
6	5.019467	3.099777	-1.998798
1	5.743680	2.911395	-1.195323
1	5.338563	2.511302	-2.868182
1	5.100710	4.157455	-2.265509
6	5.742667	-2.183622	-1.686082
6	6.406311	-3.152649	-2.336645
1	6.294556	-1.276309	-1.440591
1	7.457554	-3.037011	-2.584605
1	5.929645	-4.072388	-2.660814
6	2.597292	5.061437	-1.413093
6	2.004936	5.928296	-0.577999
1	3.187622	5.466824	-2.235796
1	2.087584	6.999916	-0.737554
1	1.458929	5.601972	0.302255
6	1.291640	0.153856	1.701764
6	1.232377	1.532978	2.273759
6	0.727889	-0.886034	2.613245
6	0.059006	2.127812	2.773799
6	2.421412	2.299934	2.355911
8	-0.314968	-0.814364	3.241729
8	1.555428	-1.965771	2.701733
6	0.050487	3.426660	3.280661
1	-0.852918	1.544337	2.759413
6	2.418219	3.604307	2.854093
8	3.637943	1.810729	1.934815
6	1.230229	4.174947	3.307219
1	-0.876918	3.851065	3.656533
1	3.359825	4.143686	2.891162
6	3.810731	0.426541	2.083090
1	1.233879	5.187995	3.701945
1	3.929785	0.116976	3.127981
1	4.598067	0.079651	1.417719
1	2.606125	-0.043362	1.687811
7	0.061668	-0.400721	-2.397655
6	-1.141922	-0.776108	-2.794616
6	0.810755	-0.218065	-3.541383
7	-1.196762	-0.841348	-4.148983
1	-1.983457	-1.007401	-2.158642
6	0.044885	-0.487547	-4.643913
1	1.842853	0.091825	-3.487393
1	-2.008726	-1.104366	-4.688338
1	0.258863	-0.462241	-5.701112

6	1.119347	-3.042900	3.553598
1	0.036396	-3.155662	3.459280
1	1.612654	-3.929843	3.145613
6	1.520488	-2.805534	5.003569
1	1.008767	-1.924486	5.400590
1	1.245298	-3.671645	5.617690
1	2.602150	-2.654343	5.087899
26	0.698164	-0.114473	-0.278298

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<sup>3</sup>D<sub>Fe(his)</sub>  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2836.5318632  
Zero-point correction=                    0.881356 (Hartree/Particle)  
Thermal correction to Energy=            0.941786  
Thermal correction to Enthalpy=         0.942730  
Thermal correction to Gibbs Free Energy= 0.781270  
Sum of electronic and zero-point Energies= -2835.650507  
Sum of electronic and thermal Energies= -2835.590077  
Sum of electronic and thermal Enthalpies= -2835.589133  
Sum of electronic and thermal Free Energies= -2835.750593

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Cartesian Coordinates  
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6	3.410104	-3.467550	-0.860494
6	2.127638	-2.875158	-0.544195
7	2.178833	-1.507242	-0.647657
6	3.455229	-1.206727	-1.036461
6	4.250338	-2.421831	-1.174029
6	0.997075	-3.603180	-0.197255
6	-0.240342	-3.068486	0.132899
7	-0.547905	-1.731392	0.165944
6	-1.865666	-1.653912	0.536123
6	-2.410843	-2.984224	0.753611
6	-1.393136	-3.866780	0.496959
6	-2.599831	-0.476044	0.618738
6	-2.139557	0.793883	0.284537
7	-0.856902	1.094143	-0.092178
6	-0.843848	2.437540	-0.367106
6	-2.156561	3.013670	-0.164943
6	-2.969254	1.987035	0.239556
6	0.261659	3.169630	-0.779365
6	1.534866	2.659582	-0.987470
7	1.865175	1.332886	-0.899877
6	3.182680	1.243063	-1.269317
6	3.710756	2.548966	-1.604145
6	2.689613	3.447365	-1.401972
6	3.924119	0.068574	-1.328158
1	0.120047	4.228341	-0.955540
1	4.953152	0.155740	-1.657077
1	1.087512	-4.683409	-0.179414

1	-3.634860	-0.560812	0.927684
6	-4.452676	2.047249	0.464899
1	-4.783819	1.252824	1.142332
1	-4.724117	2.996219	0.942158
6	-5.228116	1.932024	-0.881824
1	-5.014562	0.965515	-1.349426
1	-4.904020	2.730615	-1.553332
6	-6.712028	2.091655	-0.675194
8	-7.351958	3.113504	-0.734430
8	-7.313077	0.899402	-0.344943
1	-8.255856	1.092860	-0.180726
6	-3.823405	-3.329918	1.130433
1	-4.245085	-2.591313	1.820617
1	-3.820614	-4.280742	1.674310
6	-4.787269	-3.496039	-0.084334
1	-4.286521	-4.030802	-0.894568
1	-5.660408	-4.074476	0.237560
6	-5.284348	-2.170551	-0.617152
8	-4.919701	-1.629207	-1.645183
8	-6.189707	-1.630632	0.222842
1	-6.499279	-0.767632	-0.132639
6	-1.414247	-5.366002	0.553088
1	-2.358365	-5.740071	0.960662
1	-1.288522	-5.813983	-0.441667
1	-0.607542	-5.758450	1.184706
6	-2.506356	4.456824	-0.375954
1	-2.387382	4.758078	-1.424946
1	-3.542265	4.664866	-0.090907
1	-1.862662	5.114631	0.221256
6	3.730254	-4.930078	-0.796701
1	3.152383	-5.435465	-0.015601
1	3.516200	-5.445115	-1.743853
1	4.792530	-5.082532	-0.579335
6	5.125548	2.835087	-2.007495
1	5.811138	2.732887	-1.155471
1	5.474463	2.151252	-2.790659
1	5.232930	3.856129	-2.385539
6	5.662714	-2.442522	-1.540416
6	6.315048	-3.424498	-2.182921
1	6.236921	-1.561199	-1.254995
1	7.378941	-3.344910	-2.387471
1	5.817251	-4.319337	-2.543054
6	2.766488	4.899274	-1.565694
6	2.190953	5.826186	-0.785199
1	3.389752	5.245368	-2.391411
1	2.318264	6.885252	-0.991949
1	1.611918	5.563214	0.095107
6	1.378602	0.103401	1.718950
6	1.301456	1.494608	2.242151
6	0.753832	-0.924968	2.599510



6	0.127427	2.055130	2.778162
6	2.458734	2.309829	2.271616
8	-0.287212	-0.831266	3.227599
8	1.538724	-2.040883	2.661821
6	0.093792	3.352443	3.287121
1	-0.762077	1.439692	2.804353
6	2.431868	3.619732	2.757749
8	3.625480	1.749699	1.792778
6	1.243460	4.143940	3.265409
1	-0.833974	3.745695	3.694408
1	3.332042	4.223668	2.714516
6	4.832021	2.233316	2.190769
1	1.222881	5.163003	3.643427
1	5.654703	1.686962	1.745375
1	4.910457	2.626844	3.201554
1	2.404040	-0.180871	1.505509
7	0.010107	-0.473167	-2.419703
6	-1.200715	-0.832186	-2.806991
6	0.748918	-0.288345	-3.569155
7	-1.270661	-0.885331	-4.162524
1	-2.039320	-1.055349	-2.163926
6	-0.030797	-0.540919	-4.666650
1	1.784938	0.010432	-3.523294
1	-2.091450	-1.131402	-4.696326
1	0.173426	-0.510085	-5.725665
6	1.053623	-3.121827	3.478835
1	-0.033341	-3.183657	3.382538
1	1.506734	-4.017987	3.045019
6	1.463426	-2.946155	4.935427
1	0.990165	-2.055632	5.358244
1	1.150125	-3.817333	5.523791
1	2.550481	-2.844033	5.023404
26	0.677395	-0.186551	-0.287975

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**<sup>3</sup>TS(D-E)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2836.5308683  
Zero-point correction=                    0.879809 (Hartree/Particle)  
Thermal correction to Energy=            0.939994  
Thermal correction to Enthalpy=         0.940938  
Thermal correction to Gibbs Free Energy= 0.780007  
Sum of electronic and zero-point Energies= -2835.651060  
Sum of electronic and thermal Energies= -2835.590874  
Sum of electronic and thermal Enthalpies= -2835.589930  
Sum of electronic and thermal Free Energies= -2835.750861

.....  
Cartesian Coordinates

6	3.099777	-3.750829	-0.722060
6	1.878930	-3.037584	-0.411048

7	2.037829	-1.685740	-0.595747
6	3.319710	-1.515753	-1.041475
6	4.009556	-2.798412	-1.126616
6	0.696092	-3.651081	-0.017285
6	-0.497736	-3.003986	0.272338
7	-0.692704	-1.645395	0.245703
6	-2.004742	-1.443317	0.586891
6	-2.666243	-2.713875	0.835118
6	-1.720178	-3.688194	0.641843
6	-2.628501	-0.201219	0.642043
6	-2.046991	1.019422	0.315728
7	-0.745204	1.195902	-0.070556
6	-0.608242	2.531753	-0.346071
6	-1.858374	3.233198	-0.122558
6	-2.759695	2.287590	0.287909
6	0.551666	3.147969	-0.797524
6	1.759697	2.512728	-1.053924
7	1.964632	1.161318	-0.954491
6	3.249805	0.938004	-1.380100
6	3.882265	2.179981	-1.771850
6	2.963690	3.177709	-1.539805
6	3.879986	-0.300879	-1.419732
1	0.507419	4.213582	-0.983267
1	4.897269	-0.319749	-1.793716
1	0.699195	-4.733085	0.054447
1	-3.672038	-0.186501	0.935788
6	-4.228355	2.461987	0.542345
1	-4.563504	1.800725	1.350437
1	-4.451339	3.481409	0.872088
6	-5.053993	2.166358	-0.733281
1	-4.832671	1.171158	-1.128402
1	-4.773188	2.883935	-1.515410
6	-6.536288	2.324044	-0.498013
8	-7.080619	3.211650	0.113309
8	-7.261918	1.309183	-1.076540
1	-8.200338	1.494796	-0.875661
6	-4.113407	-2.927937	1.176627
1	-4.518809	-2.087214	1.750210
1	-4.200562	-3.804053	1.829300
6	-5.028135	-3.189990	-0.060069
1	-4.528480	-3.873947	-0.750389
1	-5.963003	-3.645978	0.281375
6	-5.367773	-1.919660	-0.807430
8	-4.780031	-1.481273	-1.779513
8	-6.412308	-1.287725	-0.234125
1	-6.602901	-0.459098	-0.727801
6	-1.873299	-5.176393	0.756630
1	-2.843328	-5.448547	1.184513
1	-1.796841	-5.672946	-0.220064
1	-1.099116	-5.614777	1.398642

6	-2.068265	4.704163	-0.325932
1	-1.936853	4.995186	-1.376415
1	-3.074440	5.010670	-0.023438
1	-1.354234	5.295053	0.261402
6	3.303263	-5.228241	-0.575167
1	2.710005	-5.636459	0.250087
1	3.020378	-5.780083	-1.482781
1	4.355875	-5.454381	-0.375251
6	5.296134	2.320564	-2.249439
1	6.010080	2.198065	-1.423572
1	5.546722	1.572686	-3.011139
1	5.474397	3.309085	-2.683389
6	5.401875	-2.957527	-1.533081
6	5.953173	-4.029108	-2.125259
1	6.052887	-2.107782	-1.327720
1	7.012067	-4.048103	-2.367109
1	5.375193	-4.903385	-2.407583
6	3.176786	4.610287	-1.743866
6	2.718919	5.613494	-0.979475
1	3.808162	4.870445	-2.594675
1	2.945857	6.647506	-1.224218
1	2.139446	5.438231	-0.078075
6	1.491763	0.092450	1.945905
6	1.584349	1.498620	2.311113
6	0.647702	-0.804916	2.763294
6	0.506413	2.233733	2.857376
6	2.820453	2.191012	2.173943
8	-0.396527	-0.529168	3.332854
8	1.230335	-2.034362	2.861068
6	0.643139	3.565605	3.230610
1	-0.436795	1.720656	2.990670
6	2.956454	3.535267	2.528264
8	3.876120	1.464053	1.683721
6	1.865329	4.224176	3.055931
1	-0.207558	4.096304	3.649383
1	3.901236	4.040753	2.360706
6	5.157663	1.866417	1.873579
1	1.972129	5.271484	3.326482
1	5.869295	1.180865	1.431503
1	5.392857	2.410400	2.784285
1	2.425560	-0.367450	1.648243
7	-0.139903	-0.527565	-2.488691
6	-1.368764	-0.881899	-2.817776
6	0.529090	-0.307917	-3.674048
7	-1.517527	-0.899367	-4.169121
1	-2.173413	-1.124050	-2.138991
6	-0.310023	-0.534587	-4.733676
1	1.565192	-0.003823	-3.679898
1	-2.368894	-1.132301	-4.659050
1	-0.166724	-0.474969	-5.801592

6	0.535007	-3.011564	3.657433
1	-0.540706	-2.900569	3.500844
1	0.861121	-3.973920	3.253354
6	0.890626	-2.882662	5.133096
1	0.543998	-1.922856	5.526082
1	0.411246	-3.684802	5.707408
1	1.973768	-2.954459	5.279604
26	0.650087	-0.233640	-0.301609

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<sup>5</sup>A<sub>Fe(his)</sub>  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2184.5613636  
 Zero-point correction=                    0.667802 (Hartree/Particle)  
 Thermal correction to Energy=            0.714818  
 Thermal correction to Enthalpy=         0.715762  
 Thermal correction to Gibbs Free Energy= 0.578878  
 Sum of electronic and zero-point Energies= -2183.893562  
 Sum of electronic and thermal Energies= -2183.846546  
 Sum of electronic and thermal Enthalpies= -2183.845602  
 Sum of electronic and thermal Free Energies= -2183.982486

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 Cartesian Coordinates  
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6	-1.667262	-3.438676	-0.692007
6	-0.363671	-2.795041	-0.630464
7	-0.523169	-1.445757	-0.444728
6	-1.867370	-1.197020	-0.385344
6	-2.604449	-2.444709	-0.540458
6	0.864149	-3.454365	-0.758125
6	2.148288	-2.891952	-0.752539
7	2.416450	-1.566495	-0.544525
6	3.762614	-1.387043	-0.692027
6	4.397698	-2.674498	-0.997145
6	3.384392	-3.611853	-1.006613
6	4.412984	-0.158031	-0.532195
6	3.835729	1.105344	-0.333701
7	2.488798	1.355358	-0.243516
6	2.330239	2.702270	-0.080672
6	3.637195	3.352295	-0.060728
6	4.575803	2.347762	-0.221913
6	1.096928	3.358753	0.056804
6	-0.181024	2.793715	0.040919
7	-0.438374	1.453425	-0.040920
6	-1.794029	1.300843	-0.091259
6	-2.443545	2.609242	-0.006697
6	-1.437887	3.538027	0.077663
6	-1.550064	5.031253	0.162491
6	-3.926284	2.846867	-0.060867
6	-4.475417	2.857743	-1.498322
6	-5.973338	3.065863	-1.549270

8	-6.709928	3.189691	-0.594725
6	-2.447527	0.069688	-0.220814
6	6.064337	2.487633	-0.325903
6	3.837760	4.792055	0.063107
6	4.908373	5.423148	0.572043
6	3.483931	-5.078493	-1.303146
6	5.809379	-2.942401	-1.263991
6	6.690250	-2.143655	-1.886713
6	-4.100757	-2.581404	-0.505194
6	-4.659418	-2.624037	0.927914
6	-6.166421	-2.756124	0.965181
8	-6.899996	-2.842901	0.004749
6	-1.893045	-4.908407	-0.891247
8	-6.428196	3.099784	-2.827232
8	-6.633443	-2.770278	2.239891
1	1.138360	4.437405	0.168719
1	-3.533034	0.100176	-0.220350
1	0.813406	-4.527550	-0.916646
1	5.494899	-0.186031	-0.578777
1	6.499769	1.708674	-0.960522
1	6.333671	3.459663	-0.752930
1	6.557519	2.418154	0.653995
1	4.522255	-5.423221	-1.291463
1	2.925870	-5.678261	-0.573330
1	3.075906	-5.318816	-2.294336
1	-1.380307	-5.277433	-1.788509
1	-1.517594	-5.497189	-0.043508
1	-2.956531	-5.139991	-1.003916
1	-2.588597	5.349139	0.297426
1	-0.971309	5.433425	1.003784
1	-1.173095	5.519485	-0.746261
1	3.018133	5.412526	-0.299388
1	4.953861	6.508219	0.597187
1	5.754499	4.892676	0.996918
1	6.163495	-3.922995	-0.942590
1	7.720097	-2.457490	-2.031663
1	6.412844	-1.177922	-2.297696
1	-4.462048	2.082018	0.513372
1	-4.177305	3.799667	0.417448
1	-3.997958	3.644782	-2.095346
1	-4.242521	1.919022	-2.016665
1	-7.393908	3.227542	-2.765376
1	-4.413907	-3.489761	-1.030292
1	-4.577357	-1.754556	-1.044314
1	-4.229235	-3.462412	1.490677
1	-4.379329	-1.723552	1.488590
1	-7.603423	-2.853277	2.168713
7	1.143789	-0.369384	2.172875
6	1.978436	-1.195907	2.775460
6	0.441389	0.274288	3.170664

7	1.842282	-1.111959	4.123621
1	2.677868	-1.850278	2.276653
6	0.861571	-0.174518	4.393880
1	-0.310173	1.011664	2.932001
1	2.368588	-1.638602	4.805462
1	0.567242	0.075337	5.401358
26	0.998223	-0.085725	-0.029698

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<sup>5</sup>BFe(his)  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0792397  
Zero-point correction=                    0.890097 (Hartree/Particle)  
Thermal correction to Energy=            0.954245  
Thermal correction to Enthalpy=         0.955189  
Thermal correction to Gibbs Free Energy= 0.777757  
Sum of electronic and zero-point Energies= -2945.189142  
Sum of electronic and thermal Energies= -2945.124995  
Sum of electronic and thermal Enthalpies= -2945.124051  
Sum of electronic and thermal Free Energies= -2945.301482

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Cartesian Coordinates  
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6	2.735071	2.412460	1.863109
6	2.149555	1.118983	1.550828
7	0.841520	1.275778	1.176660
6	0.564310	2.612802	1.196736
6	1.756287	3.355757	1.625771
6	2.830877	-0.102434	1.595227
6	2.368128	-1.365845	1.201740
7	1.116676	-1.630516	0.718921
6	1.060831	-2.970199	0.427457
6	2.330301	-3.596343	0.740723
6	3.150275	-2.598074	1.238820
6	-0.058118	-3.631911	-0.104470
6	-1.297685	-3.082675	-0.443108
7	-1.641468	-1.771655	-0.259607
6	-2.898956	-1.606057	-0.765521
6	-3.406034	-2.885656	-1.264044
6	-2.407247	-3.803969	-1.065184
7	-1.868187	1.134019	0.091472
6	-3.109196	0.876868	-0.427748
6	-3.868856	2.116145	-0.509193
6	-3.058875	3.110914	-0.010764
6	-1.802831	2.477727	0.358165
6	-3.578356	-0.383772	-0.824103
6	-0.687544	3.152423	0.875048
8	6.543753	-1.365584	-1.230426
6	6.033829	-0.135597	-0.960992
8	6.382050	0.551851	-0.013592
6	5.024596	0.255949	-1.946706

7	4.722291	-0.649541	-2.856684
7	4.452561	-1.427289	-3.639491
6	4.378123	1.584225	-2.000245
6	5.120067	2.738618	-1.716022
6	4.531831	4.002345	-1.752503
6	3.186525	4.125559	-2.093712
6	2.425319	2.992780	-2.387480
6	3.009015	1.722502	-2.334347
8	2.339461	0.564725	-2.591874
6	0.939725	0.620665	-2.842415
1	-0.803572	4.219138	1.026386
1	-4.581226	-0.414590	-1.234259
1	0.060144	-4.694275	-0.293140
1	3.857993	-0.051831	1.939576
1	6.164742	2.632464	-1.447394
1	5.124784	4.881926	-1.520044
1	1.377029	3.100547	-2.639411
1	2.716581	5.104444	-2.125389
1	0.617111	-0.415647	-2.951173
1	0.402051	1.080271	-2.005394
1	0.723690	1.171230	-3.767720
6	7.589632	-1.845863	-0.357911
1	7.481864	-2.932861	-0.376716
1	7.402893	-1.483462	0.655124
6	8.959041	-1.404497	-0.853964
1	9.050632	-0.315046	-0.809428
1	9.743164	-1.840764	-0.224006
1	9.124617	-1.731093	-1.885898
6	4.159796	2.625472	2.278966
1	4.384664	3.686629	2.418524
1	4.386397	2.109092	3.221680
1	4.854387	2.235758	1.524493
6	2.670671	-5.037656	0.510721
1	3.732925	-5.151452	0.268674
1	2.473137	-5.658084	1.396439
1	2.092026	-5.461918	-0.316336
6	1.918433	4.800799	1.768091
6	1.332934	5.772974	1.050593
1	2.628150	5.108551	2.536796
1	1.542226	6.818719	1.257555
1	0.660109	5.566018	0.224492
6	4.532302	-2.674038	1.696948
6	5.170616	-3.749033	2.189682
1	5.095099	-1.743125	1.638665
1	6.210576	-3.683026	2.497140
1	4.685276	-4.709245	2.330311
6	-3.360186	4.573682	0.132753
1	-4.330885	4.831441	-0.302194
1	-3.382525	4.881995	1.186384
1	-2.602706	5.193603	-0.363385

6	-5.268756	2.247238	-1.041834
1	-5.443661	3.272935	-1.385879
1	-5.406526	1.595681	-1.912296
6	-4.778695	-3.087883	-1.845554
1	-4.797354	-4.000608	-2.450362
1	-5.007501	-2.265646	-2.530149
6	-5.899843	-3.178215	-0.765100
1	-5.493677	-2.845237	0.199485
1	-6.241059	-4.206239	-0.621300
6	-6.356510	1.887370	0.012922
1	-6.224021	0.851446	0.332106
1	-6.258771	2.545471	0.880499
6	-7.133646	-2.321217	-0.995720
8	-8.267207	-2.654317	-0.727089
8	-6.812072	-1.096442	-1.469245
1	-7.598217	-0.497963	-1.448907
6	-7.739125	2.028693	-0.574636
8	-8.352081	1.171960	-1.192740
8	-8.254834	3.261359	-0.397108
1	-9.123631	3.266484	-0.844022
6	-2.395981	-5.263945	-1.408354
1	-2.292281	-5.891394	-0.512981
1	-3.319255	-5.565379	-1.912588
1	-1.560087	-5.516558	-2.073429
7	-1.209236	-0.630187	2.788751
6	-0.778281	0.029202	3.848351
6	-2.148961	-1.531742	3.243924
7	-1.403616	-0.410685	4.969970
1	-0.033063	0.810633	3.836269
6	-2.284881	-1.411049	4.600839
1	-2.653237	-2.198274	2.560550
1	-1.247516	-0.068415	5.906891
1	-2.904420	-1.925230	5.319105
26	-0.486562	-0.301612	0.713408

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<sup>5</sup>C<sub>Fe(his)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2946.0402448  
Zero-point correction=                    0.884815 (Hartree/Particle)  
Thermal correction to Energy=            0.951220  
Thermal correction to Enthalpy=         0.952164  
Thermal correction to Gibbs Free Energy= 0.768096  
Sum of electronic and zero-point Energies= -2945.155430  
Sum of electronic and thermal Energies= -2945.089025  
Sum of electronic and thermal Enthalpies= -2945.088081  
Sum of electronic and thermal Free Energies= -2945.272149

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Cartesian Coordinates

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6	3.198293	-3.356151	-1.285654
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6	1.992269	-2.742626	-0.757319
7	2.072271	-1.380941	-0.866870
6	3.253855	-1.086514	-1.479099
6	3.985750	-2.323114	-1.761484
6	0.866229	-3.440601	-0.299068
6	-0.386859	-2.910439	0.023144
7	-0.698403	-1.577658	0.047186
6	-2.041535	-1.474757	0.278249
6	-2.615943	-2.806924	0.428213
6	-1.582644	-3.700582	0.282732
6	-2.760202	-0.276175	0.360486
6	-2.265524	1.022079	0.207748
7	-0.966716	1.334881	-0.065587
6	-0.885627	2.693505	-0.180735
6	-2.197442	3.287688	0.055652
6	-3.057806	2.246386	0.297954
6	0.264023	3.405930	-0.535249
6	1.509083	2.881329	-0.906985
7	1.811045	1.549668	-0.944147
6	3.025080	1.415372	-1.561744
6	3.541685	2.722676	-1.915788
6	2.618628	3.649236	-1.471135
6	3.679005	0.203670	-1.815071
1	0.156854	4.481047	-0.617719
1	4.625233	0.279554	-2.341126
1	0.946495	-4.522735	-0.278047
1	-3.821654	-0.366544	0.560238
6	1.043289	0.257999	1.898818
6	1.863075	1.247190	2.571134
6	1.298372	2.125288	3.530711
6	3.248783	1.414905	2.264147
6	2.026949	3.165964	4.093118
1	0.250572	1.997603	3.779313
6	3.983423	2.450354	2.853374
6	3.370454	3.327791	3.748685
1	1.552837	3.843319	4.797409
1	5.033891	2.577097	2.620974
1	3.955781	4.132387	4.186190
6	0.019369	-0.359901	2.776182
8	-1.042495	0.146121	3.099107
8	0.412190	-1.588277	3.179633
8	3.798062	0.482352	1.452277
6	5.197219	0.520620	1.217082
1	5.410866	-0.339131	0.582483
1	5.492243	1.439141	0.694229
1	5.757712	0.436710	2.156870
7	3.500261	-3.301082	2.448790
7	3.805947	-2.384346	2.984709
6	-4.526019	2.320430	0.610758
1	-4.784596	1.572614	1.370131

1	-4.768857	3.297549	1.040957
6	-5.436511	2.106262	-0.629387
1	-5.295895	1.106632	-1.043804
1	-5.171882	2.842064	-1.396765
6	-6.886744	2.339344	-0.271749
8	-7.364046	3.387000	0.096716
8	-7.659948	1.210579	-0.380303
1	-8.562896	1.476762	-0.118679
6	-4.081152	-3.082214	0.622694
1	-4.499005	-2.352136	1.321885
1	-4.224205	-4.064555	1.085621
6	-4.886449	-3.032363	-0.712237
1	-4.299332	-2.481535	-1.458496
1	-5.061708	-4.032376	-1.115363
6	-6.223988	-2.322512	-0.643862
8	-7.259929	-2.710031	-1.137197
8	-6.115621	-1.130363	-0.005478
1	-6.948823	-0.626074	-0.116963
6	-1.634716	-5.199380	0.325750
1	-2.621137	-5.556859	0.637341
1	-1.422297	-5.642785	-0.656328
1	-0.898650	-5.611232	1.027761
6	-2.491850	4.757962	0.022515
1	-2.351868	5.177801	-0.982558
1	-3.522256	4.969735	0.323830
1	-1.829578	5.316441	0.695919
6	3.501397	-4.823827	-1.270977
1	3.016029	-5.323631	-0.426307
1	3.165616	-5.330868	-2.186976
1	4.579910	-4.995641	-1.186573
6	4.852282	2.979616	-2.598865
1	5.704428	2.680482	-1.973308
1	4.934264	2.419247	-3.538798
1	4.982783	4.040103	-2.832496
6	5.296971	-2.373048	-2.397635
6	5.836541	-3.394594	-3.083668
1	5.897594	-1.468134	-2.303201
1	6.836761	-3.316286	-3.500143
1	5.305335	-4.321839	-3.271912
6	2.742013	5.102135	-1.571334
6	2.300946	6.010751	-0.687615
1	3.280366	5.468506	-2.446258
1	2.450276	7.073243	-0.858004
1	1.806227	5.728494	0.237016
6	-0.524380	-2.310541	4.011632
1	-0.763915	-1.703171	4.890546
1	-1.448290	-2.462390	3.445320
6	0.128184	-3.627257	4.390433
1	1.053552	-3.459525	4.951050
1	-0.553199	-4.214282	5.016651

1	0.368553	-4.210832	3.496006
7	-0.161001	-0.145818	-2.750810
6	0.250188	-1.036691	-3.627538
6	-1.022271	0.683794	-3.435063
7	-0.309516	-0.820412	-4.853384
1	0.942579	-1.841843	-3.428036
6	-1.131028	0.285726	-4.743186
1	-1.504592	1.513404	-2.938766
1	-0.148245	-1.364322	-5.688139
1	-1.693870	0.668934	-5.580796
26	0.678426	0.004154	-0.093924

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<sup>5</sup>D<sub>Fe(his)</sub>  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2836.5401407  
 Zero-point correction=                    0.876852 (Hartree/Particle)  
 Thermal correction to Energy=            0.939114  
 Thermal correction to Enthalpy=         0.940058  
 Thermal correction to Gibbs Free Energy= 0.767794  
 Sum of electronic and zero-point Energies= -2835.663289  
 Sum of electronic and thermal Energies= -2835.601027  
 Sum of electronic and thermal Enthalpies= -2835.600083  
 Sum of electronic and thermal Free Energies= -2835.772347

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 Cartesian Coordinates  
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6	2.165128	-4.068680	-0.393075
6	1.013538	-3.242264	-0.088741
7	1.215675	-1.969891	-0.557755
6	2.447628	-1.936974	-1.145798
6	3.064154	-3.259202	-1.067184
6	-0.140744	-3.674444	0.581721
6	-1.272569	-2.924996	0.918429
7	-1.440531	-1.595747	0.649086
6	-2.666307	-1.230356	1.126172
6	-3.333795	-2.393367	1.707786
6	-2.457605	-3.444627	1.590044
6	-3.184267	0.070485	1.047835
6	-2.569812	1.209390	0.505540
7	-1.305530	1.253110	-0.018687
6	-1.082326	2.534126	-0.447651
6	-2.254654	3.353922	-0.179929
6	-3.183444	2.527138	0.405020
6	0.087142	2.992185	-1.068900
6	1.220269	2.244799	-1.409596
7	1.304823	0.889432	-1.286697
6	2.534884	0.507158	-1.750835
6	3.264265	1.669910	-2.233127
6	2.461559	2.764865	-1.995876

6	3.035072	-0.799277	-1.719021
1	0.114535	4.045681	-1.322181
1	4.020018	-0.935329	-2.152377
1	-0.160552	-4.720098	0.872194
1	-4.182470	0.214311	1.449985
6	-4.603830	2.845961	0.770690
1	-4.887854	2.336503	1.699996
1	-4.734965	3.916117	0.957834
6	-5.576710	2.420312	-0.356292
1	-5.445116	1.365990	-0.614105
1	-5.348905	2.997232	-1.262091
6	-7.016240	2.699186	0.000245
8	-7.453624	3.703730	0.507451
8	-7.840533	1.646278	-0.321236
1	-8.742679	1.914321	-0.057168
6	-4.728098	-2.443965	2.264273
1	-5.006249	-1.494541	2.735886
1	-4.776958	-3.199432	3.056819
6	-5.814480	-2.821437	1.209773
1	-5.464506	-3.661007	0.604421
1	-6.729451	-3.115754	1.734702
6	-6.153154	-1.674519	0.283256
8	-5.705238	-1.498581	-0.835372
8	-7.020166	-0.822452	0.868090
1	-7.219664	-0.084064	0.250540
6	-2.641696	-4.866369	2.031671
1	-3.544415	-4.988574	2.638791
1	-2.727526	-5.551997	1.177691
1	-1.792797	-5.212915	2.634216
6	-2.383793	4.810052	-0.516382
1	-2.369650	4.980258	-1.601058
1	-3.316577	5.232141	-0.129579
1	-1.558201	5.394953	-0.092003
6	2.336795	-5.503361	0.004487
1	1.745382	-5.749862	0.892138
1	2.029977	-6.194884	-0.793061
1	3.386428	-5.721704	0.231079
6	4.656906	1.647094	-2.787746
1	5.398069	1.442600	-2.003359
1	4.774884	0.871815	-3.555039
1	4.924467	2.606246	-3.241164
6	4.392013	-3.574389	-1.578961
6	4.876626	-4.780647	-1.922223
1	5.060762	-2.722218	-1.693979
1	5.895927	-4.884417	-2.283478
1	4.282142	-5.687409	-1.886148
6	2.809857	4.158072	-2.266318
6	2.468559	5.235598	-1.542736
1	3.444532	4.317576	-3.139109
1	2.790876	6.229854	-1.839182

1	1.895714	5.161549	-0.623541
6	3.803166	0.602960	1.968501
6	5.072627	1.145676	1.674278
6	2.666951	1.337719	2.517334
6	5.418058	2.516786	1.884223
6	6.110240	0.300444	1.150102
8	2.625068	2.524189	2.821391
8	1.605488	0.499016	2.672158
6	6.683823	2.995623	1.600891
1	4.648315	3.168285	2.277137
6	7.381743	0.794645	0.855958
8	5.775336	-1.007823	0.942745
6	7.669285	2.140544	1.078673
1	6.912691	4.043734	1.771612
1	8.125067	0.137253	0.418108
6	6.718748	-1.973909	0.830399
1	8.654868	2.525069	0.831488
1	6.296726	-2.946875	0.620070
1	7.651765	-1.847757	1.370313
1	3.632967	-0.449235	1.780684
7	-1.329809	-0.869579	-2.413626
6	-2.599504	-1.241862	-2.421510
6	-0.962134	-0.711649	-3.734660
7	-3.060483	-1.329158	-3.693694
1	-3.217432	-1.440335	-1.558445
6	-2.026447	-0.994162	-4.548769
1	0.038246	-0.403755	-4.000489
1	-4.003435	-1.582201	-3.951551
1	-2.142816	-0.990811	-5.621421
6	0.400362	1.073380	3.223213
1	0.274212	2.081937	2.822947
1	-0.399971	0.434440	2.846182
6	0.441859	1.085785	4.745737
1	1.239452	1.742325	5.105444
1	-0.512275	1.454886	5.140838
1	0.608984	0.076975	5.138622
26	-0.170772	-0.417273	-0.555267

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$1\text{CSS}A_{\text{FE}}(\text{eys})$

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2396.4789516  
Zero-point correction=                    0.634862 (Hartree/Particle)  
Thermal correction to Energy=            0.679956  
Thermal correction to Enthalpy=         0.680900  
Thermal correction to Gibbs Free Energy=    0.551580  
Sum of electronic and zero-point Energies=    -2395.844089  
Sum of electronic and thermal Energies=    -2395.798996  
Sum of electronic and thermal Enthalpies=   -2395.798051

Sum of electronic and thermal Free Energies= -2395.927372

.....  
Cartesian Coordinates

.....  
26 1.047720 -0.070787 -0.021412  
7 2.404005 -1.525768 -0.379996  
6 2.152694 -2.862363 -0.575321  
6 3.382245 -3.605580 -0.736558  
6 4.406542 -2.687397 -0.664317  
6 3.768527 -1.395073 -0.412389  
6 0.885567 -3.437136 -0.622073  
6 -0.317090 -2.758122 -0.502666  
7 -0.439062 -1.402095 -0.312479  
6 -1.786761 -1.160030 -0.259257  
6 -2.544275 -2.396712 -0.403607  
6 -1.622649 -3.395931 -0.560168  
6 -2.362375 0.098635 -0.127824  
6 -1.673081 1.302037 -0.042588  
7 -0.309006 1.422291 -0.025917  
6 -0.060852 2.766500 0.095588  
6 -1.302417 3.524661 0.140204  
6 -2.313565 2.608329 0.052852  
6 1.198924 3.340525 0.179489  
6 2.408819 2.656646 0.126451  
6 3.720629 3.289511 0.236889  
6 4.641828 2.266614 0.156951  
6 3.879059 1.045562 -0.003739  
7 2.528574 1.301876 -0.015061  
6 4.451354 -0.209598 -0.176948  
1 0.835539 -4.511720 -0.770072  
1 5.530907 -0.272414 -0.126704  
1 1.239083 4.416962 0.309172  
1 -3.447034 0.147350 -0.110028  
16 1.118868 -0.197752 2.302632  
6 0.585164 -1.888763 2.781387  
1 1.202582 -2.660953 2.309735  
1 0.694316 -1.982587 3.869281  
1 -0.463209 -2.081202 2.525627  
6 -1.394377 5.016943 0.261281  
1 -0.866503 5.383063 1.151803  
1 -0.949206 5.527948 -0.603940  
1 -2.434938 5.350070 0.337778  
6 -1.853969 -4.865608 -0.752220  
1 -1.353625 -5.241141 -1.654915  
1 -1.468055 -5.454161 0.091741  
1 -2.920535 -5.094901 -0.849961  
6 3.469442 -5.080696 -0.993850  
1 2.902860 -5.654519 -0.248888  
1 3.062632 -5.349177 -1.979229  
1 4.505073 -5.434364 -0.966116

6	6.136961	2.367327	0.168535
1	6.548534	2.315490	1.187156
1	6.602722	1.559130	-0.405753
1	6.466093	3.319964	-0.262787
6	5.824507	-2.985350	-0.832415
6	6.785988	-2.207085	-1.358204
1	6.121476	-3.986896	-0.514816
1	7.811974	-2.560164	-1.425126
1	6.584084	-1.217128	-1.754720
6	3.933475	4.724133	0.356150
6	4.995046	5.363633	0.879862
1	3.126284	5.347212	-0.030976
1	5.039400	6.449741	0.889574
1	5.829354	4.840155	1.335406
6	-4.041407	-2.510102	-0.344044
6	-4.577512	-2.472073	1.098347
1	-4.374720	-3.441010	-0.816162
1	-4.516989	-1.703743	-0.915760
1	-4.137414	-3.279392	1.697877
1	-4.277560	-1.545860	1.603930
6	-3.795139	2.856080	0.012869
6	-4.367147	2.788273	-1.414516
1	-4.030339	3.838459	0.436621
1	-4.328254	2.130618	0.639616
1	-3.865006	3.514636	-2.067293
1	-4.171937	1.809948	-1.870377
6	-6.080950	-2.593137	1.180148
8	-6.849374	-2.721112	0.249971
8	-6.520768	-2.546888	2.467331
1	-7.491996	-2.622776	2.412399
6	-5.852724	3.055169	-1.479660
8	-6.576282	3.359469	-0.555160
8	-6.332839	2.921905	-2.747234
1	-7.288554	3.107806	-2.682428

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**1CSSB<sub>FE(cys)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3157.9972622  
Zero-point correction=                    0.856930 (Hartree/Particle)  
Thermal correction to Energy=            0.919264  
Thermal correction to Enthalpy=         0.920209  
Thermal correction to Gibbs Free Energy=    0.750267  
Sum of electronic and zero-point Energies=    -3157.140332  
Sum of electronic and thermal Energies=    -3157.077998  
Sum of electronic and thermal Enthalpies=   -3157.077054  
Sum of electronic and thermal Free Energies=   -3157.246995

.....  
Cartesian Coordinates

.....  
6        -8.494014   -3.744776   0.542899

6	-7.437961	-4.257404	1.291505
6	-6.383488	-3.425236	1.668944
6	-6.351852	-2.072469	1.298496
6	-7.424109	-1.572562	0.516525
6	-8.489010	-2.402314	0.155785
6	-5.223608	-1.213043	1.708213
7	-5.428913	0.065753	1.952006
7	-5.594144	1.167147	2.177221
8	-7.330478	-0.259071	0.148225
6	-8.339022	0.301569	-0.673962
26	0.968228	1.042243	-0.547985
7	0.296588	2.919680	-0.227454
6	1.010838	3.998814	0.214631
6	0.175669	5.196605	0.258943
6	-1.073259	4.803884	-0.172918
6	-0.970534	3.391354	-0.478331
6	2.361783	3.971188	0.547913
6	3.177943	2.850165	0.522894
7	2.764421	1.587298	0.180737
6	3.875854	0.794891	0.292696
6	5.035789	1.576847	0.708467
6	4.595988	2.861972	0.859676
6	-2.024893	2.624639	-0.962963
6	-1.995597	1.260679	-1.222047
7	-0.907906	0.452401	-1.004646
6	-1.347064	-0.831369	-1.231225
6	-2.745244	-0.846631	-1.601769
6	-3.153536	0.468350	-1.635365
6	3.900026	-0.576697	0.079216
6	2.806694	-1.364934	-0.260471
7	1.548439	-0.892509	-0.517948
6	0.787047	-2.003292	-0.795221
6	1.580847	-3.217460	-0.696427
6	2.847504	-2.818012	-0.360810
6	-0.560137	-1.975378	-1.128297
6	-3.841216	-1.688827	1.915704
8	-3.035213	-0.695373	2.329634
8	-3.485555	-2.842830	1.742780
1	-1.045784	-2.926578	-1.322329
1	-2.973188	3.126054	-1.110345
1	2.823692	4.908872	0.838919
1	4.847355	-1.081193	0.221347
1	-5.554394	-3.822013	2.240575
1	-7.430073	-5.301870	1.590160
1	-9.308072	-2.011550	-0.437162
1	-9.324504	-4.381595	0.249452
1	-8.026403	1.329795	-0.863476
1	-8.424519	-0.234927	-1.627936
1	-9.315252	0.301690	-0.170251
6	0.733427	0.381584	-3.835160



1	-0.334483	0.626371	-3.848227
1	1.126241	0.508679	-4.851929
1	0.843697	-0.672129	-3.556616
16	1.683129	1.485779	-2.716314
6	5.368054	4.079721	1.272284
1	6.422603	3.844574	1.451717
1	5.331520	4.863347	0.503697
1	4.969893	4.521915	2.196114
6	1.056643	-4.604934	-0.920991
1	0.186762	-4.818018	-0.285893
1	0.734409	-4.754901	-1.960689
1	1.816209	-5.364041	-0.704515
6	-3.538727	-2.081080	-1.913958
1	-3.112809	-2.631757	-2.763868
1	-3.562114	-2.769184	-1.059179
1	-4.573665	-1.837209	-2.172941
6	-2.320999	5.628325	-0.271166
1	-2.426601	6.109383	-1.254864
1	-3.219389	5.022309	-0.111306
1	-2.317316	6.428486	0.477998
6	0.629906	6.497886	0.727031
6	0.131153	7.708492	0.418230
1	1.478357	6.475231	1.412027
1	0.551185	8.610345	0.856311
1	-0.679839	7.845616	-0.289766
6	-4.485992	0.937686	-2.004027
6	-4.809196	2.073329	-2.645381
1	-5.301054	0.262315	-1.739864
1	-5.846435	2.311353	-2.869794
1	-4.061741	2.782283	-2.987877
6	4.051940	-3.677115	-0.097533
6	5.075028	-3.692107	-1.274685
1	3.735381	-4.708961	0.097246
1	4.580017	-3.333524	0.799565
1	4.578367	-4.022458	-2.190179
1	5.465103	-2.682962	-1.427040
6	6.421841	1.015932	0.875862
6	6.598629	0.082450	2.113055
1	7.147771	1.833542	0.947331
1	6.685271	0.454098	-0.026221
1	7.073259	0.600834	2.950183
1	5.607328	-0.238948	2.458255
6	6.227986	-4.610418	-0.963684
8	7.183976	-4.367275	-0.241548
8	6.098212	-5.828969	-1.536909
1	6.866200	-6.350016	-1.232704
6	7.379423	-1.196603	1.863951
8	8.198416	-1.681910	2.617237
8	7.001880	-1.780573	0.705939
1	7.383542	-2.682850	0.605660

6	-1.630764	-1.027384	2.502781
6	-0.914039	0.243052	2.917049
1	-1.247922	-1.420054	1.558452
1	-1.556840	-1.813747	3.261907
1	0.149424	0.026723	3.066778
1	-0.995317	1.006395	2.137828
1	-1.323678	0.642926	3.851646

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1CSS<sup>TS</sup>(B-C)<sub>FE(cys)</sub>

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3157.9434826  
Zero-point correction=                    0.854600 (Hartree/Particle)  
Thermal correction to Energy=            0.915669  
Thermal correction to Enthalpy=         0.916613  
Thermal correction to Gibbs Free Energy= 0.758012  
Sum of electronic and zero-point Energies= -3157.088883  
Sum of electronic and thermal Energies= -3157.027814  
Sum of electronic and thermal Enthalpies= -3157.026869  
Sum of electronic and thermal Free Energies= -3157.185470

.....  
Cartesian Coordinates

.....

6	-1.116458	-3.904761	3.579630
6	0.123264	-3.305319	3.391539
6	0.204088	-2.039493	2.808166
6	-0.931894	-1.331296	2.375245
6	-2.186219	-1.976393	2.562687
6	-2.269633	-3.234286	3.170433
6	-0.785454	0.002487	1.688843
7	-2.196565	0.937988	2.272336
7	-2.959660	1.697671	1.967862
8	-3.294295	-1.296679	2.157822
6	-4.574223	-1.868496	2.335337
26	-0.746642	0.128992	-0.478109
7	-2.228666	1.466195	-0.673831
6	-2.127989	2.831096	-0.686440
6	-3.436199	3.443475	-0.910199
6	-4.326118	2.401588	-1.050296
6	-3.552196	1.182793	-0.917017
6	-0.935984	3.544962	-0.600450
6	0.338531	2.991679	-0.532128
7	0.603763	1.655906	-0.439455
6	1.965400	1.534795	-0.494413
6	2.594953	2.848185	-0.598134
6	1.575925	3.761330	-0.615157
6	-4.086946	-0.092795	-1.059204
6	-3.384894	-1.293917	-0.998736
7	-2.058358	-1.398629	-0.700180
6	-1.776201	-2.739559	-0.657149
6	-2.967050	-3.522652	-0.906267

6	-3.980479	-2.622865	-1.163156
6	2.667632	0.338034	-0.444481
6	2.115391	-0.937062	-0.372973
7	0.781935	-1.219324	-0.392522
6	0.680525	-2.583194	-0.371321
6	1.998204	-3.196964	-0.287846
6	2.898757	-2.165316	-0.289961
6	-0.511011	-3.291576	-0.468520
6	0.316664	0.855469	2.278247
8	-0.067116	2.115444	2.594464
8	1.467053	0.483745	2.434362
1	-0.445342	-4.374820	-0.444064
1	-5.152042	-0.159683	-1.240908
1	-0.998024	4.625317	-0.680673
1	3.748041	0.402024	-0.464469
1	1.172647	-1.582921	2.665533
1	1.036034	-3.809778	3.698386
1	-3.237688	-3.699870	3.314492
1	-1.199973	-4.886997	4.039469
1	-5.277589	-1.146857	1.916407
1	-4.667726	-2.814909	1.789301
1	-4.801470	-2.032072	3.398855
6	-0.655132	-1.411546	-3.605357
1	-1.686851	-1.759497	-3.482474
1	-0.446213	-1.338625	-4.680123
1	0.015981	-2.166918	-3.180206
16	-0.382558	0.242067	-2.858635
6	1.651275	5.254555	-0.739554
1	2.689286	5.601778	-0.779065
1	1.150302	5.611107	-1.649582
1	1.168943	5.762019	0.107283
6	2.251674	-4.672894	-0.208838
1	1.713964	-5.127452	0.633950
1	1.920025	-5.194122	-1.117495
1	3.316795	-4.893830	-0.078875
6	-3.017514	-5.021188	-0.946031
1	-2.468174	-5.425124	-1.807932
1	-2.569155	-5.461383	-0.045990
1	-4.045915	-5.389962	-1.020058
6	-5.808860	2.471500	-1.255780
1	-6.083439	2.489823	-2.320813
1	-6.319272	1.611935	-0.807247
1	-6.219872	3.380747	-0.802270
6	-3.676201	4.879207	-0.925638
6	-4.671355	5.545185	-1.538238
1	-2.955343	5.475864	-0.365191
1	-4.752667	6.625726	-1.451257
1	-5.411583	5.051629	-2.159799
6	-5.346100	-2.973136	-1.537680
6	-6.200520	-2.294506	-2.323014

1	-5.693368	-3.933681	-1.150754
1	-7.196152	-2.682156	-2.523932
1	-5.932185	-1.362740	-2.810091
6	4.396309	-2.241146	-0.194120
6	5.118037	-2.063989	-1.565886
1	4.691098	-3.209926	0.227311
1	4.775193	-1.470983	0.487396
1	4.748943	-2.810425	-2.273587
1	4.908497	-1.066599	-1.958844
6	4.078439	3.070076	-0.713650
6	4.880599	2.741589	0.583317
1	4.280169	4.108598	-0.999151
1	4.464092	2.450537	-1.529739
1	5.118053	3.643627	1.153485
1	4.263130	2.105671	1.231301
6	6.607909	-2.214336	-1.403863
8	7.393582	-1.363250	-1.013099
8	7.042838	-3.463726	-1.690039
1	8.001491	-3.460666	-1.503818
6	6.176889	1.979341	0.371597
8	7.224829	2.191774	0.946539
8	6.009120	0.971106	-0.511618
1	6.793809	0.377557	-0.548251
6	0.976463	2.999199	3.040617
6	0.317382	4.320780	3.396484
1	1.707341	3.117595	2.235771
1	1.486415	2.550272	3.900104
1	1.074292	5.038978	3.733443
1	-0.196594	4.736431	2.524089
1	-0.417630	4.190094	4.198272

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ICSSC<sub>FE(cys)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3157.9878355  
Zero-point correction=                    0.853058 (Hartree/Particle)  
Thermal correction to Energy=            0.916866  
Thermal correction to Enthalpy=         0.917810  
Thermal correction to Gibbs Free Energy= 0.744867  
Sum of electronic and zero-point Energies= -3157.134778  
Sum of electronic and thermal Energies= -3157.070969  
Sum of electronic and thermal Enthalpies= -3157.070025  
Sum of electronic and thermal Free Energies= -3157.242968

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Cartesian Coordinates

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6	-0.449260	-3.323849	3.958499
6	0.705476	-2.628000	3.613153
6	0.628665	-1.555539	2.719766
6	-0.591110	-1.160085	2.153890
6	-1.759641	-1.854468	2.544965

6	-1.683933	-2.936327	3.428480
6	-0.643963	-0.011458	1.207332
7	-6.837001	0.537174	1.892212
7	-6.694932	1.376566	2.596871
8	-2.931081	-1.376193	2.029573
6	-4.117005	-2.109544	2.251072
26	-0.392349	-0.053503	-0.606763
7	-2.031398	1.088889	-0.986522
6	-2.108553	2.442772	-1.070363
6	-3.484209	2.865186	-1.335171
6	-4.229502	1.707119	-1.397052
6	-3.298357	0.613156	-1.192713
6	-1.024418	3.311539	-0.952868
6	0.294367	2.930556	-0.739157
7	0.721763	1.645161	-0.574969
6	2.074541	1.708106	-0.420657
6	2.534401	3.094328	-0.485989
6	1.419484	3.858067	-0.681853
6	-3.658736	-0.729036	-1.255595
6	-2.807252	-1.824528	-1.144972
7	-1.479540	-1.755721	-0.842559
6	-1.033978	-3.044857	-0.736516
6	-2.115859	-3.978871	-0.963098
6	-3.230646	-3.222659	-1.256088
6	2.918796	0.619306	-0.236856
6	2.546330	-0.722452	-0.234215
7	1.279804	-1.192156	-0.409595
6	1.359479	-2.555751	-0.347794
6	2.733032	-2.976948	-0.115176
6	3.477225	-1.829509	-0.038196
6	0.283779	-3.422696	-0.486021
6	-0.704809	1.266400	1.974841
8	-1.936152	1.820389	2.025298
8	0.268946	1.754300	2.523634
1	0.489196	-4.486009	-0.414594
1	-4.705875	-0.946646	-1.422802
1	-1.214680	4.371821	-1.079844
1	3.971795	0.832907	-0.106880
1	1.524456	-1.011668	2.441965
1	1.668535	-2.914783	4.028028
1	-2.582444	-3.471651	3.715702
1	-0.403711	-4.165448	4.646146
1	-4.895347	-1.594211	1.685945
1	-4.027912	-3.139646	1.881441
1	-4.392156	-2.129847	3.316544
6	0.264231	-1.670122	-3.667183
1	-0.606332	-2.316501	-3.506482
1	0.448143	-1.609763	-4.747017
1	1.133332	-2.146937	-3.198955
16	-0.012365	0.024088	-3.019564

6	1.309933	5.345560	-0.836497
1	2.290035	5.829129	-0.767316
1	0.873167	5.622781	-1.805320
1	0.671727	5.788907	-0.059877
6	3.179899	-4.402329	0.018659
1	2.630903	-4.923523	0.814013
1	3.015105	-4.969517	-0.907643
1	4.247124	-4.470776	0.255677
6	-1.980554	-5.472491	-0.947989
1	-1.384740	-5.836442	-1.796750
1	-1.483023	-5.822598	-0.034450
1	-2.955888	-5.966742	-1.005379
6	-5.706748	1.565062	-1.604748
1	-5.974046	1.488722	-2.669120
1	-6.100456	0.671200	-1.108771
1	-6.240276	2.434126	-1.202576
6	-3.905428	4.252808	-1.462981
6	-4.991129	4.736064	-2.094022
1	-3.251150	4.982472	-0.984681
1	-5.201632	5.802460	-2.097040
1	-5.680450	4.104521	-2.644816
6	-4.541538	-3.752023	-1.617360
6	-5.454985	-3.222357	-2.448805
1	-4.781473	-4.721221	-1.174896
1	-6.397937	-3.730725	-2.634003
1	-5.285431	-2.295535	-2.987231
6	4.949860	-1.695289	0.230138
6	5.794053	-1.400805	-1.047522
1	5.326171	-2.618558	0.687179
1	5.136589	-0.888120	0.947614
1	5.616140	-2.178241	-1.794522
1	5.496381	-0.434566	-1.461421
6	3.975916	3.516063	-0.410660
6	4.632483	3.340595	0.994289
1	4.072998	4.564171	-0.714717
1	4.550132	2.934645	-1.139670
1	4.667299	4.283555	1.545449
1	4.024636	2.644961	1.586579
6	7.262044	-1.347678	-0.711937
8	7.863756	-0.415200	-0.200278
8	7.904763	-2.506528	-0.987721
1	8.825893	-2.377213	-0.690079
6	6.037524	2.766119	0.973183
8	6.985182	3.174877	1.611980
8	6.101481	1.680377	0.170055
1	6.972227	1.226191	0.225919
6	-2.023331	3.081541	2.714037
6	-3.482829	3.501188	2.708956
1	-1.390986	3.809273	2.194242
1	-1.632151	2.966599	3.731030

1	-3.597877	4.467723	3.214678
1	-3.852191	3.596055	1.683187
1	-4.103399	2.763573	3.228725

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**1CSS<sup>†</sup>TS(C-P)<sub>FE(cys)</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-3048.4332305  
 Zero-point correction=                    0.843437 (Hartree/Particle)  
 Thermal correction to Energy=            0.901734  
 Thermal correction to Enthalpy=         0.902678  
 Thermal correction to Gibbs Free Energy= 0.749035  
 Sum of electronic and zero-point Energies= -3047.589793  
 Sum of electronic and thermal Energies= -3047.531496  
 Sum of electronic and thermal Enthalpies= -3047.530552  
 Sum of electronic and thermal Free Energies= -3047.684195

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 Cartesian Coordinates  
 .....

6	-1.938763	3.926205	3.301445
6	-2.945945	3.112027	2.785532
6	-2.644278	1.863151	2.231777
6	-1.323461	1.399815	2.186110
6	-0.335859	2.238519	2.734800
6	-0.612365	3.481647	3.282433
6	-0.918817	0.082591	1.628826
8	0.979169	1.791091	2.682877
6	1.071628	0.427423	2.662150
26	-0.727132	-0.235785	-0.538944
7	-2.430941	0.822431	-0.808499
6	-2.553283	2.167897	-0.972206
6	-3.957274	2.543676	-1.140942
6	-4.675217	1.369001	-1.057718
6	-3.701711	0.310694	-0.862363
6	-1.485234	3.065400	-0.980174
6	-0.143267	2.739230	-0.837462
7	0.349989	1.472138	-0.672423
6	1.710598	1.596524	-0.645382
6	2.104910	2.998312	-0.765125
6	0.941508	3.710301	-0.882236
6	-4.027537	-1.039965	-0.769584
6	-3.138147	-2.100511	-0.640163
7	-1.789623	-1.969731	-0.463159
6	-1.292931	-3.237829	-0.331914
6	-2.358977	-4.217134	-0.398220
6	-3.521662	-3.513331	-0.619896
6	2.602101	0.534449	-0.512698
6	2.267235	-0.809198	-0.354267
7	0.993692	-1.301180	-0.317654
6	1.115124	-2.660711	-0.192637
6	2.515543	-3.045927	-0.103533

6	3.238494	-1.886484	-0.195290
6	0.057031	-3.559739	-0.186989
6	-1.495870	-1.072863	2.353665
8	-0.575172	-2.010363	2.710111
8	-2.683154	-1.189908	2.600918
1	0.304700	-4.613698	-0.101255
1	-5.078715	-1.295011	-0.815012
1	-1.718772	4.114091	-1.129648
1	3.656736	0.773203	-0.549469
1	-3.429831	1.236935	1.829206
1	-3.980225	3.445351	2.805087
1	0.199457	4.074436	3.692743
1	-2.176497	4.896963	3.729046
1	0.770295	-0.090828	3.572919
1	0.279193	-0.005017	1.575530
1	2.003967	0.096998	2.207691
6	-0.468994	0.937862	-3.783302
1	0.450338	1.469783	-3.512446
1	-0.439339	0.731605	-4.860680
1	-1.318936	1.601370	-3.587990
16	-0.631497	-0.658917	-2.892091
6	0.745931	5.190542	-1.026669
1	1.699768	5.728256	-1.037104
1	0.218586	5.441633	-1.956877
1	0.148027	5.599243	-0.200906
6	3.013016	-4.452730	0.050590
1	2.761375	-5.069422	-0.823083
1	4.101590	-4.485694	0.168952
1	2.573498	-4.949863	0.926028
6	-2.173391	-5.704251	-0.329815
1	-1.688247	-6.095894	-1.235080
1	-1.544639	-5.998668	0.520668
1	-3.131528	-6.224742	-0.228507
6	-6.161549	1.185216	-1.114418
1	-6.524102	1.029875	-2.141353
1	-6.483772	0.319851	-0.525186
1	-6.677122	2.069937	-0.723128
6	-4.427758	3.910922	-1.305556
6	-5.570792	4.330139	-1.878175
1	-3.764538	4.680377	-0.908769
1	-5.817080	5.388290	-1.916277
1	-6.276939	3.650896	-2.344897
6	-4.844474	-4.099438	-0.811088
6	-5.837815	-3.664912	-1.604365
1	-5.020962	-5.024944	-0.258773
1	-6.781973	-4.201419	-1.657296
1	-5.735650	-2.790295	-2.238770
6	4.726434	-1.709134	-0.107005
6	5.402062	-1.462057	-1.488784
1	5.179692	-2.602468	0.340185



1	4.975212	-0.870605	0.554239
1	5.215962	-2.304457	-2.158753
1	4.978214	-0.560732	-1.942204
6	3.509505	3.538377	-0.758784
6	4.274705	3.413248	0.595468
1	3.468041	4.600577	-1.021867
1	4.114218	3.063331	-1.539659
1	4.921922	4.293696	0.716124
1	3.583203	3.390985	1.440737
6	6.881700	-1.252670	-1.318633
8	7.415501	-0.295951	-0.774993
8	7.628416	-2.274847	-1.790409
1	8.556218	-2.042894	-1.591434
6	5.190358	2.209012	0.719625
8	5.266084	1.483588	1.693337
8	5.950629	2.042550	-0.382530
1	6.489840	1.218445	-0.296114
6	-1.109627	-3.211346	3.294927
6	0.067985	-4.080530	3.699984
1	-1.745091	-3.707876	2.555275
1	-1.736883	-2.946227	4.152987
1	-0.290683	-5.015327	4.147232
1	0.681372	-4.322381	2.826542
1	0.700618	-3.567962	4.433372

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$10SS A_{FE(cys)}$

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2396.4796783  
Zero-point correction=                    0.634414 (Hartree/Particle)  
Thermal correction to Energy=            0.679736  
Thermal correction to Enthalpy=         0.680680  
Thermal correction to Gibbs Free Energy=    0.550487  
Sum of electronic and zero-point Energies=    -2395.845264  
Sum of electronic and thermal Energies=    -2395.799942  
Sum of electronic and thermal Enthalpies=   -2395.798998  
Sum of electronic and thermal Free Energies=   -2395.929191

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Cartesian Coordinates

.....  

26	1.046559	-0.070834	-0.014089
7	2.405117	-1.524452	-0.383912
6	2.153020	-2.861318	-0.570873
6	3.383112	-3.604053	-0.734873
6	4.406489	-2.684087	-0.677240
6	3.768683	-1.390551	-0.429484
6	0.886021	-3.437914	-0.614472
6	-0.319231	-2.760674	-0.502382
7	-0.444874	-1.405405	-0.317660
6	-1.791937	-1.162585	-0.270549
6	-2.547536	-2.399871	-0.415633

6	-1.623863	-3.399291	-0.564041
6	-2.367495	0.096619	-0.136499
6	-1.678594	1.299541	-0.036147
7	-0.315018	1.420993	-0.011226
6	-0.066294	2.763293	0.122426
6	-1.308769	3.520544	0.171549
6	-2.319487	2.605133	0.070028
6	1.193652	3.338404	0.205037
6	2.406292	2.659104	0.134146
6	3.717517	3.294101	0.235975
6	4.640994	2.274353	0.135389
6	3.879931	1.052778	-0.026639
7	2.529684	1.307244	-0.021416
6	4.451879	-0.202241	-0.207268
1	0.838245	-4.513302	-0.757049
1	5.532048	-0.263232	-0.168500
1	1.232015	4.413579	0.345234
1	-3.452315	0.145525	-0.124076
16	1.133827	-0.218675	2.359200
6	0.596156	-1.916161	2.811259
1	1.214389	-2.681923	2.329485
1	0.696487	-2.032945	3.897828
1	-0.450964	-2.102230	2.544815
6	-1.402200	5.011602	0.305231
1	-0.861337	5.372228	1.190047
1	-0.971747	5.529961	-0.563130
1	-2.442194	5.341770	0.400598
6	-1.854219	-4.869916	-0.750347
1	-1.348317	-5.249999	-1.647974
1	-1.473918	-5.454265	0.099021
1	-2.920202	-5.099630	-0.853624
6	3.471402	-5.080711	-0.982104
1	2.906297	-5.649823	-0.232526
1	3.063927	-5.356472	-1.965199
1	4.507451	-5.433134	-0.953263
6	6.135867	2.378684	0.130364
1	6.559764	2.316928	1.143339
1	6.595931	1.577370	-0.458009
1	6.457904	3.336504	-0.294763
6	5.823762	-2.981327	-0.853512
6	6.778092	-2.206641	-1.397039
1	6.125899	-3.978231	-0.526461
1	7.804600	-2.557146	-1.468928
1	6.569201	-1.222131	-1.803398
6	3.928431	4.728129	0.366999
6	4.994453	5.364403	0.885280
1	3.115612	5.353255	-0.004628
1	5.036647	6.450435	0.905751
1	5.834651	4.838186	1.326577
6	-4.044583	-2.516279	-0.360503

6	-4.582874	-2.488413	1.081138
1	-4.375001	-3.444787	-0.839371
1	-4.520381	-1.707229	-0.928116
1	-4.140615	-3.297957	1.676150
1	-4.286608	-1.564432	1.592820
6	-3.800541	2.853896	0.021143
6	-4.354522	2.822329	-1.414455
1	-4.040523	3.825219	0.467218
1	-4.340211	2.112566	0.623008
1	-3.844109	3.565025	-2.041899
1	-4.152371	1.855812	-1.892043
6	-6.085978	-2.615831	1.160012
8	-6.851452	-2.751374	0.228447
8	-6.528871	-2.566280	2.445883
1	-7.499548	-2.647917	2.389471
6	-5.839263	3.090265	-1.492760
8	-6.576035	3.367489	-0.570235
8	-6.301060	2.993314	-2.770407
1	-7.257717	3.177169	-2.714259

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**10SSB<sub>FE(cys)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3158.0010275  
Zero-point correction=                    0.857468 (Hartree/Particle)  
Thermal correction to Energy=            0.919478  
Thermal correction to Enthalpy=         0.920423  
Thermal correction to Gibbs Free Energy= 0.753189  
Sum of electronic and zero-point Energies= -3157.143560  
Sum of electronic and thermal Energies= -3157.081549  
Sum of electronic and thermal Enthalpies= -3157.080605  
Sum of electronic and thermal Free Energies= -3157.247839

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Cartesian Coordinates

6	-4.997299	5.224751	-0.691243
6	-3.808803	5.862274	-1.039352
6	-2.785726	5.138068	-1.653492
6	-2.923383	3.768776	-1.921032
6	-4.135827	3.130576	-1.553150
6	-5.163384	3.861388	-0.948577
6	-1.815666	3.009053	-2.531655
7	-2.075101	1.986723	-3.322691
7	-2.277159	1.119139	-4.028042
8	-4.212734	1.800283	-1.828497
6	-5.283453	1.037751	-1.287819
26	-0.248941	-1.336464	0.689116
7	-1.394980	-2.871374	0.068568
6	-1.002998	-3.976954	-0.633801
6	-2.129098	-4.880615	-0.857585
6	-3.216778	-4.286750	-0.253882

6	-2.735122	-3.046022	0.319675
6	0.304233	-4.237521	-1.032124
6	1.400904	-3.420457	-0.796237
7	1.352753	-2.199927	-0.173150
6	2.649793	-1.760154	-0.121191
6	3.555978	-2.734892	-0.719620
6	2.767363	-3.765525	-1.157098
6	-3.536071	-2.155679	1.027277
6	-3.146588	-0.910805	1.506627
7	-1.902148	-0.368386	1.315437
6	-1.991853	0.936602	1.736131
6	-3.317607	1.233975	2.228289
6	-4.042432	0.063010	2.133157
6	3.038295	-0.521700	0.372075
6	2.179367	0.479799	0.813989
7	0.827461	0.337682	0.970738
6	0.368938	1.571418	1.371695
6	1.455878	2.534572	1.438868
6	2.593388	1.847374	1.106128
6	-0.942768	1.851988	1.723285
6	-0.385642	3.278073	-2.297523
8	0.387062	2.351295	-2.897710
8	0.043322	4.221054	-1.653366
1	-1.165518	2.865115	2.042541
1	-4.574458	-2.429653	1.165316
1	0.492685	-5.177867	-1.539458
1	4.096525	-0.293130	0.354916
1	-1.850845	5.621550	-1.907338
1	-3.671082	6.920791	-0.836571
1	-6.086189	3.367195	-0.666808
1	-5.801983	5.779068	-0.214726
1	-5.059168	-0.000696	-1.534921
1	-5.329789	1.142256	-0.198871
1	-6.244544	1.324867	-1.736544
6	-0.251899	-1.142666	4.036852
1	-1.340061	-1.021819	4.080232
1	0.087570	-1.533820	5.004242
1	0.200673	-0.156045	3.889514
16	0.260775	-2.327364	2.730179
6	3.166025	-5.032162	-1.855153
1	4.250314	-5.095666	-1.994236
1	2.854678	-5.921048	-1.290436
1	2.705504	-5.110353	-2.849777
6	1.288930	3.989697	1.760619
1	0.693624	4.492845	0.988082
1	0.778430	4.138241	2.721360
1	2.254352	4.503457	1.822545
6	-3.748575	2.559248	2.783962
1	-3.161537	2.835802	3.670252
1	-3.622027	3.365444	2.049654

1	-4.800775	2.548718	3.085732
6	-4.635386	-4.769332	-0.222246
1	-4.838855	-5.410256	0.648393
1	-5.345334	-3.935957	-0.179829
1	-4.864367	-5.361115	-1.116116
6	-2.048711	-6.119492	-1.617295
6	-2.843380	-7.200974	-1.523753
1	-1.242119	-6.162873	-2.350256
1	-2.689515	-8.060857	-2.170758
1	-3.643474	-7.279753	-0.794736
6	-5.415197	-0.123557	2.587847
6	-6.009219	-1.252764	3.012713
1	-6.015781	0.787884	2.617691
1	-7.047453	-1.245573	3.334906
1	-5.482426	-2.198657	3.084670
6	3.995029	2.374385	0.997339
6	4.900581	1.937885	2.189015
1	3.977677	3.470077	0.963270
1	4.466025	2.040821	0.065095
1	4.483321	2.302410	3.130484
1	4.946494	0.845505	2.229346
6	5.056815	-2.643929	-0.796480
6	5.641580	-1.657034	-1.853142
1	5.444015	-3.641188	-1.031175
1	5.476871	-2.385982	0.182019
1	6.596617	-2.063314	-2.215702
1	4.977523	-1.556776	-2.714522
6	6.297184	2.463201	2.005681
8	7.115734	2.064030	1.188579
8	6.592085	3.502319	2.815599
1	7.496007	3.783276	2.574520
6	5.959025	-0.263644	-1.343991
8	5.657408	0.775442	-1.903896
8	6.661337	-0.298898	-0.196107
1	6.817068	0.623008	0.130558
6	1.814427	2.431617	-2.656845
6	2.448178	1.213479	-3.300219
1	1.981982	2.455227	-1.577266
1	2.186594	3.370033	-3.083408
1	3.526663	1.212645	-3.112286
1	2.029559	0.297905	-2.870345
1	2.272825	1.204977	-4.382267

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<sup>1</sup>OSS<sup>TS(B-C)</sup>FE(cys)  
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Number of imaginary frequencies: 1	Electronic energy:	HF=-3157.9482728
Zero-point correction=	0.854026 (Hartree/Particle)	
Thermal correction to Energy=	0.915286	
Thermal correction to Enthalpy=	0.916230	
Thermal correction to Gibbs Free Energy=	0.756723	

Sum of electronic and zero-point Energies=	-3157.094247
Sum of electronic and thermal Energies=	-3157.032987
Sum of electronic and thermal Enthalpies=	-3157.032043
Sum of electronic and thermal Free Energies=	-3157.191550

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Cartesian Coordinates  
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6	-1.101709	-3.901807	3.525309
6	0.128579	-3.271712	3.379222
6	0.198052	-1.993409	2.820052
6	-0.937409	-1.287704	2.376834
6	-2.182285	-1.971193	2.515919
6	-2.255370	-3.243354	3.094578
6	-0.850239	0.089872	1.787358
7	-2.217754	0.909494	2.447753
7	-2.759588	1.857481	2.096535
8	-3.298984	-1.333686	2.053758
6	-4.572064	-1.863938	2.340470
26	-0.743312	0.116923	-0.568779
7	-2.227827	1.455699	-0.717626
6	-2.136768	2.818789	-0.675500
6	-3.454820	3.424768	-0.823378
6	-4.340891	2.381370	-0.967315
6	-3.552775	1.165760	-0.911322
6	-0.949922	3.540455	-0.625140
6	0.322906	2.985787	-0.603629
7	0.588383	1.648781	-0.526543
6	1.948654	1.524526	-0.587140
6	2.576627	2.836046	-0.697827
6	1.558874	3.750871	-0.700939
6	-4.087447	-0.107133	-1.072075
6	-3.379466	-1.303617	-1.033382
7	-2.049909	-1.412771	-0.748489
6	-1.776230	-2.755578	-0.672439
6	-2.971540	-3.532373	-0.903939
6	-3.978781	-2.630597	-1.175719
6	2.651648	0.330712	-0.517267
6	2.097180	-0.938890	-0.403774
7	0.762839	-1.227869	-0.430603
6	0.664340	-2.591386	-0.356323
6	1.979159	-3.192595	-0.226568
6	2.878355	-2.158768	-0.259729
6	-0.520236	-3.309114	-0.455464
6	0.302821	0.905358	2.258250
8	-0.013205	2.209173	2.506053
8	1.455113	0.515732	2.417018
1	-0.456360	-4.389953	-0.390603
1	-5.156534	-0.176500	-1.224592
1	-1.019846	4.621650	-0.672324
1	3.731799	0.394094	-0.531571

1	1.159074	-1.509481	2.723028
1	1.043675	-3.760251	3.707329
1	-3.217249	-3.733165	3.197551
1	-1.178366	-4.892931	3.967822
1	-5.289079	-1.140973	1.945768
1	-4.735214	-2.830640	1.844144
1	-4.728682	-1.983369	3.422773
6	-0.494440	-1.475021	-3.581943
1	-1.464234	-1.958490	-3.428659
1	-0.310398	-1.399457	-4.660341
1	0.284631	-2.104438	-3.140155
16	-0.460003	0.222457	-2.895135
6	1.635466	5.245291	-0.806296
1	2.672809	5.588316	-0.879805
1	1.101767	5.617546	-1.690795
1	1.188741	5.739387	0.067079
6	2.232214	-4.661539	-0.063456
1	1.695919	-5.060707	0.807255
1	1.897097	-5.234615	-0.938773
1	3.297383	-4.874966	0.075903
6	-3.034636	-5.030738	-0.895602
1	-2.459392	-5.469030	-1.722856
1	-2.622420	-5.440355	0.035420
1	-4.063432	-5.392063	-0.992533
6	-5.831875	2.442503	-1.101361
1	-6.157601	2.456934	-2.151906
1	-6.313309	1.580697	-0.626289
1	-6.223823	3.349873	-0.628862
6	-3.706791	4.858634	-0.770349
6	-4.710687	5.536167	-1.353221
1	-2.992237	5.434765	-0.181762
1	-4.809341	6.610260	-1.218486
1	-5.444912	5.057601	-1.993810
6	-5.350216	-2.973443	-1.537053
6	-6.191605	-2.299659	-2.339556
1	-5.710806	-3.917902	-1.124849
1	-7.194124	-2.673261	-2.532037
1	-5.906233	-1.382884	-2.845472
6	4.373484	-2.226939	-0.125322
6	5.128106	-2.118837	-1.486061
1	4.656980	-3.172764	0.351458
1	4.733826	-1.423385	0.526458
1	4.775975	-2.900854	-2.163683
1	4.930895	-1.142558	-1.934440
6	4.060508	3.055673	-0.807888
6	4.850303	2.756101	0.503997
1	4.263324	4.087878	-1.114271
1	4.453365	2.418765	-1.606917
1	5.079608	3.671085	1.056125
1	4.228705	2.132444	1.159890

6	6.613964	-2.261378	-1.281201
8	7.394406	-1.385553	-0.938910
8	7.047337	-3.529986	-1.465145
1	8.001370	-3.519019	-1.256735
6	6.150753	1.995473	0.315816
8	7.199376	2.233741	0.878222
8	5.987068	0.956083	-0.533098
1	6.777366	0.369227	-0.551340
6	1.061905	3.044447	2.945608
6	0.460380	4.393961	3.304932
1	1.802739	3.138444	2.145032
1	1.559236	2.580637	3.805097
1	1.245720	5.081387	3.642620
1	-0.040991	4.833303	2.436436
1	-0.279591	4.289631	4.105737

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<sup>10</sup>SSC<sub>FE(cys)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3157.9938429  
Zero-point correction=                    0.851169 (Hartree/Particle)  
Thermal correction to Energy=            0.915724  
Thermal correction to Enthalpy=         0.916668  
Thermal correction to Gibbs Free Energy= 0.739810  
Sum of electronic and zero-point Energies= -3157.142674  
Sum of electronic and thermal Energies= -3157.078119  
Sum of electronic and thermal Enthalpies= -3157.077175  
Sum of electronic and thermal Free Energies= -3157.254033

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Cartesian Coordinates

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6	-0.281875	-3.397592	3.961246
6	0.848998	-2.687210	3.569846
6	0.718028	-1.605908	2.694061
6	-0.527932	-1.207319	2.186309
6	-1.668984	-1.920806	2.628507
6	-1.542892	-3.012484	3.495115
6	-0.629888	-0.058449	1.251582
8	-2.875196	-1.453866	2.179404
6	-4.042435	-2.162067	2.534696
26	-0.405643	-0.145949	-0.689545
7	-1.914563	1.158393	-1.054327
6	-1.841693	2.512207	-1.170604
6	-3.150058	3.071596	-1.501167
6	-4.013734	1.997628	-1.570739
6	-3.220234	0.817882	-1.288608
6	-0.677396	3.263291	-1.017237
6	0.584911	2.748016	-0.757559
7	0.882383	1.418352	-0.634797
6	2.223702	1.345907	-0.401579
6	2.806830	2.682260	-0.356731



6	1.782235	3.557792	-0.587253
6	-3.738077	-0.474286	-1.265450
6	-3.031781	-1.647212	-1.030111
7	-1.684512	-1.721731	-0.827537
6	-1.369906	-3.048774	-0.762988
6	-2.555839	-3.862629	-0.917079
6	-3.614002	-2.991308	-1.062004
6	2.955880	0.169723	-0.268240
6	2.451080	-1.125490	-0.340696
7	1.135021	-1.452683	-0.473914
6	1.075412	-2.818134	-0.478113
6	2.408032	-3.388302	-0.346543
6	3.270945	-2.330973	-0.262099
6	-0.085631	-3.565374	-0.600637
6	-0.584326	1.236376	1.967235
8	-1.762888	1.916342	1.949115
8	0.404637	1.678084	2.534499
1	0.014419	-4.645646	-0.581168
1	-4.786936	-0.582451	-1.507785
1	-0.753809	4.338544	-1.136422
1	4.026224	0.272204	-0.120183
1	1.594839	-1.048623	2.383969
1	1.833335	-2.970165	3.935090
1	-2.421114	-3.560003	3.819611
1	-0.197731	-4.247618	4.635083
1	-4.869417	-1.639902	2.050879
1	-4.016895	-3.197954	2.170804
1	-4.202986	-2.166284	3.623714
16	-0.059951	-0.419466	-3.057321
6	-0.046776	1.218356	-3.880058
1	-1.002651	1.740575	-3.761484
1	0.746524	1.862426	-3.484968
1	0.132431	1.068749	-4.951551
6	1.821462	5.055918	-0.646923
1	1.388541	5.436426	-1.581441
1	1.255046	5.512482	0.176536
1	2.848032	5.432060	-0.584902
6	2.713424	-4.856248	-0.320639
1	2.150140	-5.370239	0.469171
1	2.452634	-5.344159	-1.269770
1	3.777363	-5.041368	-0.138599
6	-5.487992	2.013704	-1.838867
1	-5.716831	1.940253	-2.912133
1	-5.998177	1.180658	-1.344124
1	-5.937875	2.945836	-1.477913
6	-2.577240	-5.361560	-0.874803
1	-1.872101	-5.794844	-1.595838
1	-2.295394	-5.742945	0.116413
1	-3.571075	-5.758906	-1.103852
6	-5.010743	-3.382344	-1.217403

6	-6.120997	-2.722702	-0.843385
1	-5.156577	-4.362799	-1.674472
1	-7.104358	-3.148035	-1.027415
1	-6.094837	-1.763786	-0.336234
6	-3.414573	4.492575	-1.676934
6	-4.410042	5.070263	-2.373538
1	-2.712163	5.161389	-1.178481
1	-4.507093	6.152295	-2.407884
1	-5.134411	4.500289	-2.946124
6	4.770085	-2.356853	-0.168979
6	5.446227	-2.110766	-1.529637
1	5.112067	-3.320919	0.223019
1	5.130288	-1.605121	0.544063
1	5.116067	-2.855248	-2.265861
1	5.145220	-1.143230	-1.949152
6	4.243646	2.991851	-0.048135
6	4.544713	2.907338	1.459102
1	4.504335	3.995075	-0.402460
1	4.915033	2.307998	-0.581726
1	3.890322	3.584928	2.022691
1	4.318180	1.908666	1.851055
6	6.954594	-2.156528	-1.462970
8	7.629093	-2.413622	-0.487841
8	7.520842	-1.873624	-2.667784
1	8.483986	-1.924793	-2.520075
6	5.976553	3.246019	1.799052
8	6.835164	3.620696	1.027663
8	6.230219	3.091341	3.127103
1	7.169338	3.330459	3.240810
6	-1.746554	3.201104	2.589369
6	-3.158588	3.759193	2.530924
1	-1.035109	3.850635	2.066648
1	-1.393844	3.090537	3.621151
1	-3.193881	4.748261	3.004499
1	-3.492488	3.856187	1.493043
1	-3.859997	3.100510	3.053923
7	-6.213498	1.475577	2.399824
7	-6.391265	0.729927	1.603877

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**<sup>10</sup>SS<sup>TS(C-D)</sup>FE(cys)**

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Number of imaginary frequencies: 1	Electronic energy:	HF=-3048.4458203
Zero-point correction=	0.841674 (Hartree/Particle)	
Thermal correction to Energy=	0.900087	
Thermal correction to Enthalpy=	0.901031	
Thermal correction to Gibbs Free Energy=	0.747483	
Sum of electronic and zero-point Energies=	-3047.604146	
Sum of electronic and thermal Energies=	-3047.545734	
Sum of electronic and thermal Enthalpies=	-3047.544789	
Sum of electronic and thermal Free Energies=	-3047.698337	

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 Cartesian Coordinates  
 .....

6	2.718403	1.244630	3.721561
6	1.876185	2.221947	3.186037
6	0.709210	1.854609	2.513804
6	0.334372	0.508037	2.354635
6	1.178159	-0.453909	2.961181
6	2.355974	-0.097535	3.617856
6	-0.885466	0.071083	1.614308
8	0.886539	-1.805247	2.915722
6	-0.473148	-2.112049	2.872328
26	-0.835891	-0.102019	-0.499864
7	-2.492632	1.062097	-0.693811
6	-2.509197	2.419555	-0.795351
6	-3.878350	2.906130	-0.940147
6	-4.683922	1.787230	-0.925729
6	-3.796682	0.651144	-0.778853
6	-1.382208	3.236773	-0.812939
6	-0.060498	2.816360	-0.757018
7	0.360775	1.522919	-0.625503
6	1.725772	1.560978	-0.634783
6	2.202360	2.931600	-0.784424
6	1.081805	3.715567	-0.850789
6	-4.219541	-0.674741	-0.754662
6	-3.396288	-1.788723	-0.650187
7	-2.040903	-1.743760	-0.483286
6	-1.615710	-3.040839	-0.394663
6	-2.738234	-3.951204	-0.472239
6	-3.859504	-3.175234	-0.663716
6	2.547713	0.448070	-0.505668
6	2.114477	-0.865274	-0.367272
7	0.810381	-1.268835	-0.376891
6	0.829111	-2.632691	-0.274375
6	2.196993	-3.117310	-0.168498
6	3.000926	-2.010837	-0.220848
6	-0.290116	-3.455074	-0.278602
6	-2.126841	0.673543	2.147422
8	-3.121863	-0.255593	2.316025
8	-2.307810	1.846530	2.441768
1	-0.115060	-4.523870	-0.205904
1	-5.283948	-0.856805	-0.825662
1	-1.548133	4.302693	-0.922090
1	3.615640	0.615520	-0.525632
1	0.058174	2.613419	2.098037
1	2.126631	3.275928	3.287588
1	2.966199	-0.886550	4.048480
1	3.642969	1.519882	4.222205
1	-1.009914	-1.887322	3.801120
1	-0.945940	-1.168911	1.951833

1	-0.622575	-3.114455	2.479770
6	0.824862	-0.227200	-3.534757
1	1.425417	-1.052587	-3.137247
1	0.774526	-0.329570	-4.625376
1	1.333887	0.713786	-3.299487
16	-0.884584	-0.255496	-2.876994
6	0.975188	5.204243	-1.002407
1	1.960760	5.679511	-1.034674
1	0.445781	5.482358	-1.923532
1	0.422076	5.655330	-0.167802
6	2.587191	-4.556591	-0.011528
1	2.275872	-5.160252	-0.874889
1	3.671440	-4.670579	0.091870
1	2.123476	-5.004911	0.876906
6	-2.641186	-5.446966	-0.424054
1	-2.067044	-5.788831	0.446908
1	-3.630821	-5.912055	-0.372104
1	-2.141122	-5.850958	-1.315299
6	-6.179100	1.719719	-1.006424
1	-6.537609	1.644835	-2.043570
1	-6.574996	0.852966	-0.466091
1	-6.630544	2.620432	-0.575045
6	-4.245585	4.312366	-1.030021
6	-5.338612	4.841144	-1.607509
1	-3.545052	5.006628	-0.565363
1	-5.514338	5.913602	-1.586445
1	-6.072186	4.239635	-2.134876
6	-5.219058	-3.677005	-0.845350
6	-6.195413	-3.169695	-1.616002
1	-5.443404	-4.599157	-0.305482
1	-7.170727	-3.647501	-1.663164
1	-6.050554	-2.292346	-2.238303
6	4.496701	-1.938233	-0.112055
6	5.198077	-1.759739	-1.494126
1	4.880841	-2.854272	0.351401
1	4.793315	-1.108473	0.540483
1	4.937825	-2.597349	-2.146809
1	4.862315	-0.830460	-1.960516
6	3.639191	3.371845	-0.894436
6	4.515766	3.176094	0.377930
1	3.647083	4.436004	-1.152232
1	4.126859	2.862199	-1.732517
1	5.153613	4.061679	0.513244
1	3.902892	3.085767	1.277910
6	6.690932	-1.694166	-1.323802
8	7.351496	-0.694605	-1.081632
8	7.285929	-2.904406	-1.410372
1	8.232406	-2.752414	-1.224050
6	5.471098	1.993656	0.376688
8	5.806144	1.381979	1.372231

8	5.954064	1.709776	-0.852354
1	6.532958	0.909690	-0.790825
6	-4.373996	0.253598	2.789125
6	-5.299393	-0.934690	2.996565
1	-4.780100	0.956227	2.053083
1	-4.214703	0.810461	3.719845
1	-6.278256	-0.594922	3.357169
1	-5.441924	-1.480913	2.058778
1	-4.881358	-1.628351	3.734834

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<sup>10</sup>SSD<sub>FE(cys)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3048.4689254  
Zero-point correction=                    0.844887 (Hartree/Particle)  
Thermal correction to Energy=            0.904580  
Thermal correction to Enthalpy=         0.905525  
Thermal correction to Gibbs Free Energy= 0.748845  
Sum of electronic and zero-point Energies= -3047.624038  
Sum of electronic and thermal Energies= -3047.564345  
Sum of electronic and thermal Enthalpies= -3047.563401  
Sum of electronic and thermal Free Energies= -3047.720080

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Cartesian Coordinates

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6	2.148832	2.768425	3.322634
6	0.900342	3.261755	2.937807
6	-0.071397	2.403929	2.426038
6	0.141526	1.014601	2.294411
6	1.400646	0.544447	2.743872
6	2.397056	1.398761	3.219858
6	-0.874201	0.078990	1.764808
8	1.628499	-0.823304	2.667983
6	2.343247	-1.456802	3.631616
26	-0.840648	-0.083546	-0.554688
7	-2.421936	1.158325	-0.756771
6	-2.410532	2.515755	-0.851727
6	-3.767846	3.033090	-0.994400
6	-4.596071	1.933042	-0.990615
6	-3.733897	0.775410	-0.847307
6	-1.262200	3.300073	-0.898852
6	0.039172	2.818620	-0.874638
7	0.390884	1.506773	-0.737271
6	1.753494	1.465132	-0.822357
6	2.296776	2.806908	-1.012548
6	1.221325	3.652147	-1.032909
6	-4.196527	-0.535513	-0.809913
6	-3.421728	-1.677107	-0.625664
7	-2.074536	-1.679219	-0.408215
6	-1.727684	-2.969872	-0.111388
6	-2.890023	-3.827780	-0.133148

6	-3.955014	-3.032956	-0.502173
6	2.525641	0.317417	-0.702517
6	2.053644	-0.964034	-0.433568
7	0.740403	-1.316834	-0.336570
6	0.719852	-2.650189	-0.025788
6	2.071969	-3.166526	0.093665
6	2.908003	-2.112599	-0.165157
6	-0.428144	-3.418495	0.111467
6	-2.255484	0.331626	2.188593
8	-2.917247	-0.850132	2.459835
8	-2.830587	1.404043	2.335411
1	-0.299743	-4.468243	0.354696
1	-5.265597	-0.682641	-0.892282
1	-1.391265	4.370070	-1.017037
1	3.597255	0.436590	-0.791115
1	-1.037345	2.791444	2.130057
1	0.682447	4.324628	3.023558
1	3.373510	0.995560	3.468869
1	2.924247	3.433111	3.697132
1	2.743514	-0.879955	4.457695
1	-0.606410	-0.957896	1.933750
1	2.794385	-2.383352	3.299789
6	-0.590718	-2.047176	-3.321601
1	-1.454814	-2.630441	-2.986895
1	-0.515094	-2.133678	-4.411955
1	0.312428	-2.476832	-2.875651
16	-0.768104	-0.272368	-2.901214
6	1.190137	5.144286	-1.178152
1	2.193013	5.557832	-1.325135
1	0.576941	5.457096	-2.033567
1	0.766453	5.624861	-0.286001
6	2.419040	-4.584438	0.439590
1	2.081658	-5.287408	-0.334519
1	3.500115	-4.719491	0.551117
1	1.949236	-4.897945	1.380946
6	-2.875285	-5.305687	0.122017
1	-2.346919	-5.547892	1.052705
1	-3.889406	-5.710050	0.202547
1	-2.371912	-5.855558	-0.685655
6	-6.092167	1.900290	-1.061964
1	-6.459279	1.814878	-2.095323
1	-6.504061	1.053915	-0.501960
1	-6.517402	2.819161	-0.643221
6	-4.100688	4.448702	-1.075086
6	-5.174006	5.007400	-1.660651
1	-3.388794	5.121846	-0.596559
1	-5.325915	6.083311	-1.632206
1	-5.915317	4.426560	-2.200370
6	-5.322026	-3.492145	-0.726835
6	-6.220486	-3.012076	-1.602780

1	-5.623244	-4.353681	-0.128017
1	-7.212987	-3.449115	-1.677125
1	-5.992943	-2.196469	-2.281924
6	4.408049	-2.087085	-0.115561
6	5.069423	-2.061884	-1.526579
1	4.774093	-2.972809	0.417250
1	4.757737	-1.216534	0.451615
1	4.756849	-2.936719	-2.101874
1	4.755923	-1.160904	-2.061320
6	3.749507	3.172325	-1.160617
6	4.613739	3.046467	0.130967
1	3.803702	4.211763	-1.500813
1	4.217567	2.576928	-1.951929
1	5.344855	3.867819	0.145777
1	4.001375	3.136496	1.031092
6	6.568126	-2.039594	-1.399864
8	7.250737	-1.077718	-1.078978
8	7.141286	-3.241801	-1.626891
1	8.096909	-3.118006	-1.467179
6	5.433775	1.775523	0.262115
8	5.605545	1.159038	1.296295
8	6.002964	1.412921	-0.908113
1	6.498885	0.566746	-0.782525
6	-4.279582	-0.715938	2.867111
6	-4.766861	-2.093115	3.290525
1	-4.875197	-0.322446	2.034540
1	-4.349807	0.006844	3.688103
1	-5.816528	-2.045307	3.606737
1	-4.684218	-2.801213	2.459862
1	-4.170209	-2.475136	4.126658

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<sup>10</sup>SS<sup>TS(D-E)</sup><sub>FE(cys)</sub>  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-3048.4659826  
 Zero-point correction=                    0.843821 (Hartree/Particle)  
 Thermal correction to Energy=            0.903326  
 Thermal correction to Enthalpy=         0.904271  
 Thermal correction to Gibbs Free Energy= 0.746542  
 Sum of electronic and zero-point Energies= -3047.622161  
 Sum of electronic and thermal Energies= -3047.562656  
 Sum of electronic and thermal Enthalpies= -3047.561712  
 Sum of electronic and thermal Free Energies= -3047.719441

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 Cartesian Coordinates  
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6	1.985412	3.997331	2.808350
6	0.651634	4.279282	2.498612
6	-0.284866	3.255283	2.406476
6	0.068679	1.894319	2.612351
6	1.442766	1.643811	2.921195

6	2.376703	2.670270	3.027082
6	-0.862296	0.810538	2.564196
8	1.768797	0.326085	3.162795
6	3.072121	-0.068470	3.207825
26	-0.836037	-0.336557	-0.753622
7	-2.411078	0.900020	-1.007043
6	-2.387910	2.243140	-1.247433
6	-3.739279	2.758000	-1.437259
6	-4.580238	1.675290	-1.306192
6	-3.731400	0.530653	-1.038763
6	-1.232354	3.006027	-1.370811
6	0.065294	2.523813	-1.278626
7	0.406768	1.228245	-1.002330
6	1.772897	1.176754	-1.062914
6	2.322927	2.484739	-1.403767
6	1.252388	3.329726	-1.515082
6	-4.208595	-0.757753	-0.824136
6	-3.445001	-1.864140	-0.466868
7	-2.093603	-1.842323	-0.257791
6	-1.762719	-3.071348	0.253674
6	-2.934096	-3.908563	0.374539
6	-3.991691	-3.174266	-0.119379
6	2.534632	0.053650	-0.770188
6	2.045790	-1.164997	-0.307429
7	0.723574	-1.485852	-0.184178
6	0.685601	-2.753587	0.339684
6	2.028884	-3.251319	0.573944
6	2.881597	-2.260631	0.161019
6	-0.471341	-3.486017	0.566214
6	-2.293236	0.963603	2.570674
8	-2.909973	-0.245971	2.833290
8	-2.961118	1.987888	2.420258
1	-0.356446	-4.484089	0.976693
1	-5.279686	-0.903415	-0.880442
1	-1.351731	4.059345	-1.598011
1	3.608458	0.150027	-0.862231
1	-1.321541	3.468433	2.179052
1	0.336475	5.307902	2.334877
1	3.398885	2.438917	3.306212
1	2.717927	4.796072	2.898186
1	3.786925	0.429928	2.559047
1	-0.489509	-0.190119	2.732879
1	3.156018	-1.130015	3.411533
6	-0.542016	-2.754124	-3.171850
1	-1.423221	-3.257138	-2.759110
1	-0.432679	-3.058017	-4.219968
1	0.341977	-3.095164	-2.621760
16	-0.711789	-0.928826	-3.103220
6	1.231638	4.800793	-1.803438
1	0.589915	5.039510	-2.661469



1	0.848253	5.366632	-0.943797
1	2.232533	5.184500	-2.025670
6	2.355003	-4.593725	1.158578
1	2.019728	-5.413603	0.508647
1	3.432702	-4.717811	1.308100
1	1.869338	-4.739833	2.132242
6	-2.935641	-5.322009	0.876379
1	-3.954104	-5.702610	1.003038
1	-2.420706	-6.001748	0.183132
1	-2.427049	-5.406390	1.845147
6	-6.077332	1.655390	-1.359562
1	-6.455072	1.451846	-2.372226
1	-6.494407	0.887776	-0.698954
1	-6.485981	2.623596	-1.050168
6	-4.058719	4.160858	-1.665867
6	-5.123677	4.661842	-2.314801
1	-3.344883	4.874520	-1.253735
1	-5.268819	5.735642	-2.399900
1	-5.864960	4.031795	-2.796389
6	-5.366513	-3.645335	-0.258060
6	-6.258335	-3.309586	-1.204658
1	-5.679485	-4.383543	0.482433
1	-7.258151	-3.736060	-1.203411
1	-6.018037	-2.628174	-2.014812
6	4.381948	-2.249356	0.210438
6	5.039299	-2.463827	-1.186234
1	4.736460	-3.041228	0.880916
1	4.746515	-1.303227	0.626196
1	4.728801	-3.424651	-1.603662
1	4.719771	-1.668793	-1.866026
6	3.774192	2.825224	-1.613287
6	4.657327	2.883792	-0.330212
1	3.822718	3.806983	-2.095497
1	4.233942	2.125171	-2.319345
1	5.408230	3.676579	-0.458697
1	4.062408	3.133208	0.551309
6	6.538401	-2.412998	-1.071731
8	7.215494	-1.407436	-0.912900
8	7.118979	-3.631579	-1.106807
1	8.074837	-3.478626	-0.976067
6	5.445934	1.626169	-0.018605
8	5.577330	1.138836	1.090088
8	6.033281	1.107772	-1.115134
1	6.499990	0.269010	-0.874237
6	-4.334556	-0.205710	2.911599
6	-4.802487	-1.559389	3.423154
1	-4.751493	0.008534	1.920424
1	-4.644509	0.607334	3.578751
1	-5.897049	-1.579530	3.496492
1	-4.485399	-2.357175	2.744168

1 -4.384903 -1.764861 4.415486

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 $^3\text{A}_{\text{Fe(cys)}}$   
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2396.4851303  
Zero-point correction=                    0.633704 (Hartree/Particle)  
Thermal correction to Energy=            0.679384  
Thermal correction to Enthalpy=         0.680328  
Thermal correction to Gibbs Free Energy= 0.548637  
Sum of electronic and zero-point Energies= -2395.851426  
Sum of electronic and thermal Energies= -2395.805746  
Sum of electronic and thermal Enthalpies= -2395.804802  
Sum of electronic and thermal Free Energies= -2395.936493

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Cartesian Coordinates  
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26	1.042663	-0.067033	0.031487
7	2.415093	-1.515610	-0.435089
6	2.168413	-2.850429	-0.623365
6	3.402492	-3.579028	-0.810598
6	4.418157	-2.647095	-0.760434
6	3.773599	-1.363190	-0.491267
6	0.902329	-3.434545	-0.635444
6	-0.302665	-2.763656	-0.487187
7	-0.435960	-1.410099	-0.295697
6	-1.782679	-1.167932	-0.255025
6	-2.532789	-2.410614	-0.394617
6	-1.606756	-3.407428	-0.539766
6	-2.368188	0.090149	-0.147440
6	-1.692144	1.303653	-0.060069
7	-0.332335	1.440243	-0.029549
6	-0.089096	2.783026	0.094920
6	-1.335752	3.530464	0.131399
6	-2.340419	2.605062	0.032077
6	1.170029	3.359173	0.197226
6	2.383302	2.677331	0.154841
6	3.693455	3.314729	0.263478
6	4.619517	2.298252	0.158404
6	3.863767	1.073217	-0.013196
7	2.513088	1.325592	0.008442
6	4.444687	-0.170451	-0.242810
1	0.855881	-4.509392	-0.780815
1	5.525711	-0.220508	-0.217549
1	1.206802	4.435068	0.330323
1	-3.453160	0.129318	-0.142875
16	1.122056	-0.284532	2.520589
6	0.807610	-2.053677	2.910988
1	1.603443	-2.697276	2.515100
1	0.763010	-2.200002	3.997665

1	-0.142565	-2.396342	2.482944
6	-1.441059	5.021502	0.258207
1	-0.924466	5.387688	1.155163
1	-0.992588	5.539807	-0.600852
1	-2.484926	5.345653	0.326766
6	-1.830953	-4.879044	-0.724552
1	-1.334538	-5.255283	-1.629107
1	-1.436018	-5.461188	0.119476
1	-2.896730	-5.114647	-0.814349
6	3.503115	-5.053050	-1.069058
1	2.953322	-5.632561	-0.316259
1	3.086779	-5.326375	-2.049062
1	4.543101	-5.394636	-1.054817
6	6.113688	2.410284	0.154351
1	6.536625	2.337416	1.166762
1	6.578663	1.619499	-0.444174
1	6.429712	3.375593	-0.257843
6	5.836787	-2.927075	-0.955855
6	6.770375	-2.133840	-1.507761
1	6.156906	-3.921766	-0.639721
1	7.801354	-2.466654	-1.597250
1	6.538714	-1.149667	-1.902708
6	3.901128	4.748823	0.399172
6	4.960405	5.384370	0.931733
1	3.092232	5.373912	0.019138
1	5.001840	6.470325	0.955271
1	5.795048	4.857262	1.382475
6	-4.029486	-2.530775	-0.339627
6	-4.571730	-2.476966	1.099930
1	-4.355860	-3.469112	-0.801571
1	-4.506247	-1.734103	-0.923699
1	-4.132393	-3.275462	1.711528
1	-4.276689	-1.543897	1.595663
6	-3.823287	2.843775	-0.017051
6	-4.383023	2.778759	-1.449352
1	-4.068200	3.822356	0.409716
1	-4.355368	2.111370	0.602127
1	-3.878575	3.509479	-2.095490
1	-4.180402	1.802789	-1.906937
6	-6.075331	-2.600918	1.174571
8	-6.838077	-2.736138	0.240650
8	-6.521979	-2.547233	2.458688
1	-7.492800	-2.625019	2.399504
6	-5.869063	3.040797	-1.524908
8	-6.599355	3.344056	-0.605480
8	-6.339730	2.904455	-2.795465
1	-7.296411	3.087802	-2.738031

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${}^3\mathbf{B}_{\text{Fe(cys)}}$

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3158.0028436  
 Zero-point correction=                    0.855532 (Hartree/Particle)  
 Thermal correction to Energy=            0.918613  
 Thermal correction to Enthalpy=         0.919557  
 Thermal correction to Gibbs Free Energy= 0.745729  
 Sum of electronic and zero-point Energies= -3157.147312  
 Sum of electronic and thermal Energies= -3157.084231  
 Sum of electronic and thermal Enthalpies= -3157.083287  
 Sum of electronic and thermal Free Energies= -3157.257115

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 Cartesian Coordinates

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6	2.402469	-2.165540	4.566668
6	3.252146	-1.061687	4.540213
6	2.750697	0.188391	4.175808
6	1.405040	0.354713	3.823306
6	0.553904	-0.778587	3.841469
6	1.056608	-2.027811	4.220631
6	0.897471	1.678696	3.410734
7	-0.329322	2.039231	3.731810
7	-1.379188	2.364932	4.019375
8	-0.736851	-0.556237	3.479328
6	-1.600326	-1.669345	3.268710
26	-1.360095	-0.387507	-0.956869
7	-2.886563	0.961167	-0.789593
6	-2.847561	2.298934	-1.058104
6	-4.170084	2.895306	-0.902624
6	-5.009078	1.864908	-0.526452
6	-4.191727	0.671075	-0.479909
6	-1.709059	2.989654	-1.470259
6	-0.436708	2.448489	-1.595121
7	-0.102373	1.151239	-1.307201
6	1.253098	1.065477	-1.477336
6	1.797825	2.341097	-1.935600
6	0.739294	3.204194	-2.013511
6	-4.681925	-0.601996	-0.196576
6	-3.946447	-1.781396	-0.150994
7	-2.585031	-1.860713	-0.298501
6	-2.243390	-3.159488	-0.008508
6	-3.419307	-3.942251	0.303753
6	-4.498644	-3.092907	0.190321
6	2.026442	-0.058592	-1.215678
6	1.554842	-1.294655	-0.783125
7	0.239395	-1.611681	-0.597388
6	0.213792	-2.932440	-0.231697
6	1.561487	-3.471585	-0.159380
6	2.402874	-2.442424	-0.496130
6	-0.942868	-3.659936	0.026794
6	1.661195	2.653026	2.623013
8	0.929021	3.764747	2.366173

8	2.812601	2.499333	2.253355
1	-0.823370	-4.708009	0.284222
1	-5.737843	-0.682522	0.028423
1	-1.824626	4.038507	-1.722414
1	3.095749	0.039812	-1.350601
1	3.408075	1.048357	4.133771
1	4.301836	-1.166395	4.800015
1	0.405166	-2.893916	4.229090
1	2.780970	-3.144407	4.850480
1	-2.520819	-1.255525	2.856657
1	-1.170901	-2.370362	2.546385
1	-1.814973	-2.184964	4.215238
6	-1.820156	-2.667931	-3.591345
1	-2.695306	-3.032430	-3.039722
1	-1.956875	-2.922417	-4.649809
1	-0.941442	-3.212502	-3.223147
16	-1.608825	-0.850659	-3.398640
6	0.720176	4.632986	-2.471349
1	1.722607	4.978914	-2.744971
1	0.074309	4.765359	-3.349598
1	0.340826	5.311309	-1.694831
6	1.904158	-4.880431	0.225219
1	1.484800	-5.148327	1.204378
1	1.511290	-5.607674	-0.498635
1	2.987570	-5.031037	0.281153
6	-3.418325	-5.407169	0.626255
1	-3.128418	-6.013892	-0.242866
1	-2.710409	-5.646803	1.430844
1	-4.408094	-5.751221	0.943081
6	-6.467524	1.937344	-0.189562
1	-7.106639	1.820228	-1.077036
1	-6.757294	1.156604	0.521833
1	-6.714264	2.907640	0.256961
6	-4.456945	4.311422	-1.077628
6	-5.637264	4.888351	-1.366478
1	-3.601025	4.976125	-0.955660
1	-5.720553	5.968813	-1.450899
1	-6.540531	4.316747	-1.553211
6	-5.896999	-3.466954	0.375155
6	-6.977472	-2.961264	-0.242999
1	-6.066307	-4.283106	1.080404
1	-7.972895	-3.335182	-0.016987
1	-6.905391	-2.190937	-1.004112
6	3.905013	-2.450549	-0.544216
6	4.477815	-2.587320	-1.988114
1	4.289689	-3.280622	0.060471
1	4.304438	-1.528486	-0.107640
1	4.083406	-3.492725	-2.456278
1	4.176990	-1.720438	-2.580637
6	3.239534	2.566695	-2.303696

6	4.225873	2.662266	-1.096243
1	3.328138	3.481260	-2.900718
1	3.561401	1.748848	-2.956354
1	4.491302	3.699806	-0.877675
1	3.748765	2.261599	-0.192920
6	5.983021	-2.648884	-1.958376
8	6.753932	-1.704588	-1.876940
8	6.455003	-3.917524	-1.977947
1	7.425929	-3.841136	-1.906023
6	5.521557	1.893746	-1.279528
8	6.638125	2.313503	-1.055661
8	5.279348	0.630648	-1.697535
1	6.099750	0.088931	-1.732406
6	1.549769	4.751193	1.517071
6	0.579543	5.913410	1.403381
1	1.752185	4.295882	0.543101
1	2.505531	5.052369	1.959010
1	1.005975	6.693068	0.761988
1	-0.366809	5.581450	0.964611
1	0.370897	6.349454	2.386393

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**<sup>3</sup>TS(B-C)<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3157.9465852  
Zero-point correction=                    0.853586 (Hartree/Particle)  
Thermal correction to Energy=            0.915206  
Thermal correction to Enthalpy=         0.916150  
Thermal correction to Gibbs Free Energy= 0.753976  
Sum of electronic and zero-point Energies= -3157.092999  
Sum of electronic and thermal Energies= -3157.031379  
Sum of electronic and thermal Enthalpies= -3157.030435  
Sum of electronic and thermal Free Energies= -3157.192609

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Cartesian Coordinates

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6	-1.127531	-3.939846	3.489480
6	0.099489	-3.293522	3.381359
6	0.165787	-2.000156	2.859394
6	-0.970847	-1.294954	2.412350
6	-2.211684	-1.992384	2.518958
6	-2.282050	-3.280265	3.061211
6	-0.896912	0.086310	1.858449
7	-2.277071	0.930349	2.582493
7	-2.894574	1.792174	2.146167
8	-3.325097	-1.344287	2.064035
6	-4.599139	-1.874896	2.345408
26	-0.717015	0.118132	-0.629512
7	-2.214845	1.465031	-0.758464
6	-2.128432	2.823969	-0.715867
6	-3.448582	3.428130	-0.857931

6	-4.332588	2.381797	-0.993664
6	-3.539312	1.169008	-0.939583
6	-0.940644	3.544643	-0.645500
6	0.330282	2.989148	-0.612730
7	0.600272	1.649438	-0.554243
6	1.961024	1.531345	-0.603365
6	2.585006	2.845768	-0.686946
6	1.564735	3.757974	-0.684861
6	-4.070012	-0.107493	-1.084860
6	-3.361960	-1.303554	-1.045192
7	-2.029076	-1.414652	-0.773494
6	-1.757237	-2.754291	-0.687791
6	-2.955516	-3.531870	-0.902100
6	-3.963731	-2.630348	-1.170700
6	2.668892	0.339377	-0.545217
6	2.115498	-0.930429	-0.436836
7	0.781513	-1.219709	-0.470914
6	0.682563	-2.584131	-0.379677
6	1.997575	-3.182513	-0.236497
6	2.895937	-2.148724	-0.276435
6	-0.498278	-3.305316	-0.470422
6	0.264188	0.896438	2.291587
8	-0.055566	2.198557	2.560035
8	1.428956	0.520956	2.396506
1	-0.432893	-4.385041	-0.392452
1	-5.140637	-0.181042	-1.225113
1	-1.008149	4.626329	-0.682405
1	3.748758	0.406482	-0.551033
1	1.122947	-1.502538	2.789628
1	1.013130	-3.782723	3.713085
1	-3.240994	-3.780810	3.138679
1	-1.200637	-4.943506	3.903446
1	-5.315462	-1.139666	1.972420
1	-4.770454	-2.829515	1.828645
1	-4.749620	-2.018672	3.425608
6	-0.327426	-1.481384	-3.615326
1	-1.198399	-2.107008	-3.396289
1	-0.212685	-1.413854	-4.703758
1	0.563183	-1.963941	-3.200525
16	-0.534912	0.219741	-2.969377
6	1.639009	5.254325	-0.760609
1	2.676147	5.600281	-0.821350
1	1.109954	5.643067	-1.640746
1	1.186441	5.729887	0.119915
6	2.249602	-4.648859	-0.050607
1	1.714692	-5.032699	0.827755
1	1.911495	-5.235231	-0.915827
1	3.314793	-4.861289	0.089565
6	-3.020890	-5.029796	-0.875393
1	-2.434221	-5.479509	-1.688253

1	-2.622637	-5.427050	0.067113
1	-4.048736	-5.390737	-0.982604
6	-5.824515	2.438868	-1.116918
1	-6.157686	2.457294	-2.165056
1	-6.300081	1.573938	-0.641874
1	-6.215385	3.343047	-0.637441
6	-3.703529	4.861345	-0.806899
6	-4.714765	5.534610	-1.382054
1	-2.984721	5.441492	-0.227515
1	-4.814541	6.608888	-1.249890
1	-5.454474	5.052165	-2.013324
6	-5.340322	-2.972815	-1.514538
6	-6.181097	-2.308912	-2.325369
1	-5.704515	-3.905728	-1.080005
1	-7.187970	-2.677628	-2.503998
1	-5.891087	-1.404645	-2.850922
6	4.390054	-2.213686	-0.128890
6	5.156443	-2.103950	-1.482458
1	4.671126	-3.158631	0.350845
1	4.742002	-1.409023	0.525994
1	4.813208	-2.886952	-2.163505
1	4.960846	-1.128223	-1.932937
6	4.069582	3.071602	-0.771730
6	4.838896	2.754887	0.548192
1	4.273486	4.108873	-1.059593
1	4.476891	2.447915	-1.573897
1	5.059409	3.662640	1.115584
1	4.206991	2.123516	1.186762
6	6.640971	-2.241442	-1.263549
8	7.412738	-1.364915	-0.904269
8	7.082687	-3.505650	-1.456462
1	8.034572	-3.492291	-1.238470
6	6.142382	1.996633	0.371850
8	7.178510	2.222113	0.961819
8	5.997199	0.974407	-0.501410
1	6.786908	0.386593	-0.510701
6	1.025068	3.038211	2.973566
6	0.425201	4.382446	3.355736
1	1.744735	3.141676	2.154810
1	1.549377	2.574907	3.817528
1	1.214472	5.073131	3.677481
1	-0.100767	4.823853	2.502803
1	-0.293876	4.269056	4.174145

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 $^3\text{C}_{\text{Fe}(\text{cys})}$   
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Number of imaginary frequencies: 0	Electronic energy:	HF=-3157.9926334
Zero-point correction=	0.852497 (Hartree/Particle)	
Thermal correction to Energy=	0.916248	
Thermal correction to Enthalpy=	0.917192	



Thermal correction to Gibbs Free Energy=	0.746021
Sum of electronic and zero-point Energies=	-3157.140137
Sum of electronic and thermal Energies=	-3157.076385
Sum of electronic and thermal Enthalpies=	-3157.075441
Sum of electronic and thermal Free Energies=	-3157.246612

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Cartesian Coordinates  
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6	-4.896973	0.227015	3.000746
6	-4.232421	-0.986212	2.854979
6	-2.948470	-1.011882	2.301805
6	-2.288402	0.154620	1.892158
6	-2.976228	1.381446	2.081778
6	-4.267744	1.415728	2.613938
6	-0.928808	0.129566	1.308883
7	1.620863	4.059328	1.989943
7	0.637974	4.506429	1.754785
8	-2.281634	2.506461	1.719503
6	-2.935412	3.753823	1.794905
26	-0.603745	-0.441462	-0.649435
7	-2.234955	0.624813	-1.207882
6	-2.301524	1.948066	-1.513927
6	-3.673456	2.329123	-1.839280
6	-4.425587	1.178117	-1.723096
6	-3.505306	0.126801	-1.337793
6	-1.203585	2.803383	-1.588086
6	0.117642	2.425494	-1.397390
7	0.533118	1.179575	-1.025820
6	1.894946	1.207449	-1.038223
6	2.375001	2.529869	-1.431619
6	1.263499	3.295730	-1.640882
6	-3.877453	-1.199093	-1.141820
6	-3.050463	-2.237533	-0.723729
7	-1.734603	-2.101570	-0.385321
6	-1.336911	-3.298611	0.145051
6	-2.433528	-4.240505	0.148946
6	-3.503836	-3.597032	-0.437131
6	2.729010	0.157525	-0.680385
6	2.314068	-1.078422	-0.197785
7	1.022669	-1.503960	-0.119511
6	1.057681	-2.761070	0.422211
6	2.426754	-3.142141	0.731419
6	3.214324	-2.093881	0.333497
6	-0.043965	-3.591013	0.579483
6	0.132720	0.577292	2.194445
8	-0.269538	0.620626	3.529312
8	1.287988	0.883819	1.912073
1	0.127702	-4.574633	1.004898
1	-4.923045	-1.441567	-1.279455
1	-1.384771	3.828900	-1.890453

1	3.794826	0.340171	-0.717308
1	-2.430594	-1.958245	2.191814
1	-4.707668	-1.915854	3.159481
1	-4.787474	2.359584	2.739663
1	-5.902127	0.263902	3.415574
1	-2.214513	4.490742	1.435941
1	-3.831955	3.780561	1.159694
1	-3.222601	4.004789	2.827370
6	0.024537	-2.801575	-3.051832
1	-0.830325	-3.393189	-2.706613
1	0.219489	-3.054826	-4.100557
1	0.900895	-3.083546	-2.457960
16	-0.308338	-1.003113	-2.937565
6	1.173109	4.735363	-2.050262
1	2.166123	5.168329	-2.210838
1	0.605261	4.859414	-2.981937
1	0.670391	5.343472	-1.285636
6	2.832506	-4.444504	1.355285
1	2.296500	-4.627293	2.295758
1	2.619042	-5.297177	0.695830
1	3.904427	-4.468003	1.578670
6	-2.351110	-5.658755	0.630461
1	-1.757812	-6.287666	-0.048267
1	-1.880101	-5.722903	1.619525
1	-3.343154	-6.115666	0.706934
6	-5.904371	1.016847	-1.901566
1	-6.177679	0.799456	-2.944651
1	-6.297146	0.201607	-1.285485
1	-6.430411	1.935213	-1.616486
6	-4.087075	3.683585	-2.176327
6	-5.175816	4.072136	-2.864451
1	-3.423644	4.472333	-1.820275
1	-5.379549	5.126972	-3.029630
1	-5.876301	3.369019	-3.302863
6	-4.809534	-4.189433	-0.706368
6	-5.641355	-3.919682	-1.726132
1	-5.117003	-4.967647	-0.005184
1	-6.593664	-4.435537	-1.819190
1	-5.394304	-3.203447	-2.503532
6	4.705018	-1.954502	0.460599
6	5.468440	-2.160706	-0.882856
1	5.082545	-2.683388	1.187678
1	4.961369	-0.961142	0.845151
1	5.219310	-3.138221	-1.303354
1	5.171879	-1.383108	-1.590747
6	3.827521	2.896550	-1.562838
6	4.582817	3.003502	-0.201982
1	3.924830	3.848406	-2.096933
1	4.327120	2.147036	-2.184965
1	4.691013	4.042074	0.120683

1	3.996355	2.491356	0.571954
6	6.956778	-2.068058	-0.666254
8	7.617161	-1.046892	-0.548651
8	7.546091	-3.280976	-0.552009
1	8.488302	-3.102866	-0.366656
6	5.961104	2.368681	-0.169639
8	6.942173	2.834100	0.372755
8	5.960343	1.161063	-0.779185
1	6.803118	0.676722	-0.625046
6	0.731097	1.028395	4.457338
6	0.120398	0.953285	5.849014
1	1.066973	2.047043	4.224194
1	1.611068	0.378653	4.369436
1	0.851625	1.263956	6.605813
1	-0.755927	1.606380	5.923065
1	-0.201596	-0.068941	6.075776

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**<sup>3</sup>TS(C-D)<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 3    Electronic energy:    HF=-3048.4413124  
Zero-point correction=                    0.841704 (Hartree/Particle)  
Thermal correction to Energy=            0.898673  
Thermal correction to Enthalpy=         0.899617  
Thermal correction to Gibbs Free Energy= 0.748908  
Sum of electronic and zero-point Energies= -3047.599609  
Sum of electronic and thermal Energies= -3047.542639  
Sum of electronic and thermal Enthalpies= -3047.541695  
Sum of electronic and thermal Free Energies= -3047.692405

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Cartesian Coordinates

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6	1.093667	-3.222517	3.821392
6	1.803980	-2.079578	3.445898
6	1.165479	-1.047280	2.755815
6	-0.195917	-1.118909	2.408431
6	-0.897572	-2.270962	2.841697
6	-0.268313	-3.309196	3.526563
6	-0.948335	-0.077148	1.659935
8	-2.246034	-2.427031	2.577510
6	-2.987935	-1.246452	2.527183
26	-0.748416	-0.067513	-0.575100
7	-2.486159	0.978763	-0.704077
6	-2.650282	2.328219	-0.740484
6	-4.063451	2.672550	-0.870777
6	-4.743859	1.473809	-0.906880
6	-3.738418	0.433159	-0.819574
6	-1.612621	3.256894	-0.705460
6	-0.261810	2.950031	-0.627636
7	0.260045	1.689576	-0.555624
6	1.616806	1.838432	-0.551186

6	1.979669	3.251992	-0.607129
6	0.801033	3.944308	-0.648693
6	-4.024514	-0.925732	-0.885551
6	-3.105213	-1.970036	-0.841007
7	-1.761233	-1.825869	-0.642778
6	-1.242894	-3.090205	-0.544608
6	-2.288212	-4.079593	-0.673830
6	-3.457185	-3.384393	-0.895227
6	2.533706	0.797789	-0.503716
6	2.233046	-0.559783	-0.436673
7	0.979527	-1.093760	-0.459628
6	1.137487	-2.451521	-0.357506
6	2.544729	-2.794446	-0.246269
6	3.231876	-1.611724	-0.299230
6	0.110149	-3.380846	-0.382158
6	-0.790335	1.274535	2.222511
8	-2.005720	1.913553	2.349079
8	0.240840	1.826057	2.582909
1	0.389881	-4.423990	-0.288082
1	-5.066848	-1.205205	-0.970254
1	-1.875113	4.306076	-0.781360
1	3.581444	1.065153	-0.516862
1	1.716573	-0.159476	2.470423
1	2.860667	-1.987721	3.687210
1	-0.864316	-4.166413	3.828769
1	1.585731	-4.031253	4.357852
1	-3.087198	-0.734014	3.489913
1	-2.068697	-0.417750	1.805458
1	-3.906010	-1.396490	1.966179
6	-0.189745	-1.644115	-3.560499
1	-0.944953	-2.392218	-3.297891
1	-0.122789	-1.588043	-4.653396
1	0.777591	-1.976352	-3.169422
16	-0.636277	0.016880	-2.929497
6	0.571633	5.425168	-0.713773
1	1.514488	5.981127	-0.719031
1	0.017069	5.711229	-1.617554
1	-0.011520	5.781283	0.146075
6	3.072286	-4.186032	-0.063928
1	2.780005	-4.846196	-0.891511
1	4.165807	-4.198889	-0.008056
1	2.688069	-4.634767	0.861252
6	-2.128968	-5.570903	-0.612559
1	-2.636477	-5.992144	0.266879
1	-2.558116	-6.059571	-1.496450
1	-1.079370	-5.871381	-0.550784
6	-6.223461	1.250476	-0.984700
1	-6.584714	1.205315	-2.022650
1	-6.516627	0.313328	-0.499883
1	-6.764010	2.066727	-0.491935

6	-4.574992	4.035382	-0.911307
6	-5.737226	4.466896	-1.432928
1	-3.928041	4.788571	-0.460934
1	-6.012668	5.516945	-1.379789
1	-6.431642	3.809024	-1.945204
6	-4.760129	-3.997920	-1.128368
6	-5.760622	-3.550998	-1.905962
1	-4.906272	-4.958091	-0.629202
1	-6.687428	-4.111628	-1.997649
1	-5.681607	-2.638506	-2.488771
6	4.712477	-1.394040	-0.178761
6	5.397149	-1.090796	-1.546999
1	5.182942	-2.286929	0.248860
1	4.926762	-0.567756	0.509257
1	5.216917	-1.916329	-2.240302
1	4.978807	-0.175166	-1.972852
6	3.373867	3.818095	-0.649367
6	4.227114	3.625465	0.640640
1	3.296747	4.892183	-0.846921
1	3.929405	3.401567	-1.496670
1	4.807912	4.541440	0.821296
1	3.596969	3.465689	1.518554
6	6.876647	-0.895623	-1.359989
8	7.432153	0.129903	-0.993699
8	7.592477	-2.018788	-1.586869
1	8.519698	-1.793127	-1.379188
6	5.247929	2.500858	0.605354
8	5.525472	1.787562	1.549865
8	5.855966	2.395384	-0.595642
1	6.475639	1.624227	-0.576819
6	-1.959767	3.240321	2.878258
6	-3.393551	3.684784	3.122770
1	-1.454199	3.899825	2.162375
1	-1.370004	3.248387	3.801871
1	-3.412825	4.706042	3.523562
1	-3.970598	3.663721	2.192579
1	-3.886787	3.022213	3.842829

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**<sup>3</sup>D<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3048.4691061  
Zero-point correction=                    0.844884 (Hartree/Particle)  
Thermal correction to Energy=            0.904571  
Thermal correction to Enthalpy=         0.905516  
Thermal correction to Gibbs Free Energy= 0.747890  
Sum of electronic and zero-point Energies= -3047.624222  
Sum of electronic and thermal Energies= -3047.564535  
Sum of electronic and thermal Enthalpies= -3047.563590  
Sum of electronic and thermal Free Energies= -3047.721216

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Cartesian Coordinates

6	2.140429	2.790030	3.315767
6	0.887531	3.276266	2.935003
6	-0.080802	2.413072	2.426697
6	0.139387	1.024436	2.294996
6	1.403106	0.561502	2.740363
6	2.396150	1.422027	3.213082
6	-0.872326	0.083818	1.770172
8	1.637341	-0.804336	2.664942
6	2.368581	-1.433853	3.618251
26	-0.841228	-0.085211	-0.555986
7	-2.421694	1.157281	-0.758542
6	-2.409424	2.514684	-0.854905
6	-3.766442	3.032742	-0.997692
6	-4.595367	1.933222	-0.992527
6	-3.733923	0.775187	-0.848266
6	-1.260617	3.298175	-0.903082
6	0.040504	2.815968	-0.878568
7	0.391372	1.504038	-0.739953
6	1.753955	1.461397	-0.825378
6	2.298036	2.802618	-1.017189
6	1.223142	3.648571	-1.037944
6	-4.197357	-0.535420	-0.809171
6	-3.423174	-1.677170	-0.623281
7	-2.075987	-1.679639	-0.405606
6	-1.729876	-2.970073	-0.106701
6	-2.892689	-3.827363	-0.127308
6	-3.957197	-3.032544	-0.497765
6	2.525391	0.313327	-0.704117
6	2.052676	-0.967382	-0.432884
7	0.739240	-1.319182	-0.334911
6	0.717869	-2.651815	-0.021351
6	2.069676	-3.168777	0.099122
6	2.906361	-2.115918	-0.162116
6	-0.430696	-3.419130	0.117215
6	-2.255269	0.331535	2.190687
8	-2.912053	-0.852436	2.464056
8	-2.835243	1.401826	2.334078
1	-0.303019	-4.468522	0.362360
1	-5.266514	-0.682043	-0.891312
1	-1.389031	4.368142	-1.022272
1	3.597077	0.431747	-0.793104
1	-1.049797	2.794938	2.133363
1	0.664133	4.337977	3.020949
1	3.376300	1.024974	3.457334
1	2.913554	3.459555	3.686371
1	2.776632	-0.855278	4.439255
1	-0.600326	-0.951967	1.938542
1	2.820060	-2.357760	3.279762

6	-0.592805	-2.054339	-3.320173
1	-1.458332	-2.635198	-2.984923
1	-0.516360	-2.143604	-4.410257
1	0.309085	-2.484876	-2.872479
16	-0.766948	-0.278240	-2.903707
6	1.192943	5.140611	-1.184319
1	2.195895	5.553214	-1.333454
1	0.578446	5.453254	-2.038852
1	0.771310	5.622199	-0.291737
6	2.415835	-4.586220	0.447898
1	2.076770	-5.290586	-0.324195
1	3.496921	-4.722106	0.558331
1	1.946932	-4.897142	1.390565
6	-2.878808	-5.304902	0.130073
1	-2.350580	-5.546036	1.061118
1	-3.893163	-5.708562	0.211206
1	-2.375752	-5.856258	-0.676782
6	-6.091505	1.901344	-1.063288
1	-6.459045	1.814909	-2.096410
1	-6.503696	1.055902	-0.502098
1	-6.516007	2.820984	-0.645493
6	-4.098419	4.448480	-1.079722
6	-5.171594	5.007256	-1.665475
1	-3.385926	5.121675	-0.602155
1	-5.322812	6.083293	-1.638085
1	-5.913468	4.426327	-2.204322
6	-5.324403	-3.491356	-0.722008
6	-6.222406	-3.012139	-1.598887
1	-5.626200	-4.351835	-0.121966
1	-7.215109	-3.448789	-1.672822
1	-5.994251	-2.197713	-2.279237
6	4.406426	-2.091201	-0.112506
6	5.068025	-2.068520	-1.523401
1	4.771904	-2.976354	0.421666
1	4.756536	-1.220049	0.453498
1	4.755374	-2.944099	-2.097493
1	4.754821	-1.168304	-2.059654
6	3.750891	3.167124	-1.166112
6	4.614941	3.045138	0.126002
1	3.805452	4.205533	-1.509393
1	4.219017	2.569223	-1.955493
1	5.348026	3.864786	0.136706
1	4.002755	3.140758	1.025643
6	6.566721	-2.046251	-1.396462
8	7.248922	-1.085131	-1.072440
8	7.140339	-3.247529	-1.627155
1	8.095947	-3.123781	-1.467293
6	5.431874	1.772796	0.262417
8	5.599382	1.157871	1.298234
8	6.003731	1.406898	-0.905485

1	6.497820	0.560082	-0.777092
6	-4.275345	-0.723229	2.869825
6	-4.756749	-2.101355	3.296822
1	-4.871991	-0.334837	2.035614
1	-4.349481	0.001580	3.688684
1	-5.806834	-2.057298	3.612176
1	-4.670393	-2.811406	2.468215
1	-4.158993	-2.478319	4.134462

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<sup>3</sup>TS(D-E)<sub>Fe(cys)</sub>  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-3048.467686  
 Zero-point correction=                    0.844155 (Hartree/Particle)  
 Thermal correction to Energy=            0.903421  
 Thermal correction to Enthalpy=         0.904365  
 Thermal correction to Gibbs Free Energy= 0.747042  
 Sum of electronic and zero-point Energies= -3047.623531  
 Sum of electronic and thermal Energies= -3047.564265  
 Sum of electronic and thermal Enthalpies= -3047.563321  
 Sum of electronic and thermal Free Energies= -3047.720644

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 Cartesian Coordinates  
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6	-1.861691	-3.769805	2.973118
6	-0.529559	-4.037216	2.632711
6	0.368540	-2.999162	2.423872
6	-0.016871	-1.634382	2.534146
6	-1.383740	-1.401021	2.884660
6	-2.283949	-2.444950	3.103873
6	0.885072	-0.536143	2.356892
8	-1.741255	-0.084430	3.055385
6	-3.039892	0.292050	3.168290
26	0.825937	0.246411	-0.705511
7	2.394272	-0.999918	-0.944759
6	2.365781	-2.349488	-1.139589
6	3.714962	-2.873754	-1.322334
6	4.558817	-1.789040	-1.234632
6	3.713982	-0.633889	-1.001543
6	1.207284	-3.112868	-1.230315
6	-0.088285	-2.623099	-1.146446
7	-0.423803	-1.318510	-0.911611
6	-1.789307	-1.261801	-0.971459
6	-2.346338	-2.579260	-1.261146
6	-1.279723	-3.431881	-1.349383
6	4.194938	0.661423	-0.845278
6	3.436253	1.784553	-0.531299
7	2.088110	1.775392	-0.306404
6	1.763127	3.027748	0.147377
6	2.936476	3.868369	0.215103
6	3.987996	3.109437	-0.253889



6	-2.545745	-0.122777	-0.730068
6	-2.052307	1.114583	-0.325443
7	-0.729512	1.433553	-0.208757
6	-0.686059	2.724672	0.251733
6	-2.027636	3.242214	0.451368
6	-2.884090	2.237887	0.081388
6	0.474533	3.461267	0.445420
6	2.318419	-0.664684	2.455219
8	2.902491	0.562608	2.711870
8	3.008713	-1.681588	2.385675
1	0.364353	4.478374	0.807602
1	5.265575	0.802539	-0.918843
1	1.321795	-4.173304	-1.424720
1	-3.619867	-0.218047	-0.820166
1	1.402022	-3.202289	2.174901
1	-0.188453	-5.066306	2.538671
1	-3.299626	-2.222180	3.411933
1	-2.563035	-4.580176	3.158034
1	-3.796907	-0.271872	2.631564
1	0.493180	0.464063	2.479135
1	-3.132844	1.363798	3.298505
6	0.519650	2.547349	-3.231874
1	1.394729	3.074115	-2.836198
1	0.420034	2.796878	-4.295192
1	-0.370992	2.912375	-2.708585
16	0.695462	0.728519	-3.070872
6	-1.265792	-4.911684	-1.589708
1	-0.638391	-5.179308	-2.449887
1	-0.868880	-5.450620	-0.718959
1	-2.270649	-5.300601	-1.783265
6	-2.348529	4.614777	0.964598
1	-2.006548	5.398337	0.274568
1	-3.426093	4.752115	1.103381
1	-1.865541	4.808592	1.931259
6	2.943940	5.305459	0.644776
1	3.963953	5.689895	0.745002
1	2.425490	5.950543	-0.078379
1	2.442251	5.439718	1.611490
6	6.055432	-1.773484	-1.298823
1	6.427060	-1.606770	-2.320501
1	6.477292	-0.983587	-0.668276
1	6.464942	-2.730631	-0.957680
6	4.029190	-4.284058	-1.506986
6	5.091220	-4.810375	-2.140769
1	3.312901	-4.981735	-1.072197
1	5.231224	-5.887035	-2.191786
1	5.834815	-4.199575	-2.643058
6	5.361383	3.571593	-0.430257
6	6.244056	3.188294	-1.367436
1	5.682059	4.345794	0.269103

1	7.243915	3.613699	-1.396984
1	5.996002	2.467381	-2.140172
6	-4.384634	2.237734	0.123033
6	-5.035342	2.379367	-1.285643
1	-4.737619	3.066749	0.747990
1	-4.756265	1.317744	0.588369
1	-4.718062	3.313694	-1.754789
1	-4.717661	1.546307	-1.919458
6	-3.800858	-2.921340	-1.443022
6	-4.670606	-2.916456	-0.149345
1	-3.859112	-3.923713	-1.879620
1	-4.264360	-2.251599	-2.175560
1	-5.424399	-3.712718	-0.231218
1	-4.066345	-3.124562	0.736515
6	-6.535177	2.342561	-1.174582
8	-7.216135	1.354713	-0.939259
8	-7.112081	3.555899	-1.310030
1	-8.069198	3.415770	-1.174095
6	-5.453472	-1.643598	0.111301
8	-5.576307	-1.107199	1.198054
8	-6.047020	-1.173312	-1.003523
1	-6.508546	-0.322236	-0.799233
6	4.318117	0.544031	2.893631
6	4.729064	1.909391	3.423091
1	4.809152	0.326140	1.937625
1	4.589765	-0.257518	3.590226
1	5.815404	1.947631	3.572629
1	4.447476	2.695431	2.715415
1	4.239717	2.117298	4.381504

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$^5\text{A}_{\text{Fe}(\text{cys})}$

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2396.4990185  
Zero-point correction=                    0.631875 (Hartree/Particle)  
Thermal correction to Energy=            0.678217  
Thermal correction to Enthalpy=         0.679161  
Thermal correction to Gibbs Free Energy= 0.544324  
Sum of electronic and zero-point Energies= -2395.867143  
Sum of electronic and thermal Energies= -2395.820801  
Sum of electronic and thermal Enthalpies= -2395.819857  
Sum of electronic and thermal Free Energies= -2395.954695

.....  
Cartesian Coordinates

.....  
26    1.047005   -0.125685   0.481423  
7    2.428775   -1.543539   -0.405257  
6    2.153084   -2.862245   -0.630727  
6    3.380184   -3.593405   -0.887069  
6    4.404378   -2.666704   -0.855796

6	3.776008	-1.380775	-0.530639
6	0.868149	-3.426937	-0.651915
6	-0.355242	-2.765223	-0.514037
7	-0.497529	-1.425516	-0.291053
6	-1.833214	-1.162611	-0.268975
6	-2.592077	-2.397657	-0.467124
6	-1.666959	-3.399015	-0.619859
6	-2.393824	0.112586	-0.117605
6	-1.713870	1.330030	0.018667
7	-0.359649	1.465925	0.077969
6	-0.094655	2.800227	0.187390
6	-1.341522	3.560564	0.211509
6	-2.354721	2.642634	0.103322
6	1.183236	3.364373	0.241570
6	2.413074	2.698748	0.132623
6	3.728592	3.345512	0.149426
6	4.654303	2.330120	-0.004272
6	3.891994	1.095859	-0.110409
7	2.553032	1.354859	-0.010728
6	4.450668	-0.169429	-0.334794
1	0.818758	-4.497871	-0.829906
1	5.532459	-0.219171	-0.368851
1	1.223137	4.442679	0.363026
1	-3.479280	0.166653	-0.130911
16	1.089438	-0.419469	2.874761
6	1.328647	-2.239862	3.063727
1	2.281595	-2.565004	2.632709
1	1.330317	-2.491777	4.130521
1	0.523727	-2.803332	2.579464
6	-1.441197	5.053736	0.318928
1	-0.890774	5.432589	1.189932
1	-1.023206	5.557069	-0.564183
1	-2.481161	5.382349	0.420700
6	-1.903612	-4.861910	-0.854627
1	-1.376977	-5.218985	-1.749667
1	-1.548088	-5.472688	-0.013219
1	-2.967918	-5.082114	-0.991203
6	3.467990	-5.058727	-1.196220
1	2.903414	-5.657626	-0.470354
1	3.059084	-5.292247	-2.189620
1	4.503701	-5.413919	-1.184157
6	6.144440	2.451088	-0.107590
1	6.631874	2.425948	0.877971
1	6.575671	1.635781	-0.698451
1	6.428372	3.398434	-0.581265
6	5.810791	-2.952513	-1.120808
6	6.723688	-2.156403	-1.702280
1	6.139416	-3.953282	-0.833095
1	7.747917	-2.492934	-1.841551
1	6.479988	-1.166243	-2.074237

6	3.938966	4.781855	0.256601
6	5.034583	5.429426	0.692240
1	3.094978	5.398040	-0.055595
1	5.067579	6.515843	0.707424
1	5.910507	4.912782	1.070769
6	-4.090431	-2.511253	-0.456481
6	-4.667266	-2.520659	0.970382
1	-4.412152	-3.423937	-0.970612
1	-4.546487	-1.683375	-1.013023
1	-4.248994	-3.351221	1.553538
1	-4.376700	-1.614745	1.516634
6	-3.833470	2.898974	0.022612
6	-4.353628	2.877196	-1.425718
1	-4.081194	3.868350	0.468955
1	-4.388463	2.155102	0.606917
1	-3.826433	3.621265	-2.037430
1	-4.143740	1.912328	-1.903294
6	-6.173200	-2.634991	1.004257
8	-6.914111	-2.728928	0.048042
8	-6.650215	-2.626378	2.278611
1	-7.619814	-2.695021	2.193615
6	-5.835363	3.150934	-1.536248
8	-6.591163	3.427705	-0.629148
8	-6.268537	3.060004	-2.824056
1	-7.225599	3.246986	-2.789179

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**<sup>5</sup>B<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3158.0180389  
Zero-point correction=                    0.854018 (Hartree/Particle)  
Thermal correction to Energy=            0.917626  
Thermal correction to Enthalpy=        0.918570  
Thermal correction to Gibbs Free Energy=    0.742868  
Sum of electronic and zero-point Energies=    -3157.164021  
Sum of electronic and thermal Energies=    -3157.100413  
Sum of electronic and thermal Enthalpies=   -3157.099468  
Sum of electronic and thermal Free Energies=   -3157.275171

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Cartesian Coordinates

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6	8.240614	-3.950356	-0.761117
6	7.104514	-4.442470	-1.397799
6	6.058822	-3.577984	-1.723428
6	6.115863	-2.211258	-1.410876
6	7.270446	-1.731571	-0.741336
6	8.325254	-2.594777	-0.433479
6	4.995924	-1.317735	-1.766524
7	5.234704	-0.059387	-2.076084
7	5.426540	1.024902	-2.357125

8	7.265118	-0.401394	-0.422669
6	8.369325	0.145183	0.276487
26	-1.040367	1.195065	1.085284
7	-0.207356	3.014877	0.246051
6	-0.915354	4.055609	-0.268171
6	-0.057546	5.237145	-0.394083
6	1.195219	4.848011	0.042745
6	1.074801	3.453894	0.437964
6	-2.269262	3.998978	-0.633181
6	-3.105917	2.879890	-0.609392
7	-2.729591	1.634489	-0.198780
6	-3.806786	0.817884	-0.364580
6	-4.943179	1.579460	-0.888755
6	-4.502631	2.867531	-1.045723
6	2.131576	2.669861	0.920187
6	2.109801	1.310855	1.256258
7	1.013625	0.506557	1.148520
6	1.419543	-0.771389	1.414051
6	2.839723	-0.795458	1.716217
6	3.276462	0.512828	1.649262
6	-3.818396	-0.558819	-0.112283
6	-2.750959	-1.349757	0.331561
7	-1.520026	-0.880478	0.674719
6	-0.754195	-1.963264	1.005494
6	-1.536548	-3.189482	0.879842
6	-2.785046	-2.806351	0.454237
6	0.596236	-1.907263	1.365295
6	3.582079	-1.739736	-1.854432
8	2.790737	-0.728046	-2.246703
8	3.195621	-2.871019	-1.610692
1	1.076513	-2.855217	1.590149
1	3.095600	3.158651	0.997409
1	-2.715745	4.922411	-0.989506
1	-4.748809	-1.075901	-0.313921
1	5.168822	-3.958062	-2.208057
1	7.026820	-5.496373	-1.649705
1	9.207049	-2.219262	0.073061
1	9.064800	-4.612728	-0.509430
1	8.122594	1.195228	0.442407
1	8.518817	-0.351199	1.244285
1	9.293892	0.074453	-0.312507
6	-1.049920	0.264889	4.293844
1	0.043877	0.238543	4.244134
1	-1.343568	0.365681	5.344987
1	-1.434151	-0.690333	3.920150
16	-1.734092	1.688031	3.337658
6	-5.255712	4.060941	-1.554417
1	-6.294167	3.810136	-1.795876
1	-5.276281	4.872126	-0.814561
1	-4.798369	4.472499	-2.464733

6	-1.019500	-4.571469	1.151349
1	-0.113226	-4.784528	0.569768
1	-0.756764	-4.705225	2.209666
1	-1.759862	-5.339172	0.901295
6	3.633512	-2.026588	2.040907
1	3.236342	-2.541721	2.926058
1	3.612221	-2.743766	1.210223
1	4.681003	-1.787004	2.248404
6	2.455576	5.658752	0.065840
1	2.572488	6.218438	1.005522
1	3.343388	5.027133	-0.045132
1	2.461318	6.393947	-0.747436
6	-0.493118	6.517154	-0.934221
6	0.037055	7.733068	-0.711743
1	-1.358437	6.470647	-1.596289
1	-0.377043	8.615538	-1.192725
1	0.868317	7.895893	-0.033466
6	4.639679	0.971029	1.906100
6	5.015495	2.127133	2.477400
1	5.426792	0.275459	1.611308
1	6.067266	2.364571	2.619310
1	4.297458	2.856036	2.840924
6	-3.958944	-3.683680	0.119948
6	-5.068843	-3.678787	1.215016
1	-3.622734	-4.717146	-0.027063
1	-4.418324	-3.363106	-0.822455
1	-4.644049	-3.990830	2.172243
1	-5.470827	-2.668008	1.317616
6	-6.309087	1.002217	-1.146044
6	-6.380234	0.030036	-2.363855
1	-7.033975	1.809604	-1.298566
1	-6.637073	0.464711	-0.250346
1	-6.796848	0.516629	-3.249462
1	-5.361917	-0.287118	-2.623676
6	-6.194149	-4.605297	0.833602
8	-7.097798	-4.372457	0.044079
8	-6.100494	-5.816906	1.427301
1	-6.843276	-6.344977	1.076184
6	-7.162296	-1.252119	-2.134914
8	-7.921003	-1.767081	-2.930230
8	-6.860372	-1.800933	-0.938088
1	-7.240501	-2.704430	-0.841231
6	1.363041	-1.003817	-2.316826
6	0.666621	0.293267	-2.676833
1	1.035040	-1.383486	-1.347748
1	1.206609	-1.785744	-3.068332
1	-0.412618	0.118137	-2.738826
1	0.832249	1.049577	-1.905087
1	1.017226	0.677962	-3.641530

**<sup>5</sup>TS(B-C)<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3157.9521929  
Zero-point correction=                    0.851612 (Hartree/Particle)  
Thermal correction to Energy=            0.914450  
Thermal correction to Enthalpy=           0.915394  
Thermal correction to Gibbs Free Energy= 0.746060  
Sum of electronic and zero-point Energies= -3157.100581  
Sum of electronic and thermal Energies= -3157.037743  
Sum of electronic and thermal Enthalpies= -3157.036799  
Sum of electronic and thermal Free Energies= -3157.206133

.....  
Cartesian Coordinates

.....  
6      8.080383   -0.130543   -0.590995  
6      7.231989   0.965605   -0.404413  
6      6.140822   0.872314   0.456737  
6      5.826757   -0.316759   1.168290  
6      6.709801   -1.427528   0.946958  
6      7.813754   -1.325782   0.102753  
6      4.685875   -0.418874   2.018345  
7      5.111365   -1.324946   3.640364  
7      4.339718   -1.825721   4.309199  
8      6.366342   -2.594696   1.583929  
6      7.215471   -3.708232   1.453762  
26     -2.708802   -0.166656   -0.422976  
7      -4.371921   0.630693   0.421654  
6      -4.613218   1.956696   0.679568  
6      -5.957840   2.144723   1.193585  
6      -6.531178   0.889753   1.241287  
6      -5.537139   -0.030553   0.745683  
6      -3.713615   2.988025   0.449066  
6      -2.419399   2.830879   -0.013147  
7      -1.813413   1.624147   -0.288351  
6      -0.526499   1.937303   -0.664617  
6      -0.324259   3.376167   -0.668086  
6      -1.505371   3.929538   -0.247441  
6      -5.751622   -1.392541   0.591064  
6      -4.810109   -2.306304   0.144607  
7      -3.497548   -2.004445   -0.133668  
6      -2.878800   -3.209313   -0.382935  
6      -3.814290   -4.297258   -0.274508  
6      -5.038699   -3.737107   0.024363  
6      0.468413   1.013893   -0.946921  
6      0.295825   -0.361526   -0.919013  
7      -0.900734   -1.005929   -0.709964  
6      -0.609825   -2.351335   -0.801389  
6      0.802337   -2.557295   -1.046380  
6      1.375305   -1.314386   -1.113664

6	-1.531278	-3.373558	-0.675587
6	3.582050	0.443235	2.094933
8	2.851504	0.347730	3.264695
8	3.185069	1.211626	1.183100
1	-1.169633	-4.387843	-0.803457
1	-6.723579	-1.781375	0.863939
1	-4.049298	4.000038	0.642457
1	1.457043	1.389249	-1.173498
1	5.487703	1.727066	0.585072
1	7.410352	1.899803	-0.930312
1	8.466468	-2.179630	-0.047076
1	8.956182	-0.061076	-1.232372
1	6.768317	-4.501958	2.057957
1	7.292423	-4.051875	0.410351
1	8.229333	-3.499828	1.827809
6	-2.056181	0.704121	-3.662579
1	-1.156482	0.090643	-3.558495
1	-2.331634	0.744566	-4.721701
1	-1.830981	1.718530	-3.320298
16	-3.460924	-0.018601	-2.729980
6	-1.847954	5.376876	-0.054135
1	-1.000574	6.021863	-0.303558
1	-2.694249	5.682940	-0.682932
1	-2.125702	5.590283	0.986556
6	1.467476	-3.896301	-1.158731
1	2.550183	-3.788287	-1.267266
1	1.285957	-4.513402	-0.269651
1	1.101029	-4.461150	-2.026665
6	-3.484711	-5.742374	-0.501651
1	-4.340049	-6.387229	-0.279429
1	-3.197572	-5.931810	-1.544421
1	-2.647602	-6.070388	0.127477
6	-7.890525	0.509801	1.744531
1	-8.645413	0.515291	0.945226
1	-7.892275	-0.492848	2.184654
1	-8.228273	1.214853	2.511752
6	-6.506537	3.431852	1.604799
6	-7.799169	3.796573	1.619567
1	-5.775638	4.169638	1.935448
1	-8.094174	4.782597	1.967855
1	-8.594878	3.148112	1.267033
6	-6.296100	-4.462097	0.190978
6	-7.527625	-4.048621	-0.147360
1	-6.200401	-5.465599	0.608174
1	-8.393534	-4.683226	0.020951
1	-7.709010	-3.090217	-0.624077
6	2.827833	-0.957016	-1.249432
6	3.274363	-0.612713	-2.698446
1	3.444586	-1.785016	-0.889216
1	3.050674	-0.109655	-0.589745



1	3.176821	-1.498851	-3.337854
1	2.663670	0.188438	-3.120418
6	0.926955	4.065169	-1.140756
6	2.188856	3.891548	-0.245925
1	0.720441	5.134253	-1.262066
1	1.159337	3.689168	-2.142092
1	2.375406	4.780722	0.361940
1	2.078063	3.047328	0.447261
6	4.718535	-0.158063	-2.701073
8	5.105122	0.973950	-2.958637
8	5.558187	-1.138307	-2.348066
1	6.420881	-0.732891	-2.094362
6	3.464269	3.576313	-1.007567
8	4.566522	3.999799	-0.729247
8	3.230270	2.716854	-2.023360
1	4.076162	2.343936	-2.375036
6	1.629434	1.077471	3.300879
6	0.957913	0.764501	4.630064
1	0.990241	0.789168	2.457265
1	1.826237	2.153189	3.201568
1	0.005251	1.302241	4.711783
1	0.761556	-0.309221	4.718253
1	1.599046	1.060240	5.467918

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<sup>5</sup>C<sub>Fe(cys)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3157.9609089  
Zero-point correction=                    0.850194 (Hartree/Particle)  
Thermal correction to Energy=            0.915141  
Thermal correction to Enthalpy=         0.916085  
Thermal correction to Gibbs Free Energy= 0.738881  
Sum of electronic and zero-point Energies= -3157.110715  
Sum of electronic and thermal Energies= -3157.045768  
Sum of electronic and thermal Enthalpies= -3157.044823  
Sum of electronic and thermal Free Energies= -3157.222028

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Cartesian Coordinates

.....  

6	-2.173962	-3.100038	3.916346
6	-0.798834	-2.886152	3.853569
6	-0.301102	-1.800937	3.129982
6	-1.136756	-0.902043	2.434344
6	-2.536860	-1.126749	2.547177
6	-3.041961	-2.212308	3.268039
6	-0.563710	0.148072	1.596137
7	-3.642814	2.973034	2.200218
7	-2.664663	3.484101	2.145912
8	-3.334563	-0.192432	1.939295
6	-4.733036	-0.342188	2.039084

26	-0.548272	-0.110153	-0.864547
7	-2.140285	1.087771	-1.205582
6	-2.135132	2.445327	-1.337472
6	-3.484102	2.936489	-1.586681
6	-4.300011	1.823474	-1.609740
6	-3.440783	0.682851	-1.374167
6	-0.998036	3.247084	-1.312599
6	0.305058	2.787600	-1.181215
7	0.668774	1.483294	-1.015488
6	2.031525	1.470010	-0.930730
6	2.561555	2.818588	-1.073071
6	1.481633	3.643157	-1.220223
6	-3.889388	-0.630945	-1.331016
6	-3.109691	-1.751339	-1.064222
7	-1.774937	-1.723165	-0.773096
6	-1.415610	-3.005763	-0.445301
6	-2.559509	-3.881707	-0.511281
6	-3.621294	-3.112103	-0.940217
6	2.818882	0.357454	-0.673964
6	2.350367	-0.926646	-0.423592
7	1.043911	-1.311853	-0.478564
6	1.013911	-2.642322	-0.159063
6	2.354619	-3.122636	0.128962
6	3.192155	-2.049354	-0.035912
6	-0.127805	-3.430470	-0.131429
6	0.157866	1.204461	2.269276
8	-0.450687	1.593518	3.465951
8	1.181517	1.784414	1.907678
1	-0.004731	-4.474854	0.134645
1	-4.947930	-0.798192	-1.479066
1	-1.132990	4.313479	-1.452340
1	3.887127	0.514916	-0.610023
1	0.772603	-1.638552	3.072502
1	-0.112163	-3.556870	4.366440
1	-4.112583	-2.371907	3.339862
1	-2.583089	-3.940047	4.473670
1	-5.163848	0.506554	1.505082
1	-5.079057	-1.275416	1.572847
1	-5.070647	-0.319114	3.086409
6	-0.069213	-2.271269	-3.716598
1	-0.977429	-2.798198	-3.401230
1	0.086964	-2.467475	-4.784207
1	0.777794	-2.696431	-3.164521
16	-0.206138	-0.463502	-3.431783
6	1.450060	5.133321	-1.380702
1	2.460779	5.552697	-1.415297
1	0.936969	5.432439	-2.304250
1	0.922549	5.617022	-0.547780
6	2.689070	-4.526504	0.536810
1	2.117969	-4.834520	1.422032

1	2.458425	-5.246604	-0.259995
1	3.752228	-4.635166	0.775380
6	-2.538239	-5.347849	-0.197997
1	-1.882480	-5.901698	-0.883338
1	-2.171946	-5.529639	0.820458
1	-3.535924	-5.790213	-0.277998
6	-5.786014	1.771150	-1.796974
1	-6.068507	1.684805	-2.856236
1	-6.230248	0.917086	-1.274846
1	-6.256507	2.682925	-1.411896
6	-3.828052	4.344600	-1.733402
6	-4.873964	4.869993	-2.394291
1	-3.149779	5.042799	-1.242484
1	-5.035471	5.944604	-2.413196
1	-5.579215	4.263603	-2.953418
6	-4.974427	-3.596190	-1.199566
6	-5.840419	-3.163209	-2.130694
1	-5.292184	-4.432453	-0.574363
1	-6.825485	-3.612801	-2.225929
1	-5.591175	-2.377403	-2.836975
6	4.676074	-1.985560	0.192559
6	5.513425	-1.973358	-1.120707
1	4.991377	-2.844652	0.796700
1	4.933072	-1.086674	0.763592
1	5.276980	-2.853016	-1.724145
1	5.270334	-1.075719	-1.695325
6	4.023338	3.164036	-1.016298
6	4.640339	3.050510	0.412876
1	4.178739	4.182333	-1.389487
1	4.574513	2.505425	-1.694734
1	4.753193	4.030932	0.882443
1	3.956929	2.474686	1.051354
6	6.988127	-1.952140	-0.808124
8	7.630796	-1.000396	-0.391917
8	7.581038	-3.154783	-0.987146
1	8.512515	-3.035862	-0.718272
6	5.987261	2.354791	0.486715
8	6.915598	2.684382	1.195362
8	6.023072	1.259516	-0.308126
1	6.839397	0.730619	-0.160463
6	0.186216	2.666323	4.156812
6	-0.623168	2.944393	5.415038
1	0.236336	3.551249	3.510158
1	1.220546	2.392381	4.401569
1	-0.167371	3.758331	5.992884
1	-1.648676	3.232823	5.159966
1	-0.671093	2.052316	6.049112

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<sup>5</sup>TS(C-D)<sub>Fe(cys)</sub>

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Number of imaginary frequencies: 1	Electronic energy:	HF=-3048.4246379
Zero-point correction=	0.838381 (Hartree/Particle)	
Thermal correction to Energy=	0.897900	
Thermal correction to Enthalpy=	0.898844	
Thermal correction to Gibbs Free Energy=	0.740028	
Sum of electronic and zero-point Energies=	-3047.586257	
Sum of electronic and thermal Energies=	-3047.526738	
Sum of electronic and thermal Enthalpies=	-3047.525794	
Sum of electronic and thermal Free Energies=	-3047.684610	

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Cartesian Coordinates

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6	2.860525	1.178821	3.647520
6	2.020448	2.176202	3.146171
6	0.806691	1.837668	2.547859
6	0.385245	0.498861	2.428422
6	1.231224	-0.486105	3.001234
6	2.452167	-0.153204	3.587641
6	-0.866788	0.079042	1.757739
8	0.897747	-1.824487	3.000128
6	-0.478075	-2.104974	3.011319
26	-0.817427	-0.076318	-0.476264
7	-2.526181	1.121173	-0.676602
6	-2.533136	2.472219	-0.805453
6	-3.908947	2.935927	-0.999613
6	-4.704300	1.803863	-0.988126
6	-3.810463	0.672722	-0.793895
6	-1.388285	3.285528	-0.824420
6	-0.046520	2.891821	-0.761816
7	0.393879	1.612672	-0.609913
6	1.752390	1.621492	-0.671451
6	2.224271	2.996940	-0.856694
6	1.102333	3.785912	-0.903081
6	-4.202866	-0.673540	-0.751049
6	-3.390735	-1.808826	-0.614430
7	-2.041475	-1.778742	-0.441707
6	-1.596166	-3.060672	-0.296291
6	-2.724554	-3.973106	-0.347658
6	-3.849329	-3.203272	-0.577062
6	2.565193	0.486692	-0.559621
6	2.167500	-0.846699	-0.382902
7	0.881512	-1.280037	-0.344767
6	0.890057	-2.634881	-0.191989
6	2.270504	-3.101838	-0.099863
6	3.065426	-1.988372	-0.216134
6	-0.250519	-3.446892	-0.160442
6	-2.082239	0.778411	2.222653
8	-3.130127	-0.089511	2.381423
8	-2.205378	1.969680	2.470164

1	-0.072566	-4.512977	-0.047764
1	-5.266631	-0.861860	-0.831731
1	-1.560391	4.348753	-0.959090
1	3.632304	0.658436	-0.617762
1	0.158294	2.608759	2.151488
1	2.311110	3.222312	3.214811
1	3.061541	-0.953449	3.998141
1	3.821570	1.431810	4.087233
1	-0.946796	-1.918550	3.985924
1	-0.962502	-1.181945	2.153950
1	-0.652479	-3.101968	2.612508
6	-0.597060	-1.904878	-3.429811
1	-1.490552	-2.470697	-3.147322
1	-0.504868	-1.925947	-4.522652
1	0.280401	-2.398019	-2.999105
16	-0.707126	-0.153491	-2.907358
6	0.999144	5.271958	-1.081465
1	1.984824	5.744457	-1.142361
1	0.452777	5.533289	-1.997844
1	0.462713	5.741213	-0.245882
6	2.680846	-4.529550	0.105689
1	2.355669	-5.171117	-0.724876
1	3.768212	-4.630654	0.188490
1	2.241432	-4.944916	1.022136
6	-2.632969	-5.466546	-0.239489
1	-2.024876	-5.772287	0.621441
1	-3.620641	-5.925459	-0.126693
1	-2.170642	-5.912934	-1.131337
6	-6.195511	1.723721	-1.116667
1	-6.520304	1.658199	-2.165505
1	-6.598299	0.845607	-0.600224
1	-6.671392	2.614064	-0.689280
6	-4.290395	4.334800	-1.132219
6	-5.382646	4.841545	-1.731118
1	-3.596402	5.046769	-0.684466
1	-5.562184	5.913523	-1.742511
1	-6.111196	4.222722	-2.244938
6	-5.204200	-3.719242	-0.746778
6	-6.187314	-3.229314	-1.520620
1	-5.420813	-4.634812	-0.192693
1	-7.159854	-3.713573	-1.556855
1	-6.051266	-2.359134	-2.154931
6	4.562867	-1.905150	-0.146029
6	5.225244	-1.743834	-1.549146
1	4.967840	-2.809285	0.323269
1	4.868016	-1.060217	0.483005
1	4.959698	-2.596307	-2.179950
1	4.863982	-0.827804	-2.022963
6	3.656681	3.436529	-1.012748
6	4.562569	3.264372	0.242718

1	3.660031	4.495687	-1.290747
1	4.123966	2.909409	-1.851681
1	5.219582	4.141833	0.331641
1	3.971375	3.214002	1.159940
6	6.720632	-1.654344	-1.418161
8	7.370422	-0.644281	-1.190793
8	7.333799	-2.854171	-1.522760
1	8.282206	-2.685768	-1.362058
6	5.496129	2.064948	0.254042
8	5.824482	1.459371	1.255718
8	5.970321	1.760710	-0.973055
1	6.541427	0.955575	-0.905362
6	-4.368559	0.499696	2.795923
6	-5.362782	-0.631759	3.001328
1	-4.709581	1.201208	2.026727
1	-4.210834	1.073640	3.716578
1	-6.334490	-0.230490	3.314790
1	-5.499402	-1.196639	2.073797
1	-5.009534	-1.324426	3.773514

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$^5\text{D}_{\text{Fe}(\text{cys})}$

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3048.4856298  
Zero-point correction=                    0.841548 (Hartree/Particle)  
Thermal correction to Energy=            0.902976  
Thermal correction to Enthalpy=         0.903920  
Thermal correction to Gibbs Free Energy= 0.736069  
Sum of electronic and zero-point Energies= -3047.644082  
Sum of electronic and thermal Energies= -3047.582654  
Sum of electronic and thermal Enthalpies= -3047.581710  
Sum of electronic and thermal Free Energies= -3047.749561

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Cartesian Coordinates

.....

6	-0.221676	6.224046	1.949819
6	-1.558444	6.680106	1.937729
6	-2.602441	5.793055	1.796197
6	-2.378042	4.382194	1.657821
6	-0.999778	3.957267	1.697156
6	0.057456	4.870014	1.830214
6	-3.410321	3.446472	1.475621
8	-0.806452	2.617819	1.595469
6	0.364694	1.984095	1.541702
26	0.297825	-2.036936	-0.859935
7	-1.867822	-1.872767	-0.892663
6	-2.595341	-0.931497	-1.549968
6	-4.008142	-1.320290	-1.593914
6	-4.092566	-2.524525	-0.922023
6	-2.740760	-2.846373	-0.490433

6	-2.069380	0.245963	-2.099374
6	-0.755051	0.712014	-2.009010
7	0.262870	0.071218	-1.365377
6	1.360381	0.876097	-1.452566
6	1.041480	2.082565	-2.219239
6	-0.285064	1.979980	-2.557679
6	-2.396470	-3.979523	0.257287
6	-1.146123	-4.299841	0.798996
7	-0.040854	-3.509015	0.698918
6	0.921066	-4.051759	1.501605
6	0.426502	-5.263623	2.130010
6	-0.863096	-5.446100	1.670939
6	2.580407	0.620423	-0.814940
6	2.882316	-0.447538	0.042434
7	2.067491	-1.512906	0.281535
6	2.705024	-2.310952	1.190742
6	3.990569	-1.727591	1.556972
6	4.097250	-0.556838	0.848189
6	2.189511	-3.496043	1.723153
6	-4.826330	3.743886	1.400213
8	-5.533792	2.587806	1.194926
8	-5.390500	4.832239	1.490931
1	2.833125	-4.031726	2.415736
1	-3.203991	-4.661320	0.496007
1	-2.764642	0.883854	-2.635819
1	3.359684	1.361123	-0.954254
1	-3.630309	6.132709	1.777598
1	-1.765492	7.742809	2.037436
1	1.087304	4.530329	1.831497
1	0.597227	6.930393	2.056439
1	1.293432	2.532335	1.457624
1	-3.148382	2.402935	1.356618
1	0.275046	0.919755	1.382023
6	2.085158	-4.549767	-2.133275
1	1.506812	-5.249913	-1.521030
1	2.540222	-5.109969	-2.958079
1	2.888746	-4.135188	-1.515126
16	1.012573	-3.218376	-2.830048
6	-1.138425	2.948822	-3.321757
1	-0.551263	3.781770	-3.722537
1	-1.640357	2.462717	-4.168212
1	-1.924782	3.380873	-2.688080
6	4.952725	-2.314010	2.547634
1	5.340392	-3.284760	2.209497
1	5.815824	-1.659972	2.712604
1	4.478011	-2.484426	3.522912
6	1.213024	-6.143181	3.056126
1	1.673444	-5.565408	3.868092
1	0.584896	-6.914486	3.513553
1	2.028137	-6.660438	2.530941

6	-5.321979	-3.328270	-0.624835
1	-5.565312	-4.030328	-1.435834
1	-5.206786	-3.919734	0.289521
1	-6.192538	-2.674551	-0.495289
6	-5.064976	-0.510670	-2.183137
6	-6.264570	-0.917169	-2.638337
1	-4.844129	0.554096	-2.259460
1	-6.972965	-0.201801	-3.047916
1	-6.566301	-1.959477	-2.650375
6	-1.737881	-6.563320	2.011522
6	-2.680772	-7.132113	1.241934
1	-1.573764	-6.997472	2.999781
1	-3.271583	-7.966909	1.610344
1	-2.874526	-6.806871	0.224565
6	5.176507	0.482431	0.938588
6	6.148790	0.480847	-0.274123
1	5.766263	0.328554	1.850612
1	4.731178	1.480565	1.024938
1	6.665461	-0.478171	-0.355441
1	5.579124	0.637774	-1.196691
6	1.978681	3.203495	-2.579850
6	2.241129	4.263538	-1.465473
1	1.559550	3.738812	-3.438800
1	2.944879	2.810362	-2.915522
1	2.531728	5.205415	-1.949595
1	1.338827	4.447683	-0.878784
6	7.148845	1.598664	-0.149547
8	6.883404	2.790974	-0.088688
8	8.427110	1.175188	-0.066169
1	8.972666	1.979822	0.031524
6	3.369628	3.907751	-0.520213
8	3.279209	3.791428	0.691304
8	4.525623	3.742717	-1.186856
1	5.251600	3.471907	-0.572297
6	-6.953284	2.733773	1.070831
6	-7.540020	1.343544	0.889142
1	-7.178371	3.384070	0.216566
1	-7.348875	3.230341	1.964847
1	-8.629179	1.407257	0.778122
1	-7.126980	0.854598	0.000775
1	-7.317531	0.713046	1.756551

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**AIr(Me)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-1979.5214745  
Zero-point correction=                    0.636846 (Hartree/Particle)  
Thermal correction to Energy=            0.679358  
Thermal correction to Enthalpy=        0.680302  
Thermal correction to Gibbs Free Energy=    0.560149



Sum of electronic and zero-point Energies=	-1978.884629
Sum of electronic and thermal Energies=	-1978.842117
Sum of electronic and thermal Enthalpies=	-1978.841173
Sum of electronic and thermal Free Energies=	-1978.961325

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Cartesian Coordinates  
.....

6	-3.996948	-3.095273	-0.083567
6	-2.638459	-2.595259	-0.138213
7	-2.640442	-1.218189	-0.103397
6	-3.952900	-0.822693	-0.016116
6	-4.821358	-1.993724	-0.001647
6	-1.495425	-3.386323	-0.221120
6	-0.179733	-2.949140	-0.309575
7	0.214334	-1.630430	-0.324469
6	1.584816	-1.624533	-0.433554
6	2.078691	-2.992981	-0.486452
6	0.984816	-3.813191	-0.411994
6	2.375506	-0.482153	-0.512069
6	1.939901	0.838752	-0.479207
7	0.631925	1.231223	-0.320636
6	0.622116	2.606700	-0.328431
6	1.971937	3.107086	-0.520321
6	2.790061	2.011201	-0.615451
6	-0.508208	3.401650	-0.172120
6	-1.821131	2.970166	-0.012023
7	-2.216619	1.654215	-0.044035
6	-3.589758	1.641570	0.048888
6	-4.089721	2.996084	0.134183
6	-2.993684	3.829397	0.124443
77	-0.996428	0.007106	-0.128507
6	-4.381498	0.497100	0.065331
1	-0.355334	4.473386	-0.205579
1	-5.450606	0.655974	0.154234
1	-1.647633	-4.460319	-0.222804
1	3.443077	-0.638459	-0.612043
6	-0.850834	-0.004688	1.931383
1	-1.849017	-0.151372	2.353251
1	-0.189190	-0.820681	2.235475
1	-0.441007	0.954783	2.259335
6	4.276253	1.987020	-0.839182
1	4.539733	1.169560	-1.521562
1	4.596612	2.912833	-1.327374
6	5.101206	1.828069	0.466404
1	4.879335	0.877930	0.954935
1	4.841322	2.640086	1.154568
6	6.580413	1.946045	0.174462
8	7.133588	2.917900	-0.283927
8	7.280445	0.802163	0.463174
1	8.211809	0.989881	0.234646

6	3.534582	-3.359638	-0.559402
1	4.042648	-2.695041	-1.264760
1	3.647130	-4.371619	-0.961777
6	4.251573	-3.284227	0.824473
1	3.648046	-2.670290	1.505197
1	4.347776	-4.271573	1.281321
6	5.627219	-2.647740	0.809336
8	6.616740	-3.076887	1.358469
8	5.613227	-1.466612	0.139358
1	6.469577	-1.008324	0.272988
6	0.934349	-5.311652	-0.425546
1	1.927078	-5.743147	-0.584529
1	0.550014	-5.714031	0.521057
1	0.280889	-5.687515	-1.223163
6	2.336856	4.559476	-0.599128
1	2.135231	5.080291	0.346373
1	3.398422	4.695474	-0.825534
1	1.763986	5.078080	-1.378023
6	-4.383770	-4.540640	-0.163104
1	-3.699676	-5.105365	-0.806014
1	-4.377625	-5.026779	0.822519
1	-5.393998	-4.648047	-0.570792
6	-5.537099	3.366407	0.257582
1	-6.132471	2.951509	-0.565688
1	-5.972467	2.988511	1.192182
1	-5.673866	4.451170	0.253468
6	-6.278831	-1.928284	0.043196
6	-7.108940	-2.833352	0.584939
1	-6.725657	-1.045217	-0.413810
1	-8.185601	-2.695462	0.544983
1	-6.751345	-3.718448	1.101676
6	-3.024169	5.287797	0.228687
6	-2.136680	6.078613	0.851091
1	-3.890301	5.766839	-0.228608
1	-2.268730	7.156611	0.868396
1	-1.276510	5.685575	1.384590

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**BIr(Me)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2741.0390459  
Zero-point correction=                    0.858326 (Hartree/Particle)  
Thermal correction to Energy=            0.918039  
Thermal correction to Enthalpy=         0.918983  
Thermal correction to Gibbs Free Energy= 0.759223  
Sum of electronic and zero-point Energies= -2740.180720  
Sum of electronic and thermal Energies= -2740.121007  
Sum of electronic and thermal Enthalpies= -2740.120063  
Sum of electronic and thermal Free Energies= -2740.279822

## Cartesian Coordinates

6	-3.075919	2.378958	-2.026531
6	-2.527176	1.083885	-1.682828
7	-1.226845	1.223186	-1.257032
6	-0.915157	2.558872	-1.341570
6	-2.086526	3.305488	-1.793443
6	-3.219872	-0.120298	-1.763658
6	-2.766116	-1.379327	-1.383808
7	-1.516602	-1.641037	-0.881465
6	-1.460908	-2.992271	-0.622700
6	-2.725640	-3.613426	-0.957173
6	-3.539864	-2.614851	-1.449111
6	-0.345887	-3.662375	-0.123458
6	0.894537	-3.114861	0.181090
7	1.226998	-1.787763	0.038496
6	2.544099	-1.663212	0.410349
6	3.065213	-2.960793	0.818015
6	2.040690	-3.859227	0.679298
77	0.013036	-0.291984	-0.663176
7	1.524943	1.064943	-0.378978
6	2.803725	0.787251	0.041365
6	3.590877	2.010403	0.048674
6	2.767197	3.014761	-0.392972
6	1.474116	2.409262	-0.657053
6	3.268183	-0.473982	0.406669
6	0.346351	3.092547	-1.102887
8	-5.527568	-0.756533	1.315424
6	-4.936412	0.465594	1.318528
8	-5.448825	1.466963	0.846178
6	-3.620176	0.422432	1.967763
7	-3.256630	-0.768034	2.408214
7	-2.974010	-1.801524	2.783850
6	-2.756414	1.595397	2.217811
6	-3.323302	2.872957	2.362006
6	-2.534553	3.984325	2.652753
6	-1.157674	3.839730	2.817223
6	-0.568360	2.584433	2.664428
6	-1.354293	1.473730	2.353589
8	-0.812702	0.224618	2.142377
6	0.334842	-0.140012	2.916913
1	0.460993	4.153564	-1.289344
1	4.305185	-0.541525	0.713502
1	-0.450703	-4.730909	0.030514
1	-4.229130	-0.060949	-2.154599
1	-4.392563	2.984334	2.237887
1	-3.002675	4.958220	2.761965
1	0.505781	2.471958	2.759738
1	-0.536400	4.698399	3.057014
1	0.440876	-1.218934	2.800423

1	1.240880	0.347437	2.545114
1	0.177815	0.114298	3.971765
6	0.664590	-0.610536	-2.593461
1	1.710620	-0.931416	-2.570508
1	0.047923	-1.386255	-3.057670
1	0.575055	0.322555	-3.158244
6	-6.858241	-0.834791	0.757165
1	-6.940744	-1.865766	0.405532
1	-6.925517	-0.154443	-0.095291
6	-7.914568	-0.508250	1.802833
1	-7.823927	0.532031	2.128955
1	-8.915421	-0.649284	1.378317
1	-7.814917	-1.163175	2.674625
6	-4.493343	2.618593	-2.448062
1	-4.649098	3.656707	-2.755257
1	-4.782882	1.975392	-3.288797
1	-5.180787	2.411745	-1.617798
6	-3.055536	-5.059575	-0.746197
1	-4.123709	-5.186374	-0.540657
1	-2.819727	-5.673121	-1.627126
1	-2.501143	-5.479607	0.099536
6	-2.207409	4.753128	-1.959669
6	-1.656423	5.704807	-1.190891
1	-2.844614	5.074362	-2.784176
1	-1.818646	6.757332	-1.405691
1	-1.065794	5.470130	-0.310569
6	-4.916048	-2.686784	-1.924478
6	-5.550523	-3.756389	-2.433067
1	-5.480265	-1.756851	-1.866495
1	-6.587973	-3.687400	-2.747564
1	-5.063564	-4.714660	-2.579910
6	3.080982	4.469304	-0.580399
1	4.086932	4.712905	-0.225142
1	3.027192	4.762128	-1.637189
1	2.375082	5.109503	-0.036517
6	5.032795	2.110076	0.461774
1	5.251514	3.127749	0.804531
1	5.233581	1.443721	1.308367
6	4.483653	-3.202744	1.256483
1	4.537875	-4.129253	1.837342
1	4.797300	-2.402475	1.933568
6	5.493292	-3.293013	0.070597
1	5.008778	-2.922662	-0.842517
1	5.789441	-4.325452	-0.128891
6	6.021227	1.752494	-0.687149
1	5.842968	0.725882	-1.014275
1	5.864497	2.429272	-1.531099
6	6.766092	-2.475359	0.212975
8	7.867196	-2.837702	-0.137358
8	6.514080	-1.245139	0.716943

1	7.312940	-0.667548	0.643807
6	7.450729	1.856192	-0.214015
8	8.087539	0.981233	0.352444
8	7.983060	3.074291	-0.432756
1	8.886842	3.054625	-0.061977
6	2.042246	-5.333128	0.955565
1	1.893244	-5.918153	0.038307
1	2.989831	-5.655776	1.397110
1	1.241453	-5.616268	1.650552

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**TS(B-C)<sub>Ir(Me)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2740.9924631  
Zero-point correction=                    0.854747 (Hartree/Particle)  
Thermal correction to Energy=            0.914244  
Thermal correction to Enthalpy=         0.915188  
Thermal correction to Gibbs Free Energy=    0.758524  
Sum of electronic and zero-point Energies=    -2740.137716  
Sum of electronic and thermal Energies=    -2740.078219  
Sum of electronic and thermal Enthalpies=   -2740.077275  
Sum of electronic and thermal Free Energies=   -2740.233940

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Cartesian Coordinates

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6	3.082642	-3.713430	-1.006070
6	1.862039	-3.021142	-0.649454
7	2.040618	-1.659955	-0.778181
6	3.315654	-1.463428	-1.248176
6	3.988279	-2.748406	-1.393165
6	0.665462	-3.642254	-0.296615
6	-0.564727	-3.029405	-0.076192
7	-0.787130	-1.677289	-0.100434
6	-2.135791	-1.482809	0.054062
6	-2.797994	-2.771431	0.211559
6	-1.821849	-3.730617	0.140104
6	-2.776412	-0.246579	0.057744
6	-2.189652	1.005613	-0.112741
7	-0.858376	1.227625	-0.339651
6	-0.693461	2.571549	-0.536402
6	-1.971333	3.247772	-0.384612
6	-2.900899	2.276345	-0.116989
6	0.504789	3.196672	-0.874121
6	1.736376	2.588465	-1.101444
7	1.971529	1.240557	-1.028162
6	3.242253	1.017532	-1.491092
6	3.858096	2.275864	-1.858926
6	2.941676	3.264980	-1.579753
77	0.616439	-0.213461	-0.492224
6	3.858942	-0.228189	-1.586814

1	0.463627	4.267707	-1.029927
1	4.863687	-0.235644	-1.995390
1	0.678181	-4.726214	-0.254974
1	-3.850881	-0.260743	0.196883
6	0.990986	0.114144	1.764163
6	1.312440	1.479706	2.278608
6	0.300305	2.282032	2.842048
6	2.601433	2.066589	2.147920
6	0.533556	3.598264	3.237550
1	-0.691143	1.864279	2.943341
6	2.840464	3.376125	2.576500
6	1.806609	4.145364	3.110882
1	-0.282012	4.183665	3.652054
1	3.830803	3.804393	2.481744
1	2.007604	5.165422	3.427515
6	-0.053240	-0.627035	2.568136
8	-1.169630	-0.181272	2.759219
8	0.323860	-1.848604	2.987867
8	3.581351	1.274653	1.636865
6	4.913988	1.760277	1.584497
1	5.507319	0.942510	1.172299
1	4.990816	2.632963	0.925751
1	5.285989	2.017332	2.584697
7	3.148347	-1.720177	1.843216
7	2.462316	-0.910139	2.178922
6	0.044593	-0.348605	-2.515921
1	-1.040438	-0.477755	-2.587762
1	0.330397	0.566337	-3.046021
1	0.536933	-1.206228	-2.987445
6	-4.372332	2.454275	0.132497
1	-4.709553	1.752574	0.904945
1	-4.567105	3.459250	0.520666
6	-5.245958	2.256768	-1.135667
1	-5.153798	1.238752	-1.517245
1	-4.906961	2.949521	-1.914063
6	-6.691578	2.588740	-0.842021
8	-7.109901	3.663120	-0.478860
8	-7.536112	1.520052	-1.007728
1	-8.430894	1.847237	-0.790745
6	-4.285151	-2.945106	0.345237
1	-4.686844	-2.159997	0.992263
1	-4.510300	-3.894352	0.842991
6	-5.025529	-2.908509	-1.027467
1	-4.373598	-2.431300	-1.770287
1	-5.246663	-3.913916	-1.392485
6	-6.317514	-2.116284	-1.048157
8	-7.361532	-2.470083	-1.548549
8	-6.152559	-0.895011	-0.478953
1	-6.950011	-0.349691	-0.645778
6	-1.967309	-5.221661	0.215695

1	-2.993182	-5.509708	0.464790
1	-1.714857	-5.703193	-0.738319
1	-1.308883	-5.657894	0.977844
6	-2.170231	4.729015	-0.505562
1	-1.937875	5.087903	-1.516856
1	-3.203605	5.014789	-0.287584
1	-1.521061	5.279916	0.186819
6	3.286150	-5.195241	-0.916799
1	2.714565	-5.630107	-0.089556
1	2.974965	-5.713949	-1.834377
1	4.343180	-5.430261	-0.755111
6	5.246140	2.422348	-2.407811
1	6.006953	2.064099	-1.701133
1	5.375506	1.846359	-3.333023
1	5.479667	3.467018	-2.631449
6	5.373601	-2.898042	-1.826356
6	5.912216	-3.946630	-2.468733
1	6.030637	-2.058900	-1.597056
1	6.967573	-3.959221	-2.725653
1	5.327049	-4.806236	-2.779651
6	3.147135	4.703307	-1.745061
6	2.675258	5.679915	-0.954478
1	3.779490	4.992664	-2.585011
1	2.893218	6.722754	-1.167325
1	2.087063	5.473657	-0.065202
6	-0.691471	-2.625672	3.668398
1	-1.056601	-2.052333	4.526187
1	-1.527835	-2.781721	2.981846
6	-0.045574	-3.933548	4.086155
1	0.795997	-3.758659	4.764350
1	-0.779966	-4.561445	4.602676
1	0.323629	-4.478148	3.211237

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**Cr(Me)**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2741.0240614  
 Zero-point correction=                    0.853187 (Hartree/Particle)  
 Thermal correction to Energy=            0.914977  
 Thermal correction to Enthalpy=         0.915922  
 Thermal correction to Gibbs Free Energy= 0.749483  
 Sum of electronic and zero-point Energies= -2740.170874  
 Sum of electronic and thermal Energies= -2740.109084  
 Sum of electronic and thermal Enthalpies= -2740.108140  
 Sum of electronic and thermal Free Energies= -2740.274578

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 Cartesian Coordinates  
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6	3.158903	-3.247025	-1.472178
6	1.917100	-2.674204	-0.998230
7	1.981269	-1.305922	-1.076785

6	3.196865	-0.975330	-1.609836
6	3.953564	-2.192211	-1.878740
6	0.800908	-3.405866	-0.590476
6	-0.458795	-2.904991	-0.276604
7	-0.788674	-1.577504	-0.228923
6	-2.139669	-1.493988	-0.016132
6	-2.693035	-2.837890	0.103566
6	-1.648318	-3.711755	-0.044357
6	-2.872369	-0.312457	0.073347
6	-2.382258	0.989248	-0.017553
7	-1.079140	1.325971	-0.246798
6	-0.995567	2.689511	-0.282913
6	-2.312215	3.257871	-0.042830
6	-3.173402	2.202822	0.121723
6	0.159983	3.423347	-0.547339
6	1.418806	2.925174	-0.881196
7	1.735194	1.598999	-0.986479
6	2.979502	1.509835	-1.552275
6	3.505051	2.840148	-1.783680
6	2.556444	3.728041	-1.328742
77	0.498486	0.006275	-0.535785
6	3.640641	0.321978	-1.857506
1	0.052183	4.500969	-0.567999
1	4.609009	0.422619	-2.335217
1	0.904087	-4.485416	-0.592997
1	-3.937760	-0.417126	0.239223
6	0.876673	0.200711	1.470902
6	1.741717	1.165764	2.153254
6	1.171259	2.182302	2.951794
6	3.157055	1.153134	2.001404
6	1.946121	3.203436	3.493572
1	0.096222	2.176781	3.093433
6	3.934423	2.168107	2.570665
6	3.327138	3.194521	3.295971
1	1.476236	3.993774	4.071471
1	5.011812	2.161947	2.457324
1	3.946480	3.979828	3.721250
6	-0.135095	-0.366478	2.412619
8	-1.163676	0.186036	2.759195
8	0.246007	-1.585560	2.839037
8	3.677947	0.077402	1.363689
6	5.088818	-0.031694	1.250912
1	5.269804	-0.968918	0.724381
1	5.509547	0.798153	0.669460
1	5.563318	-0.066432	2.239638
7	3.225787	-3.645375	2.269009
7	3.661183	-2.809993	2.846793
6	-0.142187	0.072803	-2.582439
1	-1.144445	-0.358385	-2.687734
1	-0.164561	1.106251	-2.945810



1	0.554619	-0.499770	-3.206747
6	-4.647490	2.252163	0.410076
1	-4.915637	1.464737	1.124704
1	-4.902880	3.203925	0.886973
6	-5.534891	2.100060	-0.855553
1	-5.380962	1.125976	-1.322829
1	-5.264263	2.878129	-1.577485
6	-6.991962	2.301862	-0.506263
8	-7.484240	3.326221	-0.094895
8	-7.750355	1.170726	-0.675404
1	-8.660022	1.414102	-0.414713
6	-4.156409	-3.133512	0.281159
1	-4.587829	-2.423938	0.993498
1	-4.287880	-4.126584	0.723590
6	-4.956373	-3.068198	-1.057123
1	-4.367370	-2.510814	-1.796641
1	-5.131813	-4.064017	-1.469960
6	-6.294145	-2.359468	-0.981178
8	-7.335274	-2.752020	-1.458046
8	-6.180035	-1.162424	-0.351357
1	-7.016440	-0.661131	-0.453408
6	-1.671824	-5.211176	-0.028916
1	-2.655688	-5.592053	0.261364
1	-1.436680	-5.631080	-1.015921
1	-0.938287	-5.621915	0.676520
6	-2.610575	4.726834	0.001098
1	-2.470497	5.198347	-0.980603
1	-3.642607	4.917262	0.310117
1	-1.953015	5.252271	0.704838
6	3.485416	-4.709325	-1.473585
1	2.998228	-5.229833	-0.642433
1	3.167667	-5.204977	-2.401586
1	4.565211	-4.863651	-1.378669
6	4.852742	3.140291	-2.368142
1	5.666701	2.793310	-1.717056
1	4.989386	2.651358	-3.340989
1	4.994396	4.214776	-2.514082
6	5.302640	-2.207721	-2.434352
6	5.878373	-3.191822	-3.143947
1	5.896991	-1.312478	-2.251437
1	6.901898	-3.097008	-3.494989
1	5.353463	-4.100322	-3.420613
6	2.672617	5.185039	-1.311637
6	2.192850	6.015932	-0.373632
1	3.238138	5.621221	-2.135581
1	2.338310	7.089653	-0.451445
1	1.671689	5.654586	0.508059
6	-0.660675	-2.247553	3.755025
1	-0.833588	-1.594716	4.616452
1	-1.618427	-2.396796	3.247565

6	-0.020478	-3.563337	4.155317
1	0.937643	-3.396485	4.657723
1	-0.681273	-4.103562	4.842489
1	0.155882	-4.191642	3.276553

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**TS(C-P)<sub>Ir(Me)</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2631.4739795  
 Zero-point correction=                    0.843160 (Hartree/Particle)  
 Thermal correction to Energy=            0.899862  
 Thermal correction to Enthalpy=         0.900806  
 Thermal correction to Gibbs Free Energy= 0.748437  
 Sum of electronic and zero-point Energies= -2630.630820  
 Sum of electronic and thermal Energies= -2630.574118  
 Sum of electronic and thermal Enthalpies= -2630.573173  
 Sum of electronic and thermal Free Energies= -2630.725542

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 Cartesian Coordinates  
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6	3.396672	-3.497412	-0.993282
6	2.119741	-2.877918	-0.703992
7	2.222673	-1.510845	-0.832955
6	3.504548	-1.238167	-1.238742
6	4.262992	-2.480701	-1.339155
6	0.948636	-3.565085	-0.391663
6	-0.315763	-3.022482	-0.182636
7	-0.614835	-1.684705	-0.209978
6	-1.964537	-1.565488	-0.002276
6	-2.549097	-2.888439	0.179056
6	-1.525683	-3.791723	0.070468
6	-2.669368	-0.365131	0.028699
6	-2.156743	0.914660	-0.170949
7	-0.843810	1.203569	-0.434376
6	-0.754520	2.554418	-0.639486
6	-2.063567	3.163126	-0.467815
6	-2.933432	2.147057	-0.164716
6	0.412661	3.247972	-0.955068
6	1.687095	2.717951	-1.128396
7	1.994498	1.382845	-1.058913
6	3.304747	1.243705	-1.446168
6	3.869380	2.544310	-1.745445
6	2.877746	3.471099	-1.518663
77	0.695625	-0.149561	-0.599269
6	3.995460	0.033514	-1.529483
1	0.313530	4.315550	-1.110006
1	5.021814	0.091376	-1.875324
1	1.021426	-4.646515	-0.344209
1	-3.735951	-0.436314	0.206842
6	0.240920	-0.293316	-2.643178
1	-0.560669	-1.022335	-2.806153

1	-0.078247	0.682397	-3.025504
1	1.134334	-0.614425	-3.191157
6	-4.404288	2.251277	0.126765
1	-4.683897	1.534254	0.907964
1	-4.636615	3.246262	0.520501
6	-5.303884	2.009729	-1.116167
1	-5.177092	0.993817	-1.493669
1	-5.018474	2.713268	-1.905561
6	-6.752760	2.280262	-0.779104
8	-7.216437	3.352225	-0.467782
8	-7.538648	1.156875	-0.829216
1	-8.439801	1.445922	-0.586256
6	-4.016711	-3.141977	0.380806
1	-4.426447	-2.383903	1.054603
1	-4.166151	-4.104843	0.880605
6	-4.824992	-3.136719	-0.953635
1	-4.232146	-2.631598	-1.726930
1	-5.020503	-4.150512	-1.309965
6	-6.149681	-2.401640	-0.908838
8	-7.199966	-2.799631	-1.360522
8	-6.011691	-1.175457	-0.342734
1	-6.839742	-0.666140	-0.469839
6	-1.583385	-5.287913	0.155930
1	-2.581542	-5.633004	0.442120
1	-1.336941	-5.759663	-0.804586
1	-0.875044	-5.681511	0.896266
6	-2.346946	4.629680	-0.602802
1	-2.184136	4.980150	-1.630535
1	-3.382237	4.864661	-0.338229
1	-1.695686	5.229531	0.045507
6	3.682988	-4.964565	-0.888856
1	3.085569	-5.435868	-0.100856
1	3.463910	-5.497828	-1.824471
1	4.739585	-5.137375	-0.659067
6	5.285630	2.784491	-2.174644
1	6.003128	2.479220	-1.401132
1	5.533829	2.220329	-3.082848
1	5.465986	3.843015	-2.381159
6	5.674102	-2.547059	-1.704493
6	6.309556	-3.568644	-2.300665
1	6.264531	-1.662503	-1.464523
1	7.374052	-3.514897	-2.509896
1	5.797036	-4.469924	-2.621203
6	3.007097	4.922183	-1.645818
6	2.430330	5.852326	-0.869474
1	3.671686	5.265304	-2.439214
1	2.599303	6.910421	-1.048347
1	1.803351	5.593513	-0.021300
6	1.126998	0.089640	1.739563
6	1.280596	1.419826	2.353147

6	0.291614	-0.837361	2.552205
6	0.203037	2.308987	2.544201
6	2.524219	1.831115	2.882324
8	-0.835033	-0.566930	2.927083
8	0.906946	-2.020413	2.782277
6	0.394844	3.554543	3.133833
1	-0.779311	2.006947	2.205964
6	2.733142	3.071033	3.478833
8	3.529660	0.873124	2.980807
6	1.659346	3.949042	3.587904
1	-0.452146	4.226908	3.238047
1	3.717654	3.316224	3.863518
6	3.552014	-0.012320	1.977561
1	1.802326	4.924036	4.044264
1	4.027491	-0.952260	2.248764
1	3.731801	0.380892	0.976436
1	2.221046	-0.379825	1.576888
6	0.138960	-3.016512	3.499350
1	-0.898911	-2.968251	3.162736
1	0.576280	-3.967489	3.185094
6	0.246007	-2.822637	5.005063
1	-0.209052	-1.873954	5.302934
1	-0.277813	-3.634099	5.524007
1	1.293111	-2.829563	5.326288

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**AIr(his)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2165.6403788  
Zero-point correction=                    0.672835 (Hartree/Particle)  
Thermal correction to Energy=            0.718515  
Thermal correction to Enthalpy=         0.719459  
Thermal correction to Gibbs Free Energy= 0.588480  
Sum of electronic and zero-point Energies= -2164.967544  
Sum of electronic and thermal Energies= -2164.921864  
Sum of electronic and thermal Enthalpies= -2164.920920  
Sum of electronic and thermal Free Energies= -2165.051899

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Cartesian Coordinates

6	4.250683	-2.724075	-0.774294
6	3.631594	-1.422015	-0.564320
7	2.263649	-1.570712	-0.497930
6	1.996639	-2.918647	-0.615863
6	3.231629	-3.651232	-0.776919
6	4.306849	-0.218722	-0.398855
6	3.749912	1.047098	-0.238972
7	2.397142	1.312553	-0.196936
6	2.258574	2.674047	-0.055132
6	3.571748	3.298730	-0.014226

6	4.497540	2.281577	-0.131922
6	1.040045	3.341412	0.049468
6	-0.233264	2.781974	-0.000879
7	-0.498491	1.433894	-0.118742
6	-1.868354	1.293640	-0.115567
6	-2.493718	2.600614	-0.011855
6	-1.479213	3.521920	0.061324
6	-2.542613	0.079655	-0.201471
6	-1.982664	-1.186899	-0.331557
7	-0.631495	-1.447868	-0.382624
6	-0.492803	-2.812641	-0.520022
6	-1.802096	-3.435494	-0.572474
6	-2.726811	-2.428701	-0.457983
7	0.948825	-0.250080	1.812370
6	1.012039	0.762490	2.674686
7	1.039441	0.263305	3.927332
6	0.992268	-1.114017	3.863243
6	0.935631	-1.431006	2.535842
6	0.722274	-3.482764	-0.607645
1	-3.625623	0.127884	-0.181155
1	0.672917	-4.561862	-0.707449
1	5.388039	-0.277743	-0.401436
1	1.086679	4.418111	0.169034
1	1.037809	1.809479	2.417550
1	1.003136	-1.735391	4.744628
1	0.887963	-2.391066	2.048634
1	1.087268	0.818548	4.771042
77	0.886799	-0.081115	-0.166704
6	-2.036612	-4.906503	-0.742383
1	-3.102406	-5.131750	-0.830966
1	-1.543782	-5.291560	-1.643433
1	-1.649892	-5.480734	0.109403
6	3.328133	-5.133138	-0.979166
1	2.862092	-5.439975	-1.924280
1	4.369470	-5.462393	-1.011537
1	2.828026	-5.686991	-0.175121
6	5.989376	2.392055	-0.209273
1	6.416428	1.638694	-0.879112
1	6.282673	3.377951	-0.582004
1	6.463720	2.259677	0.772380
6	-1.578671	5.014723	0.159608
1	-1.212802	5.504268	-0.752017
1	-2.613000	5.334858	0.309731
1	-0.988975	5.408057	0.996762
6	5.676938	-3.003805	-0.953913
6	6.553041	-2.266386	-1.651245
1	6.033358	-3.926979	-0.498170
1	7.592516	-2.568450	-1.734612
1	6.263083	-1.368571	-2.189613
6	3.785905	4.741445	0.080192

6	4.821847	5.352480	0.673959
1	3.022679	5.366938	-0.381757
1	4.903273	6.435122	0.674159
1	5.605450	4.806998	1.190552
6	-4.225246	-2.538551	-0.453342
6	-4.823936	-2.588428	0.963695
1	-4.536373	-3.434966	-0.998501
1	-4.675780	-1.701750	-0.997789
1	-4.462216	-3.463329	1.517261
1	-4.519510	-1.716875	1.557562
6	-6.339955	-2.630082	0.935210
8	-7.024258	-2.563588	-0.061094
8	-6.851863	-2.746410	2.181285
1	-7.823566	-2.758678	2.083737
6	-3.975381	2.847383	-0.019813
6	-4.570469	2.924289	-1.437453
1	-4.201152	3.779370	0.508326
1	-4.501842	2.066238	0.538879
1	-4.154751	3.767445	-2.001088
1	-4.322502	2.028334	-2.021543
6	-6.081278	3.055724	-1.405039
8	-6.770249	2.966509	-0.412804
8	-6.582863	3.276885	-2.639567
1	-7.553045	3.333283	-2.542593

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**B<sub>r</sub>(his)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2927.186901  
Zero-point correction=                    0.897181 (Hartree/Particle)  
Thermal correction to Energy=            0.958570  
Thermal correction to Enthalpy=         0.959514  
Thermal correction to Gibbs Free Energy= 0.798421  
Sum of electronic and zero-point Energies= -2926.289720  
Sum of electronic and thermal Energies= -2926.228331  
Sum of electronic and thermal Enthalpies= -2926.227387  
Sum of electronic and thermal Free Energies= -2926.388480

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Cartesian Coordinates

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6	3.028252	2.350044	1.950906
6	2.506077	1.068331	1.524529
7	1.235924	1.229798	1.024239
6	0.912314	2.560435	1.141059
6	2.051955	3.286094	1.690818
6	3.190051	-0.143438	1.603146
6	2.755577	-1.390429	1.162580
7	1.533933	-1.643608	0.594987
6	1.481228	-2.989092	0.315229
6	2.729286	-3.619304	0.699045
6	3.522153	-2.629189	1.239300

6	0.379026	-3.648242	-0.228876
6	-0.854321	-3.094234	-0.568881
7	-1.189063	-1.767555	-0.439094
6	-2.484457	-1.625887	-0.876553
6	-2.994384	-2.919481	-1.307856
6	-1.982086	-3.827514	-1.113985
7	-1.486808	1.097289	0.007589
6	-2.750244	0.822577	-0.456377
6	-3.551973	2.034305	-0.409968
6	-2.746908	3.028455	0.089471
6	-1.452131	2.428106	0.349549
6	-3.191266	-0.425617	-0.894336
6	-0.342349	3.098439	0.863684
8	5.750714	-0.335001	-1.191144
6	5.020439	0.799371	-1.265151
8	5.395391	1.889840	-0.871784
6	3.704422	0.552422	-1.879662
7	3.464550	-0.693138	-2.235308
7	3.284147	-1.772451	-2.542988
6	2.707746	1.600377	-2.176036
6	3.136362	2.898002	-2.516391
6	2.223869	3.892232	-2.857975
6	0.854936	3.618647	-2.882489
6	0.402965	2.348390	-2.528857
6	1.319773	1.366736	-2.164998
8	0.851136	0.086275	-1.790994
6	0.249017	-0.653203	-2.890872
1	-0.468631	4.152138	1.081619
1	-4.203317	-0.470350	-1.276548
1	0.486013	-4.715261	-0.389315
1	4.174878	-0.105349	2.053954
1	4.196567	3.115168	-2.506278
1	2.588995	4.879273	-3.125398
1	-0.656617	2.118181	-2.515461
1	0.142232	4.385716	-3.170020
1	0.262217	-1.703496	-2.609034
1	-0.776234	-0.316145	-3.057803
1	0.853222	-0.489085	-3.785522
6	7.109769	-0.210086	-0.692778
1	7.338006	-1.205033	-0.304207
1	7.118007	0.513106	0.126015
6	8.069930	0.194093	-1.800210
1	7.836203	1.196534	-2.170035
1	9.094941	0.203454	-1.413039
1	8.024621	-0.513644	-2.633965
6	4.413121	2.581659	2.472087
1	4.514302	3.580884	2.904058
1	4.685539	1.855252	3.246865
1	5.145670	2.499070	1.659110
6	3.063508	-5.063482	0.482996

1	4.145801	-5.197749	0.394386
1	2.724540	-5.696409	1.314355
1	2.602118	-5.451652	-0.431102
6	2.151786	4.727968	1.919274
6	1.654846	5.696681	1.136229
1	2.722663	5.023999	2.799029
1	1.792960	6.743494	1.389473
1	1.137411	5.483155	0.205428
6	4.884554	-2.712303	1.759635
6	5.440919	-3.767574	2.373125
1	5.494012	-1.818670	1.631515
1	6.472187	-3.735027	2.711482
1	4.892089	-4.680866	2.580017
6	-3.089276	4.466006	0.346323
1	-4.085346	4.713142	-0.031164
1	-3.077407	4.703231	1.418006
1	-2.376599	5.143901	-0.138894
6	-5.011741	2.121778	-0.754427
1	-5.242086	3.116803	-1.152241
1	-5.270225	1.408344	-1.543564
6	-4.370897	-3.200897	-1.847423
1	-4.334371	-4.139900	-2.407896
1	-4.674380	-2.434317	-2.568846
6	-5.485549	-3.337476	-0.768581
1	-5.116505	-3.873640	0.108455
1	-6.312112	-3.910232	-1.204671
6	-5.913684	1.848338	0.482180
1	-5.683175	0.859633	0.894963
1	-5.744286	2.605313	1.251434
6	-6.053355	-2.006531	-0.313278
8	-5.969119	-1.558670	0.815924
8	-6.651411	-1.365855	-1.331397
1	-7.074299	-0.525528	-1.009559
6	-7.370588	1.826248	0.093015
8	-7.883486	0.985653	-0.631964
8	-8.077553	2.846216	0.598117
1	-8.999155	2.743087	0.287629
6	-1.975678	-5.302942	-1.383857
1	-1.879047	-5.882607	-0.456792
1	-2.897347	-5.626996	-1.873548
1	-1.140272	-5.591491	-2.033498
7	-0.671617	-0.623919	2.160706
6	-1.014022	0.303344	3.050861
6	-0.888129	-1.862524	2.741061
7	-1.441583	-0.302227	4.178165
1	-0.960987	1.369551	2.901955
6	-1.370792	-1.669016	4.003718
1	-0.684201	-2.777753	2.211296
1	-1.763590	0.176439	5.007855
1	-1.664970	-2.366742	4.771430



77 0.023220 -0.271969 0.303713

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**B'<sub>Ir(his)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2927.1665817  
Zero-point correction=                    0.895162 (Hartree/Particle)  
Thermal correction to Energy=            0.957147  
Thermal correction to Enthalpy=           0.958091  
Thermal correction to Gibbs Free Energy= 0.795187  
Sum of electronic and zero-point Energies= -2926.271420  
Sum of electronic and thermal Energies= -2926.209435  
Sum of electronic and thermal Enthalpies= -2926.208491  
Sum of electronic and thermal Free Energies= -2926.371395

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Cartesian Coordinates

.....  
6    3.169142 -3.688508 -0.628954  
6    1.924945 -3.007397 -0.334721  
7    2.077031 -1.653706 -0.541963  
6    3.357883 -1.448628 -0.993915  
6    4.060722 -2.723834 -1.053767  
6    0.731908 -3.628130 0.041694  
6    -0.509916 -3.023726 0.232735  
7    -0.756581 -1.674864 0.134571  
6    -2.104932 -1.488147 0.309786  
6    -2.743067 -2.774553 0.548219  
6    -1.754011 -3.725316 0.506816  
6    -2.758634 -0.258204 0.272731  
6    -2.190797 0.992620 0.038881  
7    -0.864280 1.223402 -0.221506  
6    -0.716770 2.565548 -0.461746  
6    -2.001802 3.228607 -0.313786  
6    -2.915081 2.255569 0.004035  
6    0.474937 3.195808 -0.816233  
6    1.719843 2.597548 -1.005277  
7    1.966790 1.252945 -0.895024  
6    3.255212 1.028959 -1.313114  
6    3.867223 2.285672 -1.691992  
6    2.930568 3.270982 -1.468446  
6    3.886755 -0.213097 -1.360311  
1    0.423114 4.261927 -0.999509  
1    4.904154 -0.216238 -1.735016  
1    0.762951 -4.706997 0.149398  
1    -3.830088 -0.279144 0.432783  
6    1.104472 0.182839 1.899099  
6    1.186687 1.655955 2.316190  
6    0.022806 2.328436 2.712931  
6    2.400722 2.386475 2.311906  
6    0.049930 3.664875 3.112337  
1    -0.916470 1.796480 2.715385

6	2.426418	3.723485	2.722209
6	1.253445	4.362008	3.123232
1	-0.872578	4.146743	3.420747
1	3.362099	4.268836	2.729984
1	1.291997	5.398726	3.445168
6	0.103958	-0.654817	2.734383
8	-1.028592	-0.303798	2.960185
8	0.642833	-1.800168	3.164649
8	3.518135	1.722159	1.898272
6	4.780076	2.382041	1.938555
1	5.507510	1.645046	1.594890
1	4.792320	3.248215	1.267833
1	5.031812	2.695969	2.958407
7	3.253070	-1.121786	2.052807
7	2.347468	-0.473162	2.038213
6	-4.382141	2.425031	0.285262
1	-4.687050	1.748921	1.092929
1	-4.577757	3.440100	0.644152
6	-5.289095	2.172749	-0.946855
1	-5.189418	1.146607	-1.304605
1	-4.995910	2.850656	-1.756417
6	-6.731756	2.483225	-0.605289
8	-7.146525	3.554221	-0.234250
8	-7.556798	1.397734	-0.737879
1	-8.455913	1.700792	-0.501620
6	-4.222544	-2.962548	0.738753
1	-4.614496	-2.151733	1.358944
1	-4.411344	-3.886348	1.294435
6	-5.010002	-3.012669	-0.606555
1	-4.378470	-2.612265	-1.410480
1	-5.267257	-4.037149	-0.883687
6	-6.288247	-2.195031	-0.647925
8	-7.336743	-2.554558	-1.128734
8	-6.097768	-0.952855	-0.132431
1	-6.896903	-0.408376	-0.303531
6	-1.877884	-5.211634	0.670357
1	-2.891852	-5.496122	0.964476
1	-1.647919	-5.744712	-0.261426
1	-1.193490	-5.596527	1.436467
6	-2.218742	4.703674	-0.471444
1	-2.001429	5.039401	-1.493504
1	-3.252212	4.983031	-0.249804
1	-1.568857	5.276738	0.201303
6	3.406403	-5.157623	-0.452228
1	2.824817	-5.563180	0.382401
1	3.135705	-5.733766	-1.347569
1	4.463891	-5.354206	-0.250462
6	5.272259	2.438111	-2.193232
1	6.007933	2.099222	-1.452298
1	5.441939	1.851416	-3.104697

1	5.502466	3.481462	-2.423040
6	5.457745	-2.866257	-1.456903
6	6.013188	-3.933829	-2.049779
1	6.100157	-2.010774	-1.250717
1	7.071101	-3.946581	-2.293721
1	5.440883	-4.812306	-2.330512
6	3.119164	4.709008	-1.669226
6	2.626568	5.691911	-0.900447
1	3.753001	4.987170	-2.510798
1	2.831554	6.733314	-1.129983
1	2.036280	5.494085	-0.010268
6	-0.231093	-2.671676	3.944044
1	-0.609199	-2.098149	4.794459
1	-1.077840	-2.949713	3.311393
6	0.593244	-3.868522	4.373073
1	1.442968	-3.562385	4.991133
1	-0.030818	-4.547893	4.963145
1	0.973242	-4.415265	3.504179
7	0.131472	-0.469549	-2.336595
6	0.004385	-1.638378	-2.952957
6	-0.103516	0.519745	-3.274258
7	-0.304334	-1.431609	-4.251614
1	0.128442	-2.607606	-2.497429
6	-0.376942	-0.071321	-4.475669
1	-0.058395	1.564517	-3.015285
1	-0.450306	-2.157441	-4.939390
1	-0.610074	0.343697	-5.443413
77	0.619521	-0.201740	-0.325698

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**TS(B-C)<sub>Ir(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2927.1600184  
Zero-point correction=                    0.891808 (Hartree/Particle)  
Thermal correction to Energy=            0.954446  
Thermal correction to Enthalpy=         0.955390  
Thermal correction to Gibbs Free Energy= 0.788107  
Sum of electronic and zero-point Energies= -2926.268210  
Sum of electronic and thermal Energies= -2926.205573  
Sum of electronic and thermal Enthalpies= -2926.204629  
Sum of electronic and thermal Free Energies= -2926.371912

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Cartesian Coordinates

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6	-3.970345	-3.017875	-0.401775
6	-3.420907	-1.666893	-0.428367
7	-2.050259	-1.734913	-0.328234
6	-1.702961	-3.066086	-0.285536
6	-2.896518	-3.880333	-0.341924
6	-4.150151	-0.496858	-0.625327
6	-3.660286	0.803820	-0.736115

7	-2.337680	1.165240	-0.626742
6	-2.257523	2.513314	-0.866377
6	-3.593167	3.043565	-1.108807
6	-4.464397	1.975188	-1.021264
6	-1.072877	3.247520	-0.924735
6	0.224589	2.766132	-0.768542
7	0.563188	1.454751	-0.541790
6	1.930748	1.377906	-0.529409
6	2.492743	2.705890	-0.730073
6	1.433858	3.565171	-0.878306
6	2.666361	0.201921	-0.393329
6	2.174095	-1.095894	-0.276636
7	0.847862	-1.439604	-0.238449
6	0.779038	-2.809829	-0.201286
6	2.123783	-3.363515	-0.184699
6	2.990215	-2.301596	-0.223796
77	-0.747430	-0.133957	-0.340400
7	-0.651906	-0.332827	-2.485307
6	-0.736757	0.659124	-3.361685
7	-0.630932	0.170973	-4.617492
6	-0.471168	-1.198042	-4.542278
6	-0.485204	-1.499266	-3.209133
6	-0.396786	-3.554510	-0.216267
1	3.745353	0.306525	-0.406442
1	-0.287611	-4.633905	-0.200636
1	-5.216811	-0.624359	-0.760598
1	-1.169213	4.307843	-1.128752
1	-0.868451	1.702257	-3.123188
1	-0.366000	-1.816995	-5.419237
1	-0.390795	-2.455821	-2.722539
1	-0.664144	0.722358	-5.463602
6	-0.745119	0.204793	1.751923
6	0.553704	0.155736	2.541490
6	1.252450	1.349030	2.791917
6	1.131911	-1.049136	3.016267
6	2.465527	1.359879	3.480155
1	0.839896	2.282005	2.437396
6	2.342003	-1.033499	3.717172
6	3.010426	0.167560	3.945921
1	2.968665	2.305004	3.659004
1	2.766568	-1.959597	4.084766
1	3.949640	0.162027	4.491238
6	-1.622704	1.412819	2.144329
8	-1.219890	2.548885	2.034390
8	-2.841769	1.087891	2.581798
8	0.438215	-2.197615	2.781398
6	0.861079	-3.410746	3.396329
1	0.107381	-4.153380	3.130373
1	1.836131	-3.727978	3.009969
1	0.909814	-3.308085	4.486607

7	-1.702407	-1.053616	2.425592
7	-2.479744	-1.837619	2.506117
6	2.443763	-4.829057	-0.159846
1	2.160320	-5.322841	-1.098597
1	3.513884	-5.000147	-0.013787
1	1.914217	-5.350297	0.647144
6	-2.914003	-5.378889	-0.296484
1	-2.308434	-5.816493	-1.099870
1	-2.514987	-5.759146	0.652804
1	-3.929968	-5.768475	-0.397019
6	-5.956846	1.982540	-1.157034
1	-6.364495	2.960246	-0.881761
1	-6.278388	1.775898	-2.186706
1	-6.426369	1.228580	-0.516630
6	1.457526	5.046684	-1.108898
1	2.477976	5.410509	-1.255996
1	0.877825	5.330135	-1.996140
1	1.032528	5.593822	-0.257752
6	-5.383097	-3.400035	-0.443243
6	-6.401523	-2.771215	0.161261
1	-5.605197	-4.310648	-0.998774
1	-7.417355	-3.144620	0.074851
1	-6.257950	-1.892262	0.783175
6	-3.875844	4.455548	-1.358924
6	-4.877283	4.950488	-2.102123
1	-3.195999	5.164811	-0.887667
1	-5.012578	6.022512	-2.209079
1	-5.575915	4.317867	-2.640530
6	4.492287	-2.327609	-0.248321
6	5.079126	-2.253776	-1.669002
1	4.859522	-3.239531	0.233208
1	4.900712	-1.503366	0.346576
1	4.740176	-3.098829	-2.280971
1	4.739582	-1.353619	-2.196563
6	3.960981	3.023494	-0.755881
6	4.560734	3.225042	0.646890
1	4.139268	3.925999	-1.349556
1	4.519549	2.229984	-1.263648
1	4.120986	4.096509	1.146256
1	4.338374	2.369122	1.297357
6	6.595286	-2.251967	-1.656038
8	7.289200	-2.290228	-0.664339
8	7.098584	-2.200165	-2.910274
1	8.070974	-2.197288	-2.820067
6	6.065639	3.399734	0.602334
8	6.761878	3.259884	-0.378684
8	6.560374	3.725630	1.818867
1	7.527670	3.807702	1.712267
6	-3.723757	2.201656	2.921656
6	-5.002379	1.609653	3.479184

1	-3.894640	2.781922	2.011398
1	-3.206149	2.836702	3.645263
1	-5.693251	2.417853	3.740931
1	-5.491126	0.965491	2.741395
1	-4.806286	1.022249	4.381575

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**C<sub>Ir(his)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2927.2069843  
 Zero-point correction=                    0.891593 (Hartree/Particle)  
 Thermal correction to Energy=            0.956107  
 Thermal correction to Enthalpy=         0.957051  
 Thermal correction to Gibbs Free Energy= 0.783300  
 Sum of electronic and zero-point Energies= -2926.315391  
 Sum of electronic and thermal Energies= -2926.250877  
 Sum of electronic and thermal Enthalpies= -2926.249933  
 Sum of electronic and thermal Free Energies= -2926.423684

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 Cartesian Coordinates  
 .....

6	3.189474	-3.132326	-1.360123
6	1.956085	-2.591558	-0.832772
7	1.984655	-1.219038	-0.914922
6	3.172920	-0.858393	-1.496526
6	3.938742	-2.057592	-1.803730
6	0.866900	-3.348089	-0.395303
6	-0.398539	-2.874083	-0.059782
7	-0.756405	-1.548507	-0.020637
6	-2.108898	-1.489502	0.210037
6	-2.631185	-2.841675	0.345420
6	-1.569136	-3.698048	0.192458
6	-2.858920	-0.319884	0.310082
6	-2.389445	0.989153	0.227306
7	-1.092398	1.352106	-0.025758
6	-1.024309	2.721968	0.005697
6	-2.343591	3.259689	0.286819
6	-3.189760	2.186693	0.422853
6	0.120791	3.480064	-0.232491
6	1.378770	3.007146	-0.605679
7	1.697418	1.684273	-0.770600
6	2.928625	1.622255	-1.376797
6	3.437036	2.962912	-1.575007
6	2.498560	3.828864	-1.056466
6	3.585697	0.449566	-1.740842
1	0.004133	4.556314	-0.199253
1	4.534654	0.572303	-2.250448
1	0.996589	-4.424543	-0.391518
1	-3.919723	-0.442672	0.491756
6	0.890043	0.194222	1.581382
6	1.822476	1.066655	2.292486

6	1.285427	1.992442	3.221228
6	3.234463	1.043643	2.108339
6	2.088638	2.936770	3.846785
1	0.215260	1.991138	3.392857
6	4.037965	1.985367	2.762269
6	3.464761	2.933659	3.608114
1	1.646053	3.663842	4.519981
1	5.112414	1.973477	2.627941
1	4.106063	3.658953	4.100629
6	-0.071954	-0.464056	2.545101
8	-1.093185	0.069011	2.929688
8	0.382877	-1.652486	2.943579
8	3.725772	0.024128	1.371000
6	5.139978	-0.141181	1.287880
1	5.294188	-1.043361	0.696994
1	5.611655	0.711277	0.785059
1	5.576103	-0.273983	2.284011
7	3.444919	-3.815067	2.327087
7	3.930062	-2.975757	2.857533
6	-4.657923	2.204872	0.743944
1	-4.890883	1.406830	1.459026
1	-4.919632	3.145484	1.237510
6	-5.571822	2.047166	-0.498917
1	-5.402201	1.088647	-0.992498
1	-5.351290	2.847611	-1.214021
6	-7.025449	2.193518	-0.099134
8	-7.516207	3.174604	0.403767
8	-7.762321	1.065035	-0.345925
1	-8.676353	1.260886	-0.059091
6	-4.083921	-3.169406	0.554741
1	-4.517122	-2.461848	1.267248
1	-4.177616	-4.157784	1.015142
6	-4.914493	-3.146896	-0.765504
1	-4.338195	-2.635429	-1.547676
1	-5.117989	-4.156197	-1.129386
6	-6.242365	-2.414197	-0.693651
8	-7.278980	-2.791846	-1.186087
8	-6.117082	-1.220990	-0.057056
1	-6.954982	-0.717045	-0.149885
6	-1.563804	-5.197560	0.226549
1	-2.536083	-5.592241	0.533688
1	-1.334506	-5.626415	-0.757665
1	-0.814575	-5.584466	0.927963
6	-2.658362	4.721514	0.397436
1	-2.516338	5.238995	-0.560002
1	-3.693934	4.885829	0.706291
1	-2.012757	5.218859	1.131366
6	3.550034	-4.586601	-1.376574
1	3.130415	-5.114102	-0.514034
1	3.187478	-5.094252	-2.280864

1	4.636603	-4.713696	-1.350139
6	4.762857	3.294081	-2.191674
1	5.597253	2.916462	-1.586310
1	4.865014	2.855451	-3.191940
1	4.898977	4.374106	-2.287671
6	5.259925	-2.045012	-2.427883
6	5.794871	-3.010539	-3.190895
1	5.858815	-1.151445	-2.255354
1	6.796173	-2.905818	-3.597373
1	5.257385	-3.915341	-3.455538
6	2.600779	5.287075	-0.995313
6	2.147905	6.073661	-0.007895
1	3.129841	5.758009	-1.823175
1	2.280192	7.150625	-0.047412
1	1.665354	5.673608	0.879367
6	-0.446458	-2.368074	3.910386
1	-0.661628	-1.693511	4.743171
1	-1.390728	-2.620022	3.419538
6	0.320606	-3.598822	4.348986
1	1.263819	-3.323368	4.830453
1	-0.279712	-4.164310	5.069604
1	0.541779	-4.249884	3.497517
7	-0.130475	0.067227	-2.469242
6	-0.331544	-1.005466	-3.218591
6	-0.384199	1.166761	-3.265319
7	-0.703494	-0.636159	-4.466143
1	-0.215365	-2.028967	-2.897617
6	-0.743494	0.743415	-4.515351
1	-0.292869	2.170901	-2.883084
1	-0.911214	-1.265579	-5.228941
1	-1.015501	1.281282	-5.409881
77	0.503889	0.065548	-0.306153

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**TS(C-P)<sub>Ir(his)</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2817.6306953  
 Zero-point correction=                    0.883861 (Hartree/Particle)  
 Thermal correction to Energy=            0.942957  
 Thermal correction to Enthalpy=         0.943901  
 Thermal correction to Gibbs Free Energy= 0.786549  
 Sum of electronic and zero-point Energies= -2816.746834  
 Sum of electronic and thermal Energies= -2816.687738  
 Sum of electronic and thermal Enthalpies= -2816.686794  
 Sum of electronic and thermal Free Energies= -2816.844146

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 Cartesian Coordinates  
 .....

6	3.483256	-3.368071	-0.771878
6	2.188394	-2.786165	-0.485312
7	2.253372	-1.418253	-0.635470



6	3.530262	-1.106144	-1.034986
6	4.320874	-2.327218	-1.123154
6	1.035646	-3.497424	-0.148237
6	-0.237840	-2.981928	0.089498
7	-0.577172	-1.651889	0.034232
6	-1.922264	-1.558382	0.287536
6	-2.461770	-2.889463	0.529519
6	-1.418496	-3.770825	0.405748
6	-2.659042	-0.376335	0.292427
6	-2.192512	0.909832	0.023472
7	-0.894277	1.232829	-0.277626
6	-0.847623	2.582343	-0.521358
6	-2.174494	3.150550	-0.354589
6	-3.006442	2.117001	-0.001349
6	0.300799	3.305482	-0.842057
6	1.594765	2.810281	-0.989722
7	1.937795	1.483891	-0.903637
6	3.259854	1.372672	-1.265375
6	3.792182	2.685206	-1.568957
6	2.770299	3.587423	-1.370833
6	3.983996	0.180068	-1.325246
1	0.173406	4.367722	-1.011868
1	5.013754	0.265998	-1.653543
1	1.137096	-4.575045	-0.078819
1	-3.718008	-0.471561	0.501273
6	-4.474004	2.184941	0.317529
1	-4.710352	1.492476	1.134083
1	-4.729064	3.185809	0.679244
6	-5.392682	1.866497	-0.890911
1	-5.236533	0.845175	-1.242406
1	-5.163534	2.555573	-1.711152
6	-6.842688	2.088881	-0.513091
8	-7.322972	3.145509	-0.182476
8	-7.586596	0.939842	-0.555060
1	-8.496841	1.185903	-0.296346
6	-3.911127	-3.181357	0.801952
1	-4.325204	-2.398257	1.442736
1	-4.000088	-4.112794	1.369553
6	-4.767127	-3.298039	-0.497039
1	-4.203286	-2.881323	-1.341985
1	-4.984161	-4.339674	-0.742814
6	-6.088417	-2.551182	-0.480584
8	-7.139287	-2.974749	-0.899948
8	-5.940831	-1.292257	0.008193
1	-6.779023	-0.797927	-0.124675
6	-1.435012	-5.264308	0.544014
1	-2.416618	-5.622580	0.865557
1	-1.200401	-5.764670	-0.404552
1	-0.701080	-5.612875	1.281133
6	-2.508318	4.601840	-0.532312

1	-2.365521	4.925461	-1.571267
1	-3.548440	4.808864	-0.266968
1	-1.874350	5.242443	0.092929
6	3.815644	-4.824555	-0.654142
1	3.231005	-5.310156	0.134077
1	3.621780	-5.371436	-1.586878
1	4.875503	-4.959251	-0.416773
6	5.207949	2.962925	-1.976292
1	5.918939	2.680607	-1.189127
1	5.486312	2.404821	-2.878902
1	5.361018	4.025158	-2.181910
6	5.736447	-2.356600	-1.483696
6	6.385050	-3.359433	-2.094859
1	6.309983	-1.466337	-1.227486
1	7.447979	-3.287458	-2.304054
1	5.886709	-4.264963	-2.425790
6	2.853227	5.041395	-1.520502
6	2.251590	5.955548	-0.745380
1	3.499186	5.395885	-2.323110
1	2.383339	7.017166	-0.931279
1	1.643528	5.682185	0.112337
6	1.219089	0.189050	1.855363
6	1.198012	1.555153	2.462186
6	0.542232	-0.852559	2.700434
6	0.085301	2.400654	2.548084
6	2.327919	1.934420	3.209703
8	-0.531595	-0.669210	3.233163
8	1.268852	-1.984657	2.802568
6	0.163492	3.607413	3.246885
1	-0.842749	2.106463	2.080051
6	2.441147	3.127439	3.906441
8	3.288926	0.935233	3.357381
6	1.338501	3.982749	3.903278
1	-0.706969	4.255296	3.285773
1	3.349322	3.357384	4.452768
6	3.347850	0.140109	2.288683
1	1.389503	4.925377	4.439550
1	3.643123	-0.881293	2.510713
1	3.724683	0.596246	1.370739
1	2.084100	-0.178140	1.257197
7	0.213666	-0.327201	-2.422895
6	0.132521	-1.490698	-3.057728
6	-0.042246	0.667359	-3.349857
7	-0.166576	-1.275077	-4.357008
1	0.282652	-2.461745	-2.614103
6	-0.281303	0.085065	-4.562723
1	-0.033606	1.709356	-3.076502
1	-0.281959	-1.995313	-5.056481
1	-0.515569	0.506311	-5.527513
6	0.692240	-3.055098	3.603378

1	-0.385397	-3.074405	3.428966
1	1.144714	-3.961045	3.193996
6	1.018468	-2.878760	5.077662
1	0.551650	-1.972225	5.472465
1	0.635335	-3.735027	5.644019
1	2.100249	-2.821391	5.237039
77	0.682372	-0.080975	-0.409914

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**Alr**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-1939.3627749  
 Zero-point correction=                    0.598678 (Hartree/Particle)  
 Thermal correction to Energy=            0.638988  
 Thermal correction to Enthalpy=         0.639932  
 Thermal correction to Gibbs Free Energy= 0.523994  
 Sum of electronic and zero-point Energies= -1938.764097  
 Sum of electronic and thermal Energies= -1938.723787  
 Sum of electronic and thermal Enthalpies= -1938.722843  
 Sum of electronic and thermal Free Energies= -1938.838781

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 Cartesian Coordinates  
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6	-3.900310	-3.106387	-0.041168
6	-2.581921	-2.617385	-0.092293
7	-2.583004	-1.197325	-0.050542
6	-3.936249	-0.822683	0.033478
6	-4.760865	-1.982063	0.043306
6	-1.441436	-3.417373	-0.163270
6	-0.139559	-2.975378	-0.230107
7	0.230056	-1.649516	-0.254576
6	1.593275	-1.643246	-0.360069
6	2.116454	-3.007764	-0.379564
6	1.036530	-3.836936	-0.301890
6	2.363087	-0.495137	-0.471099
6	1.885204	0.803719	-0.459435
7	0.527086	1.178356	-0.280954
6	0.524209	2.589051	-0.295721
6	1.845754	3.074042	-0.506732
6	2.688781	1.966464	-0.613096
6	-0.585775	3.395620	-0.112005
6	-1.884752	2.955273	0.082738
7	-2.256917	1.639036	0.039934
6	-3.629905	1.627294	0.142543
6	-4.144784	2.977772	0.267569
6	-3.056781	3.812323	0.261032
77	-1.021439	-0.009146	-0.129683
6	-4.402499	0.483913	0.129989
1	-0.427496	4.466187	-0.140863
1	-5.473295	0.619305	0.217838
1	-1.596782	-4.489133	-0.160688

1	3.434599	-0.623164	-0.563849
6	4.169262	1.979076	-0.856829
1	4.442642	1.139541	-1.505561
1	4.452607	2.889520	-1.392775
6	5.011221	1.904160	0.443341
1	4.819039	0.976571	0.984463
1	4.754781	2.744489	1.098467
6	6.483932	2.034219	0.103129
8	6.977686	2.961963	-0.489526
8	7.218171	0.962469	0.524688
1	8.147663	1.141591	0.278270
6	3.578262	-3.348633	-0.436830
1	4.076019	-2.693419	-1.158037
1	3.703986	-4.365834	-0.818885
6	4.288544	-3.233930	0.948267
1	3.657893	-2.658966	1.638569
1	4.441025	-4.216342	1.399156
6	5.631976	-2.529168	0.925861
8	6.639965	-2.911204	1.468040
8	5.558888	-1.345970	0.254091
1	6.407674	-0.866546	0.368659
6	0.992462	-5.333840	-0.285647
1	1.991283	-5.761631	-0.402818
1	0.580810	-5.714775	0.657592
1	0.368741	-5.727947	-1.097541
6	2.222213	4.519002	-0.591991
1	2.016959	5.036753	0.353705
1	3.282759	4.649880	-0.817351
1	1.647373	5.033163	-1.371518
6	-4.305108	-4.543799	-0.111499
1	-3.526337	-5.167324	-0.556002
1	-4.521510	-4.948427	0.886410
1	-5.211400	-4.660383	-0.713789
6	-5.592303	3.330495	0.419309
1	-6.190552	2.952992	-0.419277
1	-6.014275	2.907481	1.339897
1	-5.733202	4.412812	0.467126
6	-6.210899	-1.951837	0.091999
6	-7.023329	-2.935660	0.520591
1	-6.676632	-1.025836	-0.236465
1	-8.099787	-2.796377	0.518237
1	-6.661408	-3.879623	0.911304
6	-3.069132	5.269819	0.391982
6	-2.178495	6.016375	1.061065
1	-3.912908	5.774581	-0.076613
1	-2.283320	7.095723	1.111379
1	-1.346789	5.583092	1.609472

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**B<sub>Ir</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2700.8957001  
 Zero-point correction=                    0.820514 (Hartree/Particle)  
 Thermal correction to Energy=            0.878198  
 Thermal correction to Enthalpy=         0.879142  
 Thermal correction to Gibbs Free Energy= 0.718999  
 Sum of electronic and zero-point Energies= -2700.075186  
 Sum of electronic and thermal Energies= -2700.017502  
 Sum of electronic and thermal Enthalpies= -2700.016558  
 Sum of electronic and thermal Free Energies= -2700.176701

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 Cartesian Coordinates

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6	-1.780934	3.270128	-0.658294
6	-1.338200	1.889365	-0.720557
7	-0.027740	1.782801	-0.306727
6	0.372421	3.050786	0.016904
6	-0.726392	3.995567	-0.165387
6	-2.118184	0.824718	-1.125427
6	-1.714474	-0.505821	-1.180841
7	-0.436246	-0.986781	-0.844316
6	-0.484131	-2.388738	-1.068306
6	-1.756198	-2.763450	-1.532712
6	-2.538316	-1.580702	-1.613865
6	0.574141	-3.273078	-0.854782
6	1.831484	-2.946834	-0.402151
7	2.242501	-1.669217	-0.093648
6	3.540993	-1.782611	0.317728
6	3.978218	-3.177359	0.277192
6	2.912146	-3.898536	-0.178231
77	1.102752	0.053652	-0.212493
7	2.651445	1.102286	0.370490
6	3.954003	0.623948	0.668132
6	4.814860	1.721220	0.951013
6	4.053977	2.884309	0.858177
6	2.724714	2.502347	0.518428
6	4.333969	-0.705772	0.685202
6	1.670234	3.385285	0.370888
8	-7.789392	1.814687	-0.781004
6	-6.714346	1.115860	-0.361170
8	-5.583988	1.252759	-0.821582
6	-7.060175	0.169320	0.695262
7	-8.334673	0.145127	1.050214
7	-9.425710	0.114573	1.355949
6	-6.099399	-0.711693	1.393803
6	-4.815371	-0.249833	1.713032
6	-3.892600	-1.069207	2.363940
6	-4.256110	-2.366024	2.723077
6	-5.531412	-2.850393	2.424182
6	-6.451306	-2.036043	1.755626
8	-7.709160	-2.430604	1.410196

6	-8.146256	-3.735987	1.769114
1	1.882447	4.435985	0.522520
1	5.348636	-0.919666	0.992919
1	0.386654	-4.316948	-1.073892
1	-3.137786	1.042278	-1.418201
1	-4.544327	0.763816	1.442636
1	-2.906240	-0.685281	2.607104
1	-5.802347	-3.859538	2.711635
1	-3.553374	-3.008449	3.246408
1	-9.170766	-3.816034	1.403219
1	-7.527710	-4.508476	1.295185
1	-8.135309	-3.875717	2.856924
6	-7.596953	2.794356	-1.831640
1	-8.521044	2.752917	-2.412885
1	-6.760054	2.478369	-2.457621
6	-7.371728	4.178615	-1.243760
1	-6.441825	4.212982	-0.667322
1	-7.303415	4.916816	-2.050832
1	-8.200371	4.463229	-0.587939
6	-3.135898	3.763441	-1.063102
1	-3.335911	4.749332	-0.634647
1	-3.212060	3.853751	-2.155423
1	-3.933961	3.085553	-0.743818
6	-2.206232	-4.157630	-1.830363
1	-3.251272	-4.294602	-1.537161
1	-2.135436	-4.381291	-2.903435
1	-1.607074	-4.902445	-1.301207
6	-0.706826	5.434888	0.101121
6	-0.103756	6.046658	1.130959
1	-1.273939	6.047213	-0.598750
1	-0.158748	7.124606	1.248277
1	0.426983	5.500124	1.905555
6	-3.926434	-1.438715	-2.010148
6	-4.591503	-2.254588	-2.849908
1	-4.457698	-0.582466	-1.600696
1	-5.630564	-2.055963	-3.094012
1	-4.135061	-3.104228	-3.345855
6	4.512312	4.293725	1.062141
1	5.551483	4.337129	1.396140
1	4.435613	4.873221	0.133428
1	3.899108	4.806754	1.812692
6	6.288080	1.629091	1.218514
1	6.587599	2.422039	1.912932
1	6.535137	0.682804	1.707559
6	5.337343	-3.696282	0.660387
1	5.244078	-4.765091	0.874764
1	5.683075	-3.234058	1.591583
6	6.442035	-3.526069	-0.423637
1	6.045795	-3.724028	-1.421854
1	7.235105	-4.253013	-0.213689

6	7.118942	1.750543	-0.088338
1	6.808821	0.972245	-0.796005
1	6.976791	2.727862	-0.554917
6	7.084320	-2.152100	-0.429762
8	7.042219	-1.364790	-1.356373
8	7.697729	-1.897561	0.740429
1	8.171261	-1.025632	0.688432
6	8.586196	1.515422	0.181675
8	9.043027	0.506120	0.698030
8	9.366508	2.534916	-0.194732
1	10.291865	2.282062	-0.003773
6	2.798162	-5.371510	-0.426366
1	2.627740	-5.587336	-1.488852
1	3.707145	-5.900012	-0.129236
1	1.964001	-5.811476	0.134121

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**TS(B-B')<sub>IR</sub>**

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Number of imaginary frequencies: 1	Electronic energy:	HF=-2700.8748029
Zero-point correction=	0.819545 (Hartree/Particle)	
Thermal correction to Energy=	0.876418	
Thermal correction to Enthalpy=	0.877362	
Thermal correction to Gibbs Free Energy=	0.725001	
Sum of electronic and zero-point Energies=	-2700.055258	
Sum of electronic and thermal Energies=	-2699.998385	
Sum of electronic and thermal Enthalpies=	-2699.997441	
Sum of electronic and thermal Free Energies=	-2700.149802	

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 Cartesian Coordinates

6	-3.051045	3.348648	-1.607038
6	-1.840668	2.789704	-1.089808
7	-1.917159	1.406639	-1.075092
6	-3.163958	1.082258	-1.590519
6	-3.886141	2.274178	-1.932859
6	-0.735485	3.534129	-0.670721
6	0.480223	3.041501	-0.236734
7	0.808385	1.703729	-0.157642
6	2.115409	1.651226	0.235590
6	2.634133	2.993443	0.463181
6	1.617383	3.857356	0.156054
6	2.859450	0.475683	0.291878
6	2.416385	-0.787016	-0.058526
7	1.091973	-1.111966	-0.382192
6	1.079793	-2.509709	-0.583753
6	2.407370	-3.030257	-0.442578
6	3.231846	-1.971696	-0.117812
6	-0.041054	-3.272275	-0.835796
6	-1.337656	-2.796393	-1.038258
7	-1.657705	-1.474107	-1.066977

6	-2.956430	-1.394385	-1.539414
6	-3.482340	-2.725260	-1.776442
6	-2.490088	-3.609161	-1.428048
77	-0.439679	0.111554	-0.544704
6	-3.636928	-0.220295	-1.786926
1	0.107817	-4.339705	-0.939934
1	-4.631329	-0.316185	-2.206582
1	-0.828469	4.612625	-0.725837
1	3.896478	0.563683	0.590243
6	-1.692965	0.088184	2.105401
6	-1.376176	-1.290092	2.518133
6	-0.106841	-1.589249	3.054900
6	-2.319290	-2.353845	2.413405
6	0.211276	-2.870171	3.488582
1	0.621944	-0.796306	3.134644
6	-1.991312	-3.639012	2.859131
6	-0.732697	-3.895512	3.397643
1	1.194619	-3.063978	3.905123
1	-2.719386	-4.437805	2.790506
1	-0.495319	-4.896129	3.747074
6	-0.961687	1.295276	2.639244
8	0.159604	1.265383	3.097399
8	-1.723493	2.396474	2.563402
8	-3.526293	-2.039292	1.881285
6	-4.559121	-3.025198	1.847527
1	-5.431435	-2.519868	1.431303
1	-4.277709	-3.865269	1.203893
1	-4.790563	-3.384239	2.856535
7	-3.904981	0.793356	1.271403
7	-2.929707	0.405380	1.687129
6	4.720707	-2.014617	0.064360
1	5.047967	-1.251153	0.776762
1	5.009050	-2.980699	0.493414
6	5.467540	-1.816234	-1.285704
1	5.253122	-0.818995	-1.687798
1	5.144845	-2.565507	-2.011605
6	6.963044	-1.963117	-1.131280
8	7.657113	-2.833597	-1.590599
8	7.492394	-0.959515	-0.353778
1	8.455091	-1.118131	-0.301193
6	4.021488	3.352130	0.920944
1	4.381949	2.639889	1.670997
1	3.974278	4.320802	1.428687
6	5.081463	3.470880	-0.213452
1	4.662228	3.977612	-1.085221
1	5.923023	4.061192	0.165921
6	5.627157	2.131134	-0.660430
8	5.436052	1.613862	-1.742759
8	6.348391	1.549304	0.322808
1	6.728288	0.705684	-0.014729



6	1.623825	5.356971	0.164507
1	2.528176	5.750667	0.635858
1	1.584620	5.764441	-0.854072
1	0.765273	5.767611	0.709682
6	2.778369	-4.469146	-0.629728
1	2.589621	-4.799771	-1.658727
1	3.835328	-4.645029	-0.415870
1	2.193732	-5.121413	0.030967
6	-3.361767	4.807320	-1.722244
1	-2.794842	5.405899	-1.003454
1	-3.125004	5.192087	-2.723451
1	-4.426943	4.990390	-1.549303
6	-4.859039	-3.021176	-2.288817
1	-5.033393	-4.097113	-2.365898
1	-5.635244	-2.610601	-1.630428
1	-5.018405	-2.587135	-3.283872
6	-5.245759	2.295643	-2.456776
6	-5.794879	3.253180	-3.221791
1	-5.866029	1.438171	-2.201621
1	-6.824753	3.170724	-3.554843
1	-5.244667	4.122437	-3.565559
6	-2.567561	-5.069397	-1.463787
6	-1.978356	-5.919384	-0.608372
1	-3.195366	-5.487822	-2.249411
1	-2.103668	-6.992577	-0.714991
1	-1.380181	-5.578956	0.232297
6	-1.144158	3.611715	3.118783
1	-0.871753	3.413596	4.159185
1	-0.229158	3.836512	2.564411
6	-2.185299	4.705902	2.994852
1	-3.094885	4.449250	3.546433
1	-1.786541	5.638319	3.408167
1	-2.451904	4.877766	1.947077

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**B'<sub>fr</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2700.9012763  
 Zero-point correction=                    0.820439 (Hartree/Particle)  
 Thermal correction to Energy=            0.877705  
 Thermal correction to Enthalpy=         0.878649  
 Thermal correction to Gibbs Free Energy= 0.726375  
 Sum of electronic and zero-point Energies= -2700.080837  
 Sum of electronic and thermal Energies= -2700.023571  
 Sum of electronic and thermal Enthalpies= -2700.022627  
 Sum of electronic and thermal Free Energies= -2700.174901

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 Cartesian Coordinates  
 .....

6	3.324330	-3.517030	-1.095547
6	2.051983	-2.916578	-0.759758

7	2.131523	-1.542961	-0.873937
6	3.413184	-1.253796	-1.278388
6	4.176532	-2.483770	-1.426192
6	0.900548	-3.615359	-0.412009
6	-0.361015	-3.084860	-0.170603
7	-0.673649	-1.741413	-0.192430
6	-2.026914	-1.647199	0.049059
6	-2.588555	-2.974950	0.228508
6	-1.555478	-3.865577	0.093473
6	-2.749592	-0.460304	0.078466
6	-2.264169	0.818427	-0.177951
7	-0.952274	1.117141	-0.465163
6	-0.895207	2.475058	-0.700387
6	-2.216880	3.054630	-0.559073
6	-3.064992	2.030483	-0.224274
6	0.251854	3.185257	-1.026569
6	1.535060	2.675961	-1.212490
7	1.861472	1.346843	-1.112246
6	3.179690	1.223027	-1.500065
6	3.709757	2.519067	-1.856357
6	2.699963	3.434164	-1.650127
77	0.635201	-0.176992	-0.455410
6	3.888917	0.027541	-1.554452
1	0.127285	4.246195	-1.204205
1	4.915526	0.096522	-1.896303
1	0.982605	-4.696034	-0.374629
1	-3.813747	-0.547557	0.264197
6	1.130215	0.137659	1.564756
6	0.817967	1.508473	2.170118
6	-0.467377	1.735139	2.691079
6	1.745948	2.582018	2.207518
6	-0.824055	2.959326	3.248473
1	-1.194987	0.938464	2.657462
6	1.384322	3.807101	2.782647
6	0.106563	3.994775	3.302139
1	-1.825640	3.094362	3.643590
1	2.103582	4.615711	2.824596
1	-0.154728	4.950974	3.745904
6	0.557547	-1.053985	2.408976
8	-0.586356	-1.100931	2.785709
8	1.482611	-1.984862	2.640628
8	2.978674	2.360499	1.677202
6	3.989413	3.363954	1.790365
1	4.887903	2.922087	1.358220
1	3.718647	4.260790	1.223731
1	4.173661	3.619875	2.839751
7	3.661473	-0.372678	1.496290
7	2.591587	-0.086556	1.592035
6	-4.540622	2.110238	0.048597
1	-4.810835	1.411278	0.849289

1	-4.796536	3.109315	0.414416
6	-5.423812	1.815718	-1.190766
1	-5.263093	0.800378	-1.556592
1	-5.167740	2.515737	-1.993954
6	-6.883116	2.039470	-0.849987
8	-7.356208	3.079382	-0.460529
8	-7.643759	0.912324	-1.004958
1	-8.561212	1.158172	-0.772517
6	-4.048598	-3.260356	0.441368
1	-4.482456	-2.487056	1.081020
1	-4.162896	-4.201399	0.988278
6	-4.855653	-3.348639	-0.891154
1	-4.260030	-2.920754	-1.707970
1	-5.068791	-4.384557	-1.162305
6	-6.172480	-2.594993	-0.903119
8	-7.216324	-3.008805	-1.347460
8	-6.029525	-1.338746	-0.401962
1	-6.861251	-0.840361	-0.558010
6	-1.601741	-5.363525	0.147069
1	-2.580494	-5.718134	0.480957
1	-1.411352	-5.808918	-0.837923
1	-0.852485	-5.772264	0.836160
6	-2.533831	4.506576	-0.754626
1	-2.350308	4.823881	-1.788912
1	-3.581521	4.721139	-0.528460
1	-1.919206	5.143193	-0.106283
6	3.619827	-4.985213	-1.055541
1	3.062341	-5.490886	-0.259774
1	3.359998	-5.482539	-1.999494
1	4.685963	-5.158078	-0.880572
6	5.106458	2.769279	-2.340818
1	5.856666	2.418521	-1.620550
1	5.302656	2.250747	-3.287647
1	5.287070	3.834597	-2.503084
6	5.580497	-2.530054	-1.829491
6	6.173417	-3.507584	-2.530664
1	6.191741	-1.680743	-1.525252
1	7.231974	-3.458962	-2.767012
1	5.630381	-4.366537	-2.911874
6	2.792085	4.881696	-1.850698
6	2.205860	5.833846	-1.108613
1	3.434574	5.200239	-2.670630
1	2.347893	6.885160	-1.339566
1	1.589061	5.605651	-0.243695
6	1.048328	-3.150322	3.414034
1	0.657479	-2.790336	4.369207
1	0.232854	-3.626319	2.864329
6	2.251201	-4.055286	3.579738
1	3.056532	-3.549256	4.120968
1	1.960570	-4.941862	4.152841

1 2.633760 -4.382615 2.608009

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**TS(B-C)<sub>lr</sub>**

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Number of imaginary frequencies: 1 Electronic energy: HF=-2700.9005444  
Zero-point correction= 0.819333 (Hartree/Particle)  
Thermal correction to Energy= 0.876354  
Thermal correction to Enthalpy= 0.877298  
Thermal correction to Gibbs Free Energy= 0.725496  
Sum of electronic and zero-point Energies= -2700.081211  
Sum of electronic and thermal Energies= -2700.024190  
Sum of electronic and thermal Enthalpies= -2700.023246  
Sum of electronic and thermal Free Energies= -2700.175049

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Cartesian Coordinates

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6 3.305664 -3.518970 -1.106635  
6 2.039277 -2.914090 -0.759008  
7 2.123884 -1.540002 -0.870836  
6 3.403302 -1.256080 -1.290499  
6 4.158271 -2.489296 -1.447744  
6 0.886765 -3.611138 -0.411332  
6 -0.373589 -3.077248 -0.174104  
7 -0.681261 -1.732492 -0.194598  
6 -2.035666 -1.633263 0.037439  
6 -2.603376 -2.959079 0.209235  
6 -1.572533 -3.853639 0.079955  
6 -2.753895 -0.443780 0.069475  
6 -2.261622 0.834229 -0.175093  
7 -0.947585 1.130431 -0.457722  
6 -0.883790 2.489880 -0.680832  
6 -2.202588 3.073782 -0.535848  
6 -3.056211 2.050111 -0.212273  
6 0.266349 3.196726 -1.003798  
6 1.544541 2.679936 -1.198731  
7 1.865332 1.348552 -1.104232  
6 3.178375 1.218994 -1.507337  
6 3.710720 2.513076 -1.867273  
6 2.709217 3.433117 -1.645253  
77 0.637341 -0.170086 -0.440790  
6 3.881468 0.021458 -1.574334  
1 0.147847 4.259592 -1.173741  
1 4.903397 0.085692 -1.930609  
1 0.966161 -4.692018 -0.376349  
1 -3.819109 -0.527560 0.250177  
6 1.068703 0.116225 1.541446  
6 0.838338 1.487795 2.161109  
6 -0.425549 1.766010 2.713909  
6 1.807285 2.525060 2.179831  
6 -0.720257 3.002002 3.281106

1	-1.185158	0.999016	2.696994
6	1.509434	3.760901	2.767955
6	0.252219	3.998866	3.316215
1	-1.705816	3.175030	3.700956
1	2.261709	4.539529	2.795760
1	0.040031	4.963383	3.768111
6	0.488319	-1.049405	2.400634
8	-0.661565	-1.067286	2.768006
8	1.387398	-1.999690	2.655990
8	3.018393	2.257034	1.622929
6	4.083428	3.199869	1.756099
1	4.956275	2.717659	1.314429
1	3.862755	4.120997	1.206883
1	4.280554	3.425293	2.810124
7	3.695240	-0.536512	1.517882
7	2.657479	-0.173108	1.662549
6	-4.531965	2.134268	0.058700
1	-4.806584	1.429750	0.852934
1	-4.784021	3.131326	0.432580
6	-5.414037	1.854179	-1.184762
1	-5.257058	0.841293	-1.558923
1	-5.153493	2.559837	-1.981569
6	-6.873042	2.081334	-0.844827
8	-7.341947	3.119317	-0.445290
8	-7.638778	0.959709	-1.013862
1	-8.555565	1.207617	-0.780982
6	-4.065948	-3.238946	0.411621
1	-4.499491	-2.467984	1.054308
1	-4.188034	-4.183297	0.951070
6	-4.865785	-3.313471	-0.926013
1	-4.264688	-2.879796	-1.735732
1	-5.079974	-4.346419	-1.207456
6	-6.180634	-2.556305	-0.938226
8	-7.223383	-2.963718	-1.390940
8	-6.036619	-1.304578	-0.426221
1	-6.866202	-0.802475	-0.581689
6	-1.624945	-5.351554	0.129590
1	-2.606558	-5.703146	0.458246
1	-1.432016	-5.795149	-0.855706
1	-0.880255	-5.764803	0.820863
6	-2.512889	4.528793	-0.719051
1	-2.328304	4.853814	-1.750746
1	-3.559503	4.746232	-0.490683
1	-1.895016	5.157043	-0.065723
6	3.595711	-4.988284	-1.068611
1	3.046344	-5.490323	-0.264985
1	3.322114	-5.485801	-2.008560
1	4.663226	-5.165056	-0.906648
6	5.102353	2.757433	-2.368966
1	5.860084	2.400906	-1.659493

1	5.283609	2.240452	-3.319600
1	5.286133	3.822297	-2.530688
6	5.557292	-2.542185	-1.867315
6	6.136893	-3.522336	-2.575857
1	6.176136	-1.695995	-1.569988
1	7.192763	-3.478851	-2.824886
1	5.585102	-4.378484	-2.950766
6	2.806576	4.881223	-1.840116
6	2.240293	5.830871	-1.079789
1	3.434916	5.201289	-2.670362
1	2.383604	6.883191	-1.305348
1	1.639801	5.598766	-0.204456
6	0.915297	-3.139048	3.444978
1	0.527573	-2.753292	4.391367
1	0.090568	-3.601604	2.897449
6	2.090946	-4.074814	3.634805
1	2.906356	-3.582880	4.173958
1	1.771379	-4.943474	4.219809
1	2.471264	-4.428607	2.671472

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**Cr**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2700.9575091  
Zero-point correction=                    0.817889 (Hartree/Particle)  
Thermal correction to Energy=            0.877395  
Thermal correction to Enthalpy=         0.878339  
Thermal correction to Gibbs Free Energy= 0.716051  
Sum of electronic and zero-point Energies= -2700.139620  
Sum of electronic and thermal Energies= -2700.080114  
Sum of electronic and thermal Enthalpies= -2700.079170  
Sum of electronic and thermal Free Energies= -2700.241458

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Cartesian Coordinates

.....  

6	3.091668	-3.065728	-1.763396
6	1.875149	-2.533685	-1.204085
7	1.908132	-1.150107	-1.234786
6	3.121411	-0.791343	-1.788897
6	3.859173	-1.983713	-2.156686
6	0.801898	-3.299607	-0.760281
6	-0.446431	-2.829386	-0.379597
7	-0.789865	-1.498153	-0.298206
6	-2.144119	-1.448811	-0.056168
6	-2.671016	-2.798588	0.049863
6	-1.614545	-3.654158	-0.138740
6	-2.891044	-0.281221	0.042621
6	-2.417170	1.018534	-0.077805
7	-1.105742	1.372204	-0.335404
6	-1.050245	2.752878	-0.307388
6	-2.371477	3.287142	-0.066073

6	-3.218050	2.213852	0.077170
6	0.093767	3.518208	-0.491885
6	1.360380	3.049596	-0.818817
7	1.674267	1.721552	-0.983899
6	2.925575	1.673637	-1.562064
6	3.440891	3.012433	-1.729872
6	2.489499	3.873590	-1.229123
77	0.501816	0.109124	-0.456126
6	3.574578	0.510964	-1.954481
1	-0.029371	4.593550	-0.458387
1	4.534472	0.635978	-2.441938
1	0.925870	-4.375676	-0.796598
1	-3.953140	-0.397968	0.220255
6	0.871144	0.175301	1.392074
6	1.867003	0.987625	2.093540
6	1.388891	1.957522	3.006073
6	3.271340	0.835242	1.935654
6	2.261277	2.814389	3.665127
1	0.318573	2.049860	3.152901
6	4.141394	1.692772	2.619754
6	3.636801	2.681294	3.463641
1	1.871468	3.574204	4.334660
1	5.213244	1.584349	2.509680
1	4.329848	3.337921	3.981468
6	-0.127644	-0.467661	2.330968
8	-1.125459	0.119146	2.698057
8	0.264879	-1.675190	2.725812
8	3.682118	-0.205199	1.175688
6	5.079022	-0.486515	1.099675
1	5.163835	-1.379100	0.480735
1	5.625249	0.339195	0.628622
1	5.492166	-0.686714	2.094247
7	3.153077	-4.034747	1.943274
7	3.628711	-3.264023	2.576540
6	-4.693108	2.238581	0.362801
1	-4.946852	1.445259	1.075807
1	-4.961368	3.182388	0.846450
6	-5.575839	2.080406	-0.901901
1	-5.398319	1.119861	-1.388579
1	-5.336380	2.877365	-1.614626
6	-7.037667	2.233365	-0.533684
8	-7.533313	3.217458	-0.041877
8	-7.771042	1.107048	-0.794271
1	-8.692182	1.304182	-0.531875
6	-4.123768	-3.130694	0.249983
1	-4.568204	-2.417510	0.949726
1	-4.212423	-4.113274	0.723676
6	-4.943711	-3.135353	-1.078045
1	-4.356062	-2.658300	-1.873090
1	-5.160483	-4.152338	-1.410846

6	-6.261517	-2.383465	-1.030641
8	-7.306012	-2.767163	-1.499428
8	-6.118683	-1.166629	-0.441000
1	-6.953822	-0.660630	-0.548942
6	-1.619282	-5.153205	-0.166342
1	-2.575824	-5.553555	0.180111
1	-1.452810	-5.538596	-1.180514
1	-0.834085	-5.573935	0.473110
6	-2.695981	4.749016	0.001915
1	-2.540004	5.239807	-0.967042
1	-3.737365	4.914653	0.288773
1	-2.065970	5.268975	0.733579
6	3.424312	-4.523016	-1.860620
1	3.030485	-5.083471	-1.006675
1	3.012417	-4.977854	-2.771351
1	4.508040	-4.669112	-1.886551
6	4.775186	3.347595	-2.324744
1	5.597260	2.897983	-1.753433
1	4.859935	2.984508	-3.356597
1	4.944026	4.426922	-2.337843
6	5.176731	-1.967827	-2.790358
6	5.659131	-2.886496	-3.640268
1	5.814226	-1.118218	-2.548663
1	6.659157	-2.791177	-4.052020
1	5.076580	-3.738900	-3.974612
6	2.581758	5.332453	-1.163012
6	2.106219	6.110063	-0.179424
1	3.120409	5.809316	-1.980759
1	2.231293	7.188063	-0.210534
1	1.610924	5.701999	0.697289
6	-0.604868	-2.353957	3.687852
1	-0.776601	-1.676426	4.528180
1	-1.562937	-2.542503	3.195661
6	0.089783	-3.632424	4.108654
1	1.049997	-3.419139	4.587923
1	-0.540157	-4.168108	4.826553
1	0.266078	-4.286900	3.249452

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**TS(C-P)<sub>Ir</sub>**

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Number of imaginary frequencies: 3    Electronic energy:    HF=-2591.3873191  
Zero-point correction=                    0.808646 (Hartree/Particle)  
Thermal correction to Energy=            0.860904  
Thermal correction to Enthalpy=         0.861849  
Thermal correction to Gibbs Free Energy= 0.721229  
Sum of electronic and zero-point Energies= -2590.578673  
Sum of electronic and thermal Energies= -2590.526415  
Sum of electronic and thermal Enthalpies= -2590.525470  
Sum of electronic and thermal Free Energies= -2590.666090

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## Cartesian Coordinates

6	3.219182	-3.428930	-1.394331
6	1.976871	-2.809187	-1.003611
7	2.098235	-1.432351	-1.058685
6	3.380105	-1.159960	-1.486980
6	4.095608	-2.404250	-1.710053
6	0.810798	-3.493112	-0.656543
6	-0.427048	-2.941443	-0.365375
7	-0.698402	-1.590049	-0.310948
6	-2.042281	-1.463925	-0.057352
6	-2.647560	-2.782982	0.056915
6	-1.643988	-3.697714	-0.128079
6	-2.721013	-0.253715	0.049112
6	-2.184083	1.016252	-0.116312
7	-0.857877	1.290542	-0.391407
6	-0.760922	2.660536	-0.544198
6	-2.061533	3.269521	-0.350922
6	-2.940325	2.253133	-0.071865
6	0.404857	3.354664	-0.836628
6	1.668001	2.812635	-1.055459
7	1.949472	1.467527	-1.049143
6	3.258416	1.330265	-1.473610
6	3.831242	2.632762	-1.728634
6	2.853806	3.560420	-1.443312
6	3.906602	0.115614	-1.665422
1	0.316551	4.428246	-0.949081
1	4.925157	0.165976	-2.030604
1	0.864908	-4.575909	-0.668508
1	-3.786696	-0.310707	0.236061
6	-4.408737	2.366713	0.226425
1	-4.694320	1.623263	0.979745
1	-4.621568	3.345823	0.666249
6	-5.314943	2.195189	-1.019888
1	-5.198765	1.202078	-1.456882
1	-5.038836	2.939128	-1.775372
6	-6.760741	2.452550	-0.646909
8	-7.192235	3.488830	-0.203893
8	-7.562121	1.359530	-0.839871
1	-8.466643	1.624982	-0.580031
6	-4.116268	-3.028267	0.262488
1	-4.517643	-2.284134	0.956039
1	-4.263193	-4.000138	0.743856
6	-4.934709	-2.993581	-1.065456
1	-4.328871	-2.532222	-1.856083
1	-5.188075	-3.999553	-1.405852
6	-6.222632	-2.192483	-1.012793
8	-7.282229	-2.533522	-1.480824
8	-6.030512	-0.984062	-0.419832
1	-6.842460	-0.442719	-0.532039

6	-1.733681	-5.194246	-0.141313
1	-2.723443	-5.535641	0.173431
1	-1.552328	-5.600543	-1.144632
1	-0.998084	-5.652417	0.531120
6	-2.336397	4.739264	-0.455514
1	-2.182356	5.104315	-1.478934
1	-3.366407	4.974362	-0.175558
1	-1.676095	5.322544	0.197741
6	3.474485	-4.905304	-1.423990
1	2.900122	-5.433954	-0.656220
1	3.205324	-5.347560	-2.392347
1	4.534866	-5.116931	-1.255677
6	5.225331	2.924047	-2.199982
1	5.216569	3.447618	-3.164362
1	5.755753	3.568667	-1.489435
1	5.823010	2.018686	-2.331130
6	5.485278	-2.479973	-2.155950
6	6.033115	-3.460853	-2.888888
1	6.125932	-1.648268	-1.865126
1	7.083459	-3.428834	-3.161642
1	5.460996	-4.303293	-3.263633
6	3.005758	5.010660	-1.552536
6	2.462467	5.939321	-0.751736
1	3.667538	5.347437	-2.350341
1	2.650851	6.995910	-0.915159
1	1.844893	5.683106	0.104409
6	1.178986	-0.193937	1.436678
6	1.954755	0.895048	2.140008
6	0.037340	-0.665158	2.345707
6	1.489192	2.209721	2.267916
6	3.109967	0.567713	2.872611
8	-0.863126	0.070238	2.682280
8	0.204017	-1.934762	2.740917
6	2.196820	3.151346	3.017081
1	0.564886	2.484907	1.777864
6	3.828065	1.479276	3.631415
8	3.456080	-0.793848	2.956679
6	3.369024	2.795623	3.687376
1	1.825474	4.169549	3.079649
1	4.709675	1.153591	4.173049
6	3.269162	-1.468154	1.836244
1	3.915588	3.531385	4.268582
1	3.180001	-2.542575	1.973553
1	3.718828	-1.077221	0.924357
1	1.918598	-1.108808	1.427586
6	-0.797037	-2.474665	3.659333
1	-1.772203	-2.076532	3.373030
1	-0.771526	-3.549117	3.468632
6	-0.451449	-2.143463	5.101124
1	-0.492353	-1.064396	5.274622

1	-1.174847	-2.623534	5.769328
1	0.547245	-2.509407	5.360101
77	0.668859	-0.058155	-0.512902

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**A<sub>Ir(Cl)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2399.8125195  
Zero-point correction=                    0.599343 (Hartree/Particle)  
Thermal correction to Energy=            0.642032  
Thermal correction to Enthalpy=         0.642976  
Thermal correction to Gibbs Free Energy= 0.518876  
Sum of electronic and zero-point Energies= -2399.213177  
Sum of electronic and thermal Energies= -2399.170487  
Sum of electronic and thermal Enthalpies= -2399.169543  
Sum of electronic and thermal Free Energies= -2399.293644

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Cartesian Coordinates

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6	3.586597	3.295475	0.244171
6	2.279040	2.661538	0.149864
7	2.429922	1.307059	-0.008175
6	3.782583	1.049554	-0.000358
6	4.520782	2.285805	0.148778
6	1.056851	3.321041	0.225782
6	-0.207609	2.752412	0.143583
7	-0.462035	1.408718	-0.001946
6	-1.828553	1.260394	-0.014933
6	-2.465230	2.562698	0.095772
6	-1.458598	3.486731	0.196990
6	-2.494062	0.043164	-0.105744
6	-1.921370	-1.220124	-0.209717
7	-0.571123	-1.468726	-0.249402
6	-0.418964	-2.833049	-0.342013
6	-1.721800	-3.471546	-0.384909
6	-2.655206	-2.471887	-0.304193
6	0.799695	-3.495422	-0.395344
6	2.067958	-2.922117	-0.384089
7	2.324952	-1.572930	-0.297403
6	3.690889	-1.419495	-0.318320
6	4.324821	-2.723585	-0.476324
6	3.309711	-3.653897	-0.487306
77	0.931277	-0.091548	-0.033092
6	4.353572	-0.211023	-0.141999
1	0.760098	-4.577683	-0.461631
1	5.434159	-0.262730	-0.097529
1	1.092356	4.395316	0.369035
1	-3.577999	0.082883	-0.091225
17	0.940586	-0.310922	2.288582
6	-1.941184	-4.950517	-0.496827

1	-3.002333	-5.188524	-0.614045
1	-1.412118	-5.373945	-1.359850
1	-1.581550	-5.482016	0.394102
6	3.415298	-5.141864	-0.634585
1	2.964408	-5.487982	-1.574069
1	4.458296	-5.469564	-0.636643
1	2.902813	-5.665589	0.182176
6	6.014168	2.402755	0.137860
1	6.474303	1.649002	-0.510064
1	6.321096	3.389746	-0.222625
1	6.444393	2.273067	1.140430
6	-1.564267	4.975918	0.335311
1	-1.128994	5.496754	-0.527726
1	-2.606854	5.295525	0.419054
1	-1.037423	5.335639	1.228122
6	5.753885	-3.007092	-0.604107
6	6.671797	-2.267402	-1.244542
1	6.084552	-3.941378	-0.150105
1	7.711569	-2.579162	-1.280987
1	6.418432	-1.353937	-1.774293
6	3.787626	4.736161	0.366962
6	4.808319	5.355478	0.979896
1	3.019781	5.360699	-0.089751
1	4.871556	6.439637	0.997328
1	5.591607	4.814602	1.501361
6	-4.152295	-2.596329	-0.280409
6	-4.729772	-2.591079	1.146219
1	-4.462643	-3.519171	-0.781337
1	-4.617903	-1.785946	-0.852568
1	-4.330568	-3.424909	1.736580
1	-4.435600	-1.684708	1.690554
6	-3.948317	2.802312	0.070812
6	-4.527040	2.833856	-1.354695
1	-4.185207	3.748963	0.566847
1	-4.474232	2.033927	0.648836
1	-4.058940	3.626262	-1.952056
1	-4.314267	1.900921	-1.891892
6	-6.240956	-2.677986	1.157343
8	-6.959303	-2.699429	0.181483
8	-6.726816	-2.728191	2.421911
1	-7.698313	-2.771286	2.336982
6	-6.024975	3.053014	-1.366743
8	-6.733622	3.178409	-0.392059
8	-6.510470	3.095148	-2.632291
1	-7.473478	3.230793	-2.547844

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**B<sub>IR</sub>(Cl)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3161.3263613  
Zero-point correction=                      0.821602 (Hartree/Particle)

Thermal correction to Energy=	0.881397
Thermal correction to Enthalpy=	0.882341
Thermal correction to Gibbs Free Energy=	0.719563
Sum of electronic and zero-point Energies=	-3160.504759
Sum of electronic and thermal Energies=	-3160.444964
Sum of electronic and thermal Enthalpies=	-3160.444020
Sum of electronic and thermal Free Energies=	-3160.606798

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Cartesian Coordinates  
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6	-4.113223	3.581354	0.658929
6	-2.779814	3.057782	0.450407
7	-2.847838	1.768480	-0.024926
6	-4.179807	1.462016	-0.158734
6	-4.991704	2.592155	0.271537
6	-1.598709	3.755892	0.687092
6	-0.302681	3.297128	0.497514
7	0.034428	2.041489	0.046663
6	1.404828	1.994585	-0.022282
6	1.960242	3.269544	0.408909
6	0.901058	4.073368	0.737499
6	2.147037	0.887152	-0.423641
6	1.651772	-0.344321	-0.838550
7	0.317740	-0.659376	-0.941687
6	0.247077	-1.942727	-1.429583
6	1.585375	-2.474168	-1.613454
6	2.457890	-1.488635	-1.235543
6	-0.926173	-2.639777	-1.684456
6	-2.227516	-2.197154	-1.470131
7	-2.559700	-0.940770	-1.024355
6	-3.933974	-0.853950	-1.040251
6	-4.499331	-2.103878	-1.492220
6	-3.444003	-2.957567	-1.733772
77	-1.263045	0.586786	-0.583555
6	-4.671547	0.258753	-0.648254
1	-0.817747	-3.634901	-2.096982
1	-5.749188	0.173767	-0.734913
1	-1.701488	4.773649	1.047612
1	3.225103	0.998565	-0.421078
6	1.247968	-1.876937	3.106502
6	0.838088	-3.197444	2.584526
6	1.796352	-4.194530	2.350621
6	-0.520664	-3.494291	2.309569
6	1.431075	-5.451330	1.867129
1	2.837730	-3.967594	2.540131
6	-0.887057	-4.762470	1.848161
6	0.088953	-5.737288	1.625869
1	2.194931	-6.204475	1.697419
1	-1.927741	-4.991448	1.651061
1	-0.210319	-6.718815	1.268011

6	2.552779	-1.245477	2.867016
8	3.448540	-1.724174	2.192427
8	2.651183	-0.052359	3.503527
8	-1.409638	-2.480368	2.521466
6	-2.793769	-2.722227	2.303133
1	-3.297150	-1.781224	2.529781
1	-2.991910	-2.997838	1.261434
1	-3.168218	-3.508994	2.970915
7	-0.249999	-0.605102	4.579169
7	0.435043	-1.199851	3.895592
6	3.958464	-1.555984	-1.196908
1	4.329404	-1.054345	-0.296677
1	4.277199	-2.599363	-1.114167
6	4.633167	-0.945059	-2.455355
1	4.408745	0.119601	-2.539700
1	4.249656	-1.451384	-3.347594
6	6.126575	-1.175986	-2.421467
8	6.678429	-2.248139	-2.496699
8	6.849342	-0.018585	-2.266807
1	7.788734	-0.286221	-2.247364
6	3.427228	3.596287	0.408104
1	3.990907	2.747171	0.805377
1	3.623735	4.434281	1.084651
6	3.974522	3.951579	-1.008122
1	3.268423	3.590548	-1.767094
1	4.064636	5.031286	-1.145872
6	5.310543	3.328204	-1.362898
8	6.227168	3.886592	-1.921869
8	5.342302	2.012255	-1.030896
1	6.142417	1.596750	-1.418277
6	0.914790	5.488732	1.232310
1	1.936017	5.844922	1.396211
1	0.441002	6.171948	0.515449
1	0.373524	5.591287	2.181415
6	1.888613	-3.863888	-2.086448
1	1.445505	-4.061437	-3.070844
1	2.965971	-4.030341	-2.173056
1	1.493347	-4.616134	-1.392027
6	-4.426207	4.927688	1.236570
1	-3.679426	5.231092	1.978401
1	-4.456026	5.710809	0.466409
1	-5.404101	4.918433	1.728342
6	-5.967384	-2.383130	-1.612529
1	-6.473193	-2.325347	-0.639523
1	-6.460731	-1.660760	-2.274929
1	-6.152871	-3.382945	-2.013910
6	-6.451080	2.582704	0.304757
6	-7.265300	3.638388	0.150773
1	-6.913557	1.609585	0.470509
1	-8.343557	3.523150	0.212430

1	-6.894910	4.635421	-0.065572
6	-3.549506	-4.350718	-2.167615
6	-2.753728	-5.374586	-1.821922
1	-4.394379	-4.567975	-2.821338
1	-2.936400	-6.372998	-2.208852
1	-1.920738	-5.264108	-1.133870
6	3.908028	0.641111	3.359257
1	4.704470	0.021616	3.785472
1	4.121882	0.769176	2.293712
6	3.773851	1.971569	4.076890
1	3.545011	1.823240	5.137138
1	4.713327	2.530172	4.001647
1	2.974913	2.572829	3.631148
17	-1.284318	1.406246	-2.766667

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**TS(B-B')<sub>Ir(Cl)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3162.34307388  
Zero-point correction=                    0.821764 (Hartree/Particle)  
Thermal correction to Energy=            0.880181  
Thermal correction to Enthalpy=         0.881125  
Thermal correction to Gibbs Free Energy= 0.725972  
Sum of electronic and zero-point Energies= -3160.504447  
Sum of electronic and thermal Energies= -3160.446029  
Sum of electronic and thermal Enthalpies= -3160.445085  
Sum of electronic and thermal Free Energies= -3160.600239

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Cartesian Coordinates

.....

6	-3.368022	3.475295	-1.045374
6	-2.078884	2.897766	-0.725656
7	-2.140244	1.527762	-0.824234
6	-3.408953	1.211173	-1.241013
6	-4.200094	2.427336	-1.375004
6	-0.936981	3.621778	-0.393678
6	0.327176	3.116743	-0.111568
7	0.668930	1.786608	-0.107121
6	2.006625	1.711685	0.192179
6	2.529901	3.049454	0.426550
6	1.488140	3.919912	0.225103
6	2.748968	0.535263	0.222676
6	2.295436	-0.748468	-0.064073
7	0.995388	-1.078213	-0.354951
6	0.961274	-2.428606	-0.592500
6	2.291438	-2.986624	-0.436842
6	3.119984	-1.945884	-0.108502
6	-0.172976	-3.161659	-0.922349
6	-1.464329	-2.675598	-1.095950
7	-1.815039	-1.350883	-1.032654
6	-3.130001	-1.256082	-1.420684

6	-3.651263	-2.573073	-1.709849
6	-2.629468	-3.467613	-1.477449
77	-0.562971	0.224103	-0.613878
6	-3.856585	-0.073307	-1.522493
1	-0.033207	-4.223005	-1.085351
1	-4.878301	-0.166374	-1.873431
1	-1.037926	4.701621	-0.376212
1	3.796474	0.632232	0.481293
6	-1.252895	-0.226592	2.324746
6	-0.960512	-1.670493	2.539625
6	0.353891	-2.085341	2.805724
6	-1.970014	-2.666862	2.506156
6	0.661706	-3.424042	3.049179
1	1.136754	-1.341920	2.829441
6	-1.657471	-4.006852	2.748417
6	-0.342054	-4.386691	3.022603
1	1.690493	-3.703145	3.256123
1	-2.439131	-4.756762	2.727396
1	-0.115921	-5.431758	3.216562
6	-0.403064	0.863734	2.892040
8	0.747265	0.729737	3.258247
8	-1.079368	2.028908	2.971295
8	-3.237206	-2.235967	2.237663
6	-4.286591	-3.187121	2.135700
1	-5.182593	-2.612303	1.894316
1	-4.089420	-3.910934	1.336244
1	-4.440470	-3.716300	3.085038
7	-3.513507	0.657866	1.898872
7	-2.505241	0.190159	2.100379
6	4.609088	-1.989160	0.084468
1	4.931622	-1.227691	0.802333
1	4.897966	-2.956539	0.512491
6	5.372695	-1.788423	-1.255960
1	5.153673	-0.795188	-1.665183
1	5.057375	-2.539375	-1.983342
6	6.864806	-1.924110	-1.091980
8	7.576857	-2.791181	-1.536565
8	7.389306	-0.914934	-0.314232
1	8.350396	-1.078127	-0.261600
6	3.938568	3.404830	0.818687
1	4.325107	2.699296	1.561767
1	3.919076	4.380634	1.315223
6	4.955729	3.501456	-0.355750
1	4.492042	3.937433	-1.243062
1	5.780537	4.153943	-0.041595
6	5.578246	2.179442	-0.754406
8	5.546487	1.685613	-1.862620
8	6.207651	1.597809	0.293641
1	6.618245	0.759176	-0.017767
6	1.487114	5.418313	0.301430



1	2.438080	5.803255	0.680957
1	1.323883	5.870805	-0.685570
1	0.694288	5.793728	0.960792
6	2.632429	-4.435488	-0.614905
1	2.454404	-4.770735	-1.644793
1	3.683766	-4.631894	-0.384450
1	2.025303	-5.071821	0.041434
6	-3.696989	4.935184	-0.975885
1	-3.139118	5.437087	-0.177532
1	-3.461157	5.457367	-1.913520
1	-4.764643	5.081220	-0.782912
6	-5.058097	-2.859259	-2.142408
1	-5.210732	-3.925941	-2.328140
1	-5.788671	-2.553412	-1.381634
1	-5.312063	-2.321332	-3.064553
6	-5.611196	2.445460	-1.747553
6	-6.258491	3.422615	-2.401404
1	-6.186132	1.565689	-1.458363
1	-7.321107	3.342353	-2.611767
1	-5.756474	4.311911	-2.769141
6	-2.717243	-4.922617	-1.593494
6	-2.093835	-5.834496	-0.830218
1	-3.390370	-5.287858	-2.369466
1	-2.236460	-6.896968	-1.006335
1	-1.448369	-5.557174	-0.002203
6	-0.345831	3.148631	3.521425
1	0.022889	2.870228	4.513584
1	0.518349	3.346886	2.881538
6	-1.300875	4.326102	3.576202
1	-2.164171	4.103371	4.211652
1	-0.786106	5.200946	3.988785
1	-1.664565	4.575410	2.574413
17	-0.022223	0.466871	-2.878359

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**B'<sub>IR(CI)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-3161.3256228  
 Zero-point correction=                    0.821722 (Hartree/Particle)  
 Thermal correction to Energy=            0.880696  
 Thermal correction to Enthalpy=         0.881640  
 Thermal correction to Gibbs Free Energy= 0.725671  
 Sum of electronic and zero-point Energies= -3160.503901  
 Sum of electronic and thermal Energies= -3160.444927  
 Sum of electronic and thermal Enthalpies= -3160.443983  
 Sum of electronic and thermal Free Energies= -3160.599952

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 Cartesian Coordinates  
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6	3.148348	-3.698927	-0.902415
6	1.913320	-3.020239	-0.567840

7	2.079134	-1.661381	-0.692757
6	3.356209	-1.447651	-1.145592
6	4.049145	-2.723533	-1.274300
6	0.719912	-3.653810	-0.226230
6	-0.514325	-3.053688	0.001125
7	-0.753265	-1.703086	-0.006578
6	-2.099645	-1.524441	0.173344
6	-2.743474	-2.819900	0.336648
6	-1.759582	-3.768552	0.233647
6	-2.756194	-0.296826	0.177277
6	-2.192479	0.955510	-0.051086
7	-0.867813	1.191527	-0.305066
6	-0.732392	2.526701	-0.574051
6	-2.021195	3.184269	-0.440367
6	-2.927144	2.211712	-0.106002
6	0.451842	3.165464	-0.929116
6	1.702030	2.579558	-1.103457
7	1.964889	1.241419	-0.979534
6	3.252042	1.030631	-1.402528
6	3.853977	2.291608	-1.780094
6	2.906647	3.267345	-1.562287
77	0.618039	-0.224383	-0.445154
6	3.890528	-0.205480	-1.471277
1	0.386840	4.226918	-1.133349
1	4.904999	-0.199364	-1.854164
1	0.740453	-4.737980	-0.195816
1	-3.827761	-0.322922	0.335962
6	1.130770	0.145869	1.865463
6	1.154472	1.614731	2.256973
6	-0.040992	2.255384	2.609953
6	2.341661	2.388458	2.268873
6	-0.069428	3.599437	2.984052
1	-0.960203	1.690270	2.593324
6	2.311441	3.733937	2.648289
6	1.107162	4.339805	3.006965
1	-1.017275	4.055844	3.252752
1	3.227297	4.312153	2.661866
1	1.101057	5.385657	3.301831
6	0.150459	-0.745552	2.637995
8	-0.968025	-0.411050	2.952142
8	0.684925	-1.941896	2.926711
8	3.492975	1.751990	1.906611
6	4.708124	2.485563	1.847940
1	5.463505	1.774842	1.508421
1	4.635664	3.311454	1.131434
1	4.989767	2.872335	2.835720
7	3.285150	-1.120875	1.867019
7	2.369645	-0.479743	1.922172
6	-4.398419	2.375805	0.153796
1	-4.718484	1.692824	0.950012

1	-4.603543	3.389122	0.514249
6	-5.281498	2.128780	-1.098586
1	-5.179916	1.100890	-1.449637
1	-4.958743	2.800525	-1.901748
6	-6.727319	2.453944	-0.798107
8	-7.152351	3.534176	-0.460497
8	-7.562183	1.372709	-0.923134
1	-8.458549	1.697206	-0.708618
6	-4.226150	-3.011548	0.490080
1	-4.630398	-2.228585	1.138076
1	-4.433181	-3.961161	0.995057
6	-4.979570	-2.991533	-0.875620
1	-4.343568	-2.503987	-1.625593
1	-5.184586	-4.001870	-1.236238
6	-6.286048	-2.224017	-0.885367
8	-7.326386	-2.595962	-1.379940
8	-6.141155	-1.000242	-0.314666
1	-6.946765	-0.468849	-0.487446
6	-1.892434	-5.261885	0.286084
1	-2.904563	-5.561267	0.574885
1	-1.681205	-5.721030	-0.688637
1	-1.198228	-5.710521	1.008201
6	-2.251364	4.652731	-0.636356
1	-2.050112	4.958917	-1.671146
1	-3.284511	4.931309	-0.408235
1	-1.596070	5.251195	0.009178
6	3.366049	-5.178745	-0.815600
1	2.780419	-5.625759	-0.004709
1	3.081039	-5.693937	-1.743387
1	4.421667	-5.403555	-0.631486
6	5.256798	2.453861	-2.284600
1	5.998997	2.122426	-1.545871
1	5.426693	1.864205	-3.194380
1	5.478693	3.498412	-2.520080
6	5.442798	-2.856336	-1.686404
6	6.000917	-3.898391	-2.322338
1	6.087115	-2.010225	-1.447063
1	7.059583	-3.899452	-2.565452
1	5.428202	-4.762336	-2.643926
6	3.087677	4.705022	-1.760031
6	2.566138	5.691933	-1.014462
1	3.743626	4.985193	-2.584635
1	2.769063	6.733185	-1.248641
1	1.946688	5.496802	-0.144001
6	-0.187687	-2.883932	3.605052
1	-0.540443	-2.420845	4.531345
1	-1.052052	-3.071670	2.963128
6	0.623257	-4.139537	3.860286
1	1.491229	-3.927371	4.493017
1	-0.000037	-4.882741	4.369443

1	0.977150	-4.568488	2.917694
17	0.038148	-0.479077	-2.755733

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**TS(B-C)<sub>Ir(Cl)</sub>**  
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Number of imaginary frequencies: 1	Electronic energy:	HF=-3161.3184563
Zero-point correction=	0.819821 (Hartree/Particle)	
Thermal correction to Energy=	0.878548	
Thermal correction to Enthalpy=	0.879492	
Thermal correction to Gibbs Free Energy=	0.724744	
Sum of electronic and zero-point Energies=	-3160.498635	
Sum of electronic and thermal Energies=	-3160.439909	
Sum of electronic and thermal Enthalpies=	-3160.438964	
Sum of electronic and thermal Free Energies=	-3160.593713	

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 Cartesian Coordinates  
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6	3.062944	-3.708229	-0.978624
6	1.858162	-3.017191	-0.576757
7	2.044813	-1.654398	-0.682414
6	3.305848	-1.456447	-1.190873
6	3.963917	-2.741415	-1.375122
6	0.667639	-3.638830	-0.208149
6	-0.558079	-3.025731	0.031130
7	-0.780125	-1.674378	0.030074
6	-2.128895	-1.480101	0.176093
6	-2.791154	-2.769521	0.315367
6	-1.815218	-3.728378	0.234678
6	-2.772554	-0.246681	0.176714
6	-2.191057	1.003943	-0.017059
7	-0.861859	1.231809	-0.244058
6	-0.706587	2.568373	-0.485694
6	-1.989043	3.238011	-0.357002
6	-2.911502	2.267813	-0.060200
6	0.486058	3.195900	-0.835401
6	1.721091	2.592129	-1.047568
7	1.968927	1.249703	-0.944604
6	3.231958	1.023766	-1.421939
6	3.838088	2.278965	-1.814887
6	2.917612	3.266823	-1.547184
77	0.622842	-0.204543	-0.370170
6	3.847743	-0.220850	-1.526293
1	0.435374	4.261397	-1.021827
1	4.842664	-0.228830	-1.957390
1	0.676074	-4.723169	-0.187514
1	-3.847662	-0.263472	0.309962
6	1.008152	0.108835	1.693692
6	1.311366	1.510204	2.200545
6	0.262684	2.314058	2.676298
6	2.605986	2.089092	2.164957

6	0.472605	3.623745	3.108880
1	-0.736273	1.904736	2.698741
6	2.818390	3.395566	2.617601
6	1.753366	4.164179	3.085870
1	-0.370110	4.208174	3.465858
1	3.814577	3.820162	2.595612
1	1.935936	5.178926	3.429180
6	-0.015503	-0.628921	2.575189
8	-1.107461	-0.173512	2.836158
8	0.401145	-1.832855	2.995821
8	3.618114	1.307077	1.696334
6	4.947385	1.805548	1.693247
1	5.561892	0.996799	1.294377
1	5.037057	2.684208	1.044189
1	5.283997	2.057251	2.707088
7	3.106595	-1.614352	1.791603
7	2.392081	-0.800083	2.049735
6	-4.385754	2.442087	0.174069
1	-4.728153	1.746354	0.949553
1	-4.587490	3.449820	0.551659
6	-5.245483	2.230433	-1.100641
1	-5.145662	1.209756	-1.472604
1	-4.900892	2.916318	-1.882576
6	-6.694289	2.561906	-0.822148
8	-7.116034	3.636001	-0.461639
8	-7.536840	1.493890	-0.998673
1	-8.434651	1.821611	-0.795369
6	-4.279757	-2.945139	0.424691
1	-4.693367	-2.165939	1.071372
1	-4.511888	-3.898902	0.910556
6	-4.993707	-2.897444	-0.961349
1	-4.332465	-2.404631	-1.685604
1	-5.197550	-3.900288	-1.342859
6	-6.292509	-2.117645	-0.994890
8	-7.322423	-2.472370	-1.522690
8	-6.152129	-0.904037	-0.401605
1	-6.948115	-0.362551	-0.587174
6	-1.964557	-5.220323	0.275903
1	-2.985045	-5.510645	0.543679
1	-1.739767	-5.676065	-0.697363
1	-1.288836	-5.679628	1.008685
6	-2.201894	4.711853	-0.531719
1	-2.004312	5.029093	-1.563930
1	-3.230010	4.999663	-0.292666
1	-1.535358	5.294580	0.116524
6	3.257978	-5.192904	-0.929008
1	2.701912	-5.644892	-0.100436
1	2.922447	-5.684965	-1.852326
1	4.316672	-5.438514	-0.796953
6	5.217695	2.423533	-2.384672

1	5.988516	2.060867	-1.691404
1	5.329590	1.851248	-3.314373
1	5.449464	3.468554	-2.608156
6	5.333971	-2.893234	-1.855080
6	5.839437	-3.932785	-2.537144
1	6.006065	-2.064928	-1.630510
1	6.884944	-3.949369	-2.831208
1	5.234393	-4.778439	-2.847856
6	3.107780	4.703577	-1.743254
6	2.638072	5.688138	-0.961662
1	3.722897	4.983271	-2.598847
1	2.840674	6.729635	-1.194990
1	2.064881	5.489846	-0.060652
6	-0.564801	-2.614906	3.746629
1	-0.889605	-2.028420	4.611117
1	-1.432385	-2.791289	3.105474
6	0.121977	-3.905641	4.149914
1	0.994327	-3.708285	4.781389
1	-0.576089	-4.533645	4.714134
1	0.451920	-4.460768	3.266175
17	-0.016517	-0.416085	-2.726622

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**CIr(Cl)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3161.3663639  
Zero-point correction=                    0.818590 (Hartree/Particle)  
Thermal correction to Energy=            0.879805  
Thermal correction to Enthalpy=         0.880749  
Thermal correction to Gibbs Free Energy= 0.715130  
Sum of electronic and zero-point Energies= -3160.547774  
Sum of electronic and thermal Energies= -3160.486559  
Sum of electronic and thermal Enthalpies= -3160.485615  
Sum of electronic and thermal Free Energies= -3160.651234

.....  
Cartesian Coordinates

.....  

6	3.175986	-3.129729	-1.487037
6	1.938990	-2.590071	-0.967367
7	1.978587	-1.219916	-1.019110
6	3.171110	-0.856048	-1.581490
6	3.939634	-2.052419	-1.894167
6	0.845913	-3.352208	-0.556754
6	-0.417747	-2.883084	-0.217075
7	-0.772518	-1.563409	-0.125835
6	-2.124158	-1.511366	0.091171
6	-2.650090	-2.866811	0.173747
6	-1.589695	-3.716849	-0.003580
6	-2.880686	-0.349306	0.207808
6	-2.420729	0.961365	0.113130
7	-1.129663	1.330825	-0.139269

6	-1.079617	2.696900	-0.176295
6	-2.405599	3.230860	0.079423
6	-3.237743	2.154779	0.259275
6	0.051468	3.461216	-0.449643
6	1.315926	2.994193	-0.800008
7	1.665365	1.676729	-0.906139
6	2.898667	1.618247	-1.500517
6	3.383769	2.960170	-1.743821
6	2.422270	3.824083	-1.270482
77	0.476150	0.053827	-0.437900
6	3.581847	0.450613	-1.826333
1	-0.084823	4.535328	-0.470296
1	4.533259	0.576653	-2.330748
1	0.968131	-4.429003	-0.591710
1	-3.942031	-0.478660	0.381191
6	0.867799	0.194808	1.442328
6	1.732887	1.164793	2.140827
6	1.126552	2.138781	2.959192
6	3.146189	1.164641	2.025154
6	1.878656	3.141564	3.566481
1	0.048877	2.116103	3.075385
6	3.898231	2.164425	2.652511
6	3.263263	3.153996	3.404627
1	1.384476	3.901740	4.163819
1	4.978019	2.171455	2.565592
1	3.863603	3.926172	3.877984
6	-0.014650	-0.534115	2.423184
8	-1.039495	-0.061119	2.873909
8	0.496310	-1.723863	2.763867
8	3.689855	0.119515	1.353796
6	5.103829	0.044591	1.241142
1	5.305149	-0.862627	0.671621
1	5.506908	0.910292	0.701256
1	5.576360	-0.027978	2.228507
7	3.613115	-3.719716	2.091057
7	4.027684	-2.884142	2.683715
6	-4.710554	2.169218	0.557106
1	-4.956878	1.372405	1.269206
1	-4.984894	3.112112	1.040856
6	-5.599605	2.003449	-0.704308
1	-5.423454	1.038360	-1.181739
1	-5.352599	2.792546	-1.423134
6	-7.059521	2.165763	-0.345215
8	-7.564827	3.158352	0.124503
8	-7.802991	1.038071	-0.584364
1	-8.717743	1.256044	-0.318818
6	-4.108574	-3.195118	0.329911
1	-4.561796	-2.512645	1.054943
1	-4.224702	-4.201524	0.745779
6	-4.891792	-3.110816	-1.016987

1	-4.309936	-2.514042	-1.731035
1	-5.032059	-4.098207	-1.462085
6	-6.250485	-2.444445	-0.936163
8	-7.273731	-2.851243	-1.438507
8	-6.180064	-1.264745	-0.266841
1	-7.028158	-0.784264	-0.372436
6	-1.588891	-5.216004	-0.043283
1	-2.562801	-5.622552	0.245414
1	-1.361700	-5.593679	-1.048806
1	-0.839707	-5.641635	0.636407
6	-2.742457	4.691514	0.115518
1	-2.638235	5.153831	-0.874743
1	-3.771850	4.857005	0.446683
1	-2.083461	5.242750	0.797768
6	3.524267	-4.585971	-1.536308
1	3.081243	-5.133354	-0.697893
1	3.173907	-5.062914	-2.462111
1	4.609299	-4.724811	-1.491352
6	4.706912	3.293764	-2.364528
1	5.546607	2.949531	-1.745673
1	4.818727	2.824287	-3.349883
1	4.824917	4.372881	-2.495412
6	5.271364	-2.033051	-2.491349
6	5.831587	-2.987722	-3.250929
1	5.861986	-1.137525	-2.298459
1	6.841605	-2.871418	-3.633125
1	5.304113	-3.890438	-3.541106
6	2.497689	5.284073	-1.261082
6	2.020824	6.102709	-0.311196
1	3.026336	5.733223	-2.102065
1	2.132479	7.179996	-0.394411
1	1.533862	5.728513	0.584698
6	-0.295243	-2.506571	3.698352
1	-0.478952	-1.902924	4.592024
1	-1.259501	-2.723374	3.229558
6	0.483152	-3.770216	4.008341
1	1.443807	-3.535619	4.477329
1	-0.092869	-4.397463	4.697628
1	0.674409	-4.342184	3.095046
17	-0.255152	0.041121	-2.827355

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**TS(C-P)<sub>Ir(Cl)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3051.7914464  
Zero-point correction=                    0.809954 (Hartree/Particle)  
Thermal correction to Energy=            0.866073  
Thermal correction to Enthalpy=        0.867017  
Thermal correction to Gibbs Free Energy=    0.716183  
Sum of electronic and zero-point Energies=    -3050.981492  
Sum of electronic and thermal Energies=    -3050.925373



Sum of electronic and thermal Enthalpies= -3050.924429  
Sum of electronic and thermal Free Energies= -3051.075263

.....  
Cartesian Coordinates

.....  
6 3.445351 -3.367911 -1.073446  
6 2.162719 -2.787506 -0.735870  
7 2.241046 -1.416798 -0.805800  
6 3.509056 -1.098732 -1.218475  
6 4.288911 -2.319711 -1.381146  
6 1.012006 -3.508536 -0.425596  
6 -0.253021 -2.998622 -0.151166  
7 -0.581794 -1.669404 -0.110788  
6 -1.925776 -1.586291 0.136837  
6 -2.474779 -2.927261 0.289786  
6 -1.437394 -3.802676 0.110464  
6 -2.662383 -0.406548 0.192832  
6 -2.196246 0.884757 -0.045340  
7 -0.899780 1.215078 -0.334301  
6 -0.862276 2.559012 -0.591339  
6 -2.190667 3.122975 -0.425035  
6 -3.017555 2.086978 -0.071330  
6 0.275483 3.287863 -0.928745  
6 1.568593 2.801363 -1.089697  
7 1.925534 1.481866 -0.993558  
6 3.237210 1.379328 -1.384848  
6 3.755875 2.693704 -1.702317  
6 2.730770 3.588403 -1.494032  
77 0.675009 -0.090540 -0.517277  
6 3.965418 0.192393 -1.474626  
1 0.135328 4.345472 -1.115378  
1 4.986990 0.284912 -1.826342  
1 1.102676 -4.589382 -0.433310  
1 -3.722654 -0.508600 0.392177  
6 -4.489949 2.147524 0.223756  
1 -4.745021 1.435132 1.017385  
1 -4.753225 3.141047 0.601581  
6 -5.381902 1.856850 -1.013750  
1 -5.225152 0.838418 -1.372334  
1 -5.116584 2.552592 -1.816833  
6 -6.837534 2.093444 -0.679722  
8 -7.329027 3.157424 -0.383760  
8 -7.592907 0.949188 -0.712606  
1 -8.502394 1.217486 -0.477005  
6 -3.931344 -3.224138 0.510066  
1 -4.356331 -2.481425 1.191141  
1 -4.045779 -4.192793 1.008096  
6 -4.751289 -3.238928 -0.817029  
1 -4.181274 -2.713808 -1.594253  
1 -4.918402 -4.257090 -1.175243

6	-6.097021	-2.544964	-0.758256
8	-7.135724	-2.967964	-1.213546
8	-5.995420	-1.322400	-0.175656
1	-6.836819	-0.835921	-0.305410
6	-1.464878	-5.301954	0.128770
1	-2.443397	-5.678360	0.441765
1	-1.253983	-5.722659	-0.863209
1	-0.717825	-5.716234	0.817971
6	-2.534951	4.569602	-0.619748
1	-2.420554	4.873014	-1.668567
1	-3.569157	4.778097	-0.330165
1	-1.886401	5.225038	-0.024936
6	3.759493	-4.832745	-1.049517
1	3.172187	-5.359638	-0.289813
1	3.549589	-5.315332	-2.013998
1	4.819432	-4.997647	-0.829429
6	5.160963	2.975992	-2.142094
1	5.893845	2.676958	-1.380890
1	5.412173	2.432249	-3.061746
1	5.311972	4.041700	-2.333947
6	5.696703	-2.341752	-1.764960
6	6.343804	-3.323709	-2.412360
1	6.272708	-1.457090	-1.492840
1	7.404144	-3.239308	-2.632100
1	5.844570	-4.219473	-2.767063
6	2.806398	5.040135	-1.653641
6	2.191740	5.965433	-0.901255
1	3.460225	5.389151	-2.453067
1	2.320930	7.024699	-1.104184
1	1.568963	5.703000	-0.051131
6	1.219990	0.127532	1.722387
6	1.221128	1.473122	2.364092
6	0.573711	-0.936033	2.554923
6	0.106931	2.311970	2.491726
6	2.378211	1.857640	3.065418
8	-0.479037	-0.774609	3.137453
8	1.296424	-2.078003	2.584243
6	0.201375	3.516664	3.191432
1	-0.830130	2.015661	2.042476
6	2.505235	3.051606	3.760624
8	3.364585	0.879684	3.168566
6	1.396970	3.897911	3.805478
1	-0.670213	4.161301	3.256627
1	3.434464	3.289250	4.267254
6	3.406715	0.082231	2.093326
1	1.462892	4.841128	4.339896
1	3.723756	-0.933872	2.309298
1	3.753646	0.542092	1.165505
1	2.117045	-0.221372	1.148467
6	0.717472	-3.187397	3.316880

1	-0.361670	-3.190229	3.150033
1	1.158171	-4.071657	2.850814
6	1.052594	-3.107866	4.798854
1	0.592528	-2.224996	5.251115
1	0.670200	-3.996984	5.313699
1	2.135990	-3.062565	4.953598
17	0.079970	-0.305827	-2.842099

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N<sub>2</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-109.5207179  
Zero-point correction=                    0.005599 (Hartree/Particle)  
Thermal correction to Energy=            0.007960  
Thermal correction to Enthalpy=         0.008904  
Thermal correction to Gibbs Free Energy= -0.012850  
Sum of electronic and zero-point Energies= -109.515119  
Sum of electronic and thermal Energies= -109.512758  
Sum of electronic and thermal Enthalpies= -109.511814  
Sum of electronic and thermal Free Energies= -109.533568

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Cartesian Coordinates

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7	0.000000	0.000000	0.552657
7	0.000000	0.000000	-0.552657

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Q-A<sub>Ir(Me)</sub>

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Number of imaginary frequencies: 7    Electronic energy:    HF=-4752.0971348  
Zero-point correction=                    2.098008 (Hartree/Particle)  
Thermal correction to Energy=            2.224168  
Thermal correction to Enthalpy=         2.225112  
Thermal correction to Gibbs Free Energy= 1.885693  
Sum of electronic and zero-point Energies= -4749.999127  
Sum of electronic and thermal Energies= -4749.872967  
Sum of electronic and thermal Enthalpies= -4749.872023  
Sum of electronic and thermal Free Energies= -4750.211442

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Cartesian Coordinates

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6	3.151403	5.228463	-3.997654
6	3.990290	5.444093	-2.732417
6	5.466412	5.012060	-2.844985
6	6.255845	5.459941	-1.605503
6	5.621290	3.498926	-3.063308
6	4.366490	-5.858215	-4.628565
6	5.647028	-5.118141	-4.269336
8	6.752776	-5.646338	-4.273202
6	4.083932	-7.105585	-3.750160
6	5.055631	-8.260557	-4.033836

6	4.051701	-6.752011	-2.255445
7	5.479844	-3.800339	-3.906125
6	6.622923	-2.934762	-3.639836
6	7.106944	-2.965243	-2.177176
8	8.145731	-2.387437	-1.866208
6	6.326162	-1.489182	-4.054600
7	6.304847	-3.623026	-1.302379
6	6.614996	-3.770246	0.107121
6	5.592687	-3.101775	1.039604
6	5.402388	-1.599983	0.893991
6	4.198519	-1.024715	1.333617
6	6.391655	-0.750920	0.377161
6	3.988553	0.354982	1.273400
6	6.183059	0.631190	0.312377
6	4.987477	1.191291	0.763258
6	-0.927719	-3.733838	-4.409033
6	-1.521012	-4.543342	-3.271621
8	-0.884664	-4.829846	-2.250598
6	0.552184	-4.053773	-4.642758
7	-2.811364	-4.902390	-3.453961
6	-3.566330	-5.563878	-2.413101
6	-1.617903	-7.905760	1.915245
6	-0.856694	-7.092502	0.868269
8	-1.834776	-6.451696	0.048667
6	0.079669	-7.959384	0.021872
6	2.671298	-4.685533	6.500144
6	3.354977	-3.310060	6.552363
6	4.477627	-3.289858	7.599807
6	3.883988	-2.895885	5.170689
6	7.147739	1.571371	5.629657
6	6.776526	0.851672	4.337715
8	5.375461	0.551523	4.411340
6	7.599668	-0.421171	4.128613
6	-3.123992	1.025949	6.166375
6	-4.161227	1.319758	5.067000
6	-5.039564	0.124199	4.760894
6	-6.214071	-0.109533	5.490446
6	-4.676411	-0.800968	3.771866
6	-6.999313	-1.237689	5.247606
6	-5.458441	-1.931015	3.523207
6	-6.621579	-2.154993	4.264074
6	-6.318716	0.989128	-1.409473
6	-7.351552	-0.122230	-1.335968
8	-7.444332	-0.976048	-2.219647
6	-6.410668	1.750019	-2.736688
16	-7.954186	2.737878	-2.948952
7	-8.172524	-0.080025	-0.254848
6	-9.230700	-1.052934	-0.037548
6	-8.750254	-2.320409	0.686390
6	-9.841477	-3.393632	0.870387

6	-9.222637	-4.702400	1.384578
6	-10.973489	-2.931375	1.802587
6	0.808111	5.273354	0.412476
6	0.455655	1.048949	2.760707
6	-2.211833	-0.745611	-0.869158
6	-1.842930	3.477703	-3.225500
7	0.443128	3.013704	1.290940
6	0.993116	4.272308	1.361121
6	1.776475	4.401556	2.580790
6	1.674945	3.207365	3.246428
6	0.826457	2.348730	2.435263
6	2.315398	2.806550	4.543094
6	2.571212	5.615073	2.971953
6	3.969524	5.678626	2.318897
6	4.760770	6.923479	2.731412
7	-0.840439	0.476692	0.756405
6	-0.310848	0.176481	1.991003
6	-0.640783	-1.187993	2.354464
6	-1.379724	-1.706519	1.313771
6	-1.503289	-0.646036	0.322083
6	-0.188940	-1.879950	3.604220
6	-1.891701	-3.063563	1.131494
6	-2.414476	-3.853506	2.082228
7	-1.790485	1.491883	-1.791565
6	-2.342338	0.230142	-1.855908
6	-3.045986	0.064907	-3.109770
6	-2.879339	1.237545	-3.817021
6	-2.120557	2.138692	-2.958083
6	-3.801789	-1.160393	-3.538387
6	-3.376692	1.496348	-5.168060
6	-2.785080	2.227566	-6.125577
7	-0.548283	4.047904	-1.219263
6	-1.123899	4.360692	-2.429271
6	-0.845926	5.747719	-2.762343
6	-0.089745	6.258295	-1.739394
6	0.088113	5.181934	-0.774953
6	-1.324999	6.434288	-4.006733
6	0.435327	7.657121	-1.575894
6	-0.452607	8.553630	-0.685019
6	0.107780	9.970266	-0.526640
1	7.615679	-3.356145	0.248243
1	6.668743	-4.837524	0.358162
1	4.458504	-6.174096	-5.675694
1	3.504475	-5.180672	-4.572742
1	1.845783	-4.694440	5.777910
1	3.384486	-5.464879	6.199897
1	2.264314	-4.967057	7.478939
1	8.204000	1.861492	5.620859
1	6.538582	2.472276	5.756969
1	6.974162	0.917317	6.492208

1	2.128615	5.592387	-3.850831
1	3.581740	5.763623	-4.854036
1	3.083905	4.168681	-4.267778
1	-0.923387	-8.413133	2.593999
1	-2.269859	-7.256989	2.509089
1	-2.242351	-8.661974	1.425407
1	-2.506393	1.908762	6.368586
1	-3.614092	0.730539	7.101078
1	-2.459251	0.207356	5.867096
1	-4.520020	-5.898274	-2.828534
1	-3.021816	-6.427102	-2.027056
1	-3.766161	-4.895626	-1.567296
1	-1.032028	-2.673505	-4.140272
1	-1.506241	-3.881553	-5.328945
1	-5.323730	0.530079	-1.344378
1	-6.410721	1.689721	-0.572159
1	-9.629731	-1.321881	-1.020937
1	-10.027777	-0.553886	0.522930
1	-0.541345	10.586219	0.105894
1	1.104021	9.955208	-0.067053
1	0.200346	10.472173	-1.497836
1	5.746873	6.943698	2.253941
1	4.233467	7.842568	2.446348
1	4.914853	6.954462	3.817136
1	3.524247	4.909989	-1.890867
1	3.960865	6.511124	-2.468123
1	5.896521	5.525079	-3.719858
1	7.315231	5.187904	-1.685719
1	6.197798	6.546204	-1.464867
1	5.859663	4.985761	-0.697179
1	6.679180	3.221263	-3.145063
1	5.194473	2.935686	-2.222428
1	5.121285	3.161710	-3.977677
1	3.075054	-7.439513	-4.032334
1	4.792834	-9.138168	-3.430968
1	5.017679	-8.555402	-5.089493
1	6.085166	-7.972283	-3.806500
1	3.739700	-7.615699	-1.657611
1	5.047261	-6.453168	-1.903026
1	3.346927	-5.936066	-2.047913
1	4.575304	-3.368668	-4.038586
1	7.463751	-3.322022	-4.223622
1	7.193448	-0.865668	-3.827272
1	6.115589	-1.429319	-5.127555
1	5.467550	-1.086149	-3.502737
1	5.492514	-4.089945	-1.680985
1	5.900609	-3.328773	2.071623
1	4.618374	-3.594068	0.914043
1	3.411150	-1.667014	1.723181
1	7.320905	-1.158635	-0.007893

1	3.045439	0.773087	1.612937
1	6.962051	1.267797	-0.098979
1	4.826434	2.264873	0.714570
1	0.979387	-3.378877	-5.391678
1	1.106530	-3.944720	-3.706223
1	0.683712	-5.083119	-4.994608
1	-3.292257	-4.583155	-4.281753
1	-0.257024	-6.326901	1.388655
1	-1.383198	-5.915446	-0.633929
1	0.588681	-7.351401	-0.736101
1	0.846314	-8.440661	0.641334
1	-0.490423	-8.740537	-0.494948
1	2.598899	-2.570642	6.857142
1	4.945874	-2.300392	7.661563
1	4.099443	-3.547315	8.596723
1	5.262362	-4.014691	7.344701
1	4.337379	-1.897510	5.190592
1	4.647742	-3.604525	4.820765
1	3.077735	-2.887753	4.425669
1	6.954726	1.531631	3.489193
1	5.102398	0.211314	3.542327
1	7.315867	-0.917607	3.193875
1	8.671031	-0.192846	4.073516
1	7.434877	-1.119273	4.957592
1	-3.638499	1.636915	4.155931
1	-4.786217	2.165824	5.380804
1	-6.515383	0.601419	6.257462
1	-3.771594	-0.636586	3.190136
1	-7.905262	-1.400367	5.826329
1	-5.153996	-2.633732	2.752222
1	-7.226708	-3.038619	4.078070
1	-6.323725	1.054426	-3.573600
1	-5.597051	2.475376	-2.811716
1	-8.015895	0.631653	0.443583
1	-8.331508	-2.046602	1.665459
1	-7.926483	-2.741589	0.096845
1	-10.279210	-3.597660	-0.119283
1	-11.724255	-3.720751	1.926891
1	-10.582175	-2.685823	2.798829
1	-11.492409	-2.045207	1.420280
1	1.279830	6.227794	0.619451
1	0.813861	0.669221	3.711621
1	-2.712955	-1.690187	-1.050420
1	-2.240442	3.874350	-4.151883
1	1.613364	2.268116	5.191145
1	3.188440	2.155229	4.397580
1	2.659923	3.684920	5.098135
1	2.692112	5.636575	4.062552
1	2.016828	6.528537	2.715299
1	3.858487	5.652931	1.226748

1	4.528294	4.773770	2.591790
1	-0.214031	-2.966009	3.471528
1	0.832492	-1.593113	3.880128
1	-0.832761	-1.643457	4.462770
1	-1.817601	-3.469357	0.122323
1	-2.723695	-4.862671	1.830104
1	-2.556781	-3.516780	3.105417
1	-3.857869	-1.222913	-4.630058
1	-3.324457	-2.078859	-3.180663
1	-4.833341	-1.167565	-3.157935
1	-4.317536	1.006046	-5.418249
1	-3.248517	2.346417	-7.100703
1	-1.820363	2.705253	-5.983286
1	-0.934851	7.453875	-4.075221
1	-1.010542	5.899452	-4.912047
1	-2.420517	6.499472	-4.037546
1	0.535688	8.129633	-2.561271
1	1.450252	7.630128	-1.155515
1	-0.565565	8.084081	0.300748
1	-1.460376	8.596251	-1.118242
1	-8.766276	-4.558712	2.373062
1	-9.980492	-5.488955	1.481680
1	-8.441574	-5.068082	0.707780
77	-0.741423	2.279406	-0.209110
6	-2.488512	2.914896	0.686722
1	-2.248294	3.355295	1.658765
1	-2.964501	3.660928	0.043827
1	-3.150328	2.053528	0.816852
1	-8.785523	1.689309	-3.130020

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**Q-B<sub>Ir(Me)</sub>**

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Number of imaginary frequencies: 7    Electronic energy:    HF=-5513.603695  
Zero-point correction=                    2.318349 (Hartree/Particle)  
Thermal correction to Energy=            2.462486  
Thermal correction to Enthalpy=         2.463430  
Thermal correction to Gibbs Free Energy= 2.081834  
Sum of electronic and zero-point Energies= -5511.285346  
Sum of electronic and thermal Energies= -5511.141209  
Sum of electronic and thermal Enthalpies= -5511.140265  
Sum of electronic and thermal Free Energies= -5511.521861

.....  
Cartesian Coordinates

.....

6	0.798185	6.668201	-1.381094
6	1.982552	6.182001	-0.537268
6	3.365804	6.687667	-0.994073
6	4.445717	6.306613	0.030325
6	3.746123	6.176423	-2.392178



6	5.428838	-2.493878	-5.785644
6	6.412018	-1.469515	-5.231743
8	7.611068	-1.501453	-5.495792
6	5.666293	-3.939603	-5.275744
6	6.965031	-4.552159	-5.820167
6	5.607905	-4.015497	-3.742426
7	5.876025	-0.500950	-4.419460
6	6.725353	0.536798	-3.849080
6	7.449215	0.121824	-2.548566
8	8.525834	0.619929	-2.249573
6	5.943162	1.836558	-3.622743
7	6.784198	-0.776411	-1.759773
6	7.422886	-1.415737	-0.618164
6	7.092050	-0.811120	0.764182
6	7.635666	0.579563	1.022838
6	6.780286	1.684361	1.114816
6	9.011657	0.786983	1.200248
6	7.283847	2.962359	1.374484
6	9.518664	2.059332	1.458576
6	8.654470	3.154367	1.547615
6	-0.203551	-2.500023	-4.854907
6	-0.395221	-3.743217	-4.009731
8	0.348406	-4.027781	-3.063869
6	1.259047	-2.304269	-5.273519
7	-1.453730	-4.504387	-4.372165
6	-1.862714	-5.662449	-3.613355
6	1.225231	-8.463470	-0.352396
6	1.568757	-7.136696	-1.033461
8	0.331661	-6.473918	-1.309292
6	2.382418	-7.330523	-2.315286
6	4.755783	-5.639708	5.065465
6	4.372328	-6.908906	4.290191
6	3.402723	-7.779699	5.102285
6	3.783857	-6.560672	2.915081
6	6.850724	1.691665	6.405301
6	6.710434	0.646026	5.297801
8	5.627711	-0.256866	5.589418
6	8.007329	-0.120757	5.041260
6	-2.564511	-2.473659	6.709767
6	-3.914678	-2.329499	5.983278
6	-4.231100	-3.519070	5.100389
6	-4.856079	-4.657463	5.629435
6	-3.866301	-3.530041	3.746730
6	-5.101111	-5.778023	4.834406
6	-4.108122	-4.648596	2.945704
6	-4.723661	-5.778604	3.489398
6	-6.437907	-1.146219	-0.420109
6	-7.052085	-2.498463	-0.739743
8	-7.011820	-2.976508	-1.874770
6	-7.015611	-0.048567	-1.321973

16	-8.800991	0.319266	-1.037023
7	-7.676511	-3.111018	0.300205
6	-8.358506	-4.387238	0.162260
6	-7.431397	-5.595028	0.369919
6	-8.116436	-6.960871	0.166622
6	-7.071702	-8.087335	0.165366
6	-9.204589	-7.238247	1.216861
6	-2.540313	5.575518	1.108537
6	-0.951362	1.295367	2.737229
6	-2.563014	-0.844215	-1.299012
6	-4.201715	3.428798	-2.908439
7	-1.857813	3.272257	1.599991
6	-1.952649	4.606970	1.916978
6	-1.364980	4.845417	3.227059
6	-0.929633	3.631044	3.689039
6	-1.243804	2.651758	2.663545
6	-0.252807	3.309417	4.987594
6	-1.250532	6.189261	3.890342
6	-0.034404	7.016763	3.419573
6	0.052058	8.384687	4.103254
7	-1.851591	0.564493	0.576862
6	-1.206155	0.327265	1.769822
6	-0.816731	-1.066902	1.854884
6	-1.243164	-1.670991	0.691587
6	-1.911456	-0.636559	-0.088644
6	-0.031802	-1.677968	2.974297
6	-1.006888	-3.031581	0.212731
6	-0.902165	-4.145646	0.955991
7	-3.236016	1.463414	-1.810804
6	-3.191589	0.114656	-2.091817
6	-3.858800	-0.148821	-3.347818
6	-4.257723	1.071232	-3.851237
6	-3.885801	2.073548	-2.858552
6	-4.083374	-1.510303	-3.938015
6	-4.935229	1.287353	-5.129921
6	-4.779170	2.324188	-5.967366
7	-3.215823	4.174985	-0.785829
6	-3.887431	4.400836	-1.965023
6	-4.222994	5.809849	-2.077504
6	-3.747438	6.423612	-0.948444
6	-3.127536	5.384869	-0.139002
6	-4.953052	6.419312	-3.236926
6	-3.860275	7.870376	-0.557211
6	-5.061791	8.173210	0.364984
6	-5.149841	9.651480	0.756107
1	8.504017	-1.371244	-0.783655
1	7.123483	-2.469770	-0.615610
1	5.534942	-2.477776	-6.877333
1	4.397874	-2.199129	-5.552602
1	5.475539	-5.030803	4.504591

1	3.870130	-5.019857	5.260651
1	5.208113	-5.884234	6.034304
1	7.610295	2.438487	6.147723
1	5.898753	2.206836	6.569851
1	7.153719	1.220209	7.350631
1	-0.151671	6.322418	-0.958146
1	0.767447	7.764739	-1.421528
1	0.850118	6.302237	-2.412788
1	2.137434	-9.001663	-0.071677
1	0.631030	-8.287147	0.550194
1	0.640180	-9.097018	-1.029208
1	-2.364639	-1.601868	7.343858
1	-2.553889	-3.366539	7.345113
1	-1.741425	-2.568679	5.992175
1	-2.440384	-6.329607	-4.259364
1	-0.991146	-6.197862	-3.236618
1	-2.484115	-5.388235	-2.750877
1	-0.529815	-1.643628	-4.248296
1	-0.855848	-2.525951	-5.736223
1	-5.359588	-1.213395	-0.611592
1	-6.571993	-0.873473	0.632443
1	-8.782200	-4.419994	-0.846686
1	-9.188715	-4.397778	0.875955
1	-6.011243	9.840130	1.406701
1	-4.249362	9.975758	1.292798
1	-5.254234	10.291371	-0.128960
1	0.924006	8.949698	3.754876
1	-0.840365	8.989066	3.897983
1	0.135855	8.280171	5.192167
1	1.993419	5.080949	-0.522661
1	1.823966	6.494576	0.504734
1	3.317761	7.787254	-1.038968
1	5.429971	6.688130	-0.266182
1	4.213860	6.710299	1.023608
1	4.528806	5.215440	0.124499
1	4.731429	6.551640	-2.692934
1	3.794020	5.078850	-2.405521
1	3.026354	6.490320	-3.155910
1	4.826377	-4.531521	-5.668473
1	7.077129	-5.586237	-5.471440
1	6.964723	-4.565036	-6.916859
1	7.836278	-3.975374	-5.498300
1	5.656099	-5.056238	-3.401509
1	6.454519	-3.482425	-3.291692
1	4.680830	-3.578448	-3.351020
1	4.890231	-0.520539	-4.180293
1	7.534690	0.712796	-4.561087
1	6.610086	2.595772	-3.204635
1	5.533726	2.208237	-4.568414
1	5.117294	1.686609	-2.917385

1	5.973325	-1.226314	-2.162402
1	7.508809	-1.505170	1.509155
1	6.007462	-0.819232	0.913593
1	5.710553	1.546387	0.984064
1	9.694232	-0.057107	1.129095
1	6.600402	3.805358	1.441574
1	10.589288	2.197994	1.586176
1	9.048678	4.147362	1.748113
1	1.371678	-1.382850	-5.855001
1	1.900993	-2.238499	-4.392240
1	1.604280	-3.138962	-5.894193
1	-2.052308	-4.174426	-5.114595
1	2.160521	-6.526116	-0.330779
1	0.509644	-5.641502	-1.792041
1	2.585906	-6.365286	-2.794349
1	3.344577	-7.813030	-2.105166
1	1.829295	-7.955827	-3.026512
1	5.291215	-7.491395	4.125467
1	3.153212	-8.703790	4.567363
1	3.832184	-8.058475	6.072183
1	2.463822	-7.243844	5.295093
1	3.536654	-7.464510	2.345453
1	2.860799	-5.975084	3.020641
1	4.487950	-5.970734	2.315395
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1	5.860436	-0.735346	6.402252
1	7.855457	-0.878060	4.265803
1	8.802912	0.553522	4.706392
1	8.351400	-0.625003	5.955403
1	-3.902433	-1.414079	5.378385
1	-4.710009	-2.200996	6.728827
1	-5.153572	-4.664340	6.676333
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1	-3.807227	-4.636314	1.901765
1	-4.904997	-6.652890	2.869795
1	-6.872524	-0.310457	-2.371579
1	-6.500873	0.896794	-1.136947
1	-7.653081	-2.667684	1.206578
1	-6.990648	-5.548743	1.376220
1	-6.603038	-5.497739	-0.342900
1	-8.596365	-6.949409	-0.824409
1	-9.660787	-8.222297	1.056274
1	-8.779673	-7.230751	2.229443
1	-10.010664	-6.496560	1.187651
1	-2.547938	6.588577	1.495973
1	-0.450806	0.960174	3.638697
1	-2.588306	-1.866000	-1.662152
1	-4.769631	3.757597	-3.770115
1	-0.822435	2.573418	5.569957

1	0.746026	2.885195	4.824194
1	-0.136018	4.201541	5.609779
1	-1.185893	6.057055	4.977884
1	-2.165543	6.772637	3.717251
1	-0.086028	7.145982	2.330540
1	0.881061	6.442726	3.614511
1	0.592199	-2.494912	2.596893
1	0.623398	-0.942865	3.452412
1	-0.681379	-2.099578	3.753918
1	-0.864806	-3.134461	-0.863039
1	-0.667647	-5.096582	0.484181
1	-1.056748	-4.144739	2.031225
1	-4.357397	-1.442447	-4.995081
1	-3.186530	-2.137667	-3.869715
1	-4.891117	-2.043947	-3.416821
1	-5.615073	0.491640	-5.434687
1	-5.335411	2.375804	-6.898862
1	-4.083219	3.134364	-5.770963
1	-5.020297	7.506703	-3.138604
1	-4.452951	6.204410	-4.189983
1	-5.977762	6.033664	-3.319068
1	-3.944997	8.489211	-1.459703
1	-2.937180	8.197920	-0.059237
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1	-5.984804	7.865017	-0.142947
1	-6.556950	-8.145538	1.133756
1	-7.538587	-9.062175	-0.019544
1	-6.310765	-7.925838	-0.607114
6	3.096281	-0.414530	-0.455717
6	3.036275	0.408905	0.773477
6	2.798541	1.792673	0.707539
6	3.289537	-0.149664	2.055490
6	2.814379	2.594659	1.848789
1	2.599991	2.246749	-0.252610
6	3.330808	0.658084	3.195857
6	3.094204	2.030224	3.090294
1	2.620730	3.658624	1.753932
1	3.586046	0.229496	4.157951
1	3.142942	2.649661	3.981651
6	2.773621	-0.049439	-1.848526
8	3.202987	-0.670889	-2.818414
8	1.958669	1.010330	-1.956718
6	1.597476	1.409835	-3.304592
1	2.508509	1.700350	-3.837573
1	1.167527	0.545293	-3.817421
6	0.609581	2.554902	-3.192648
1	-0.294408	2.244562	-2.659076
1	1.050037	3.408740	-2.667800
1	0.318520	2.883798	-4.196376
8	3.507694	-1.495428	2.086512

6	3.792238	-2.127652	3.332697
1	4.673475	-1.694322	3.816857
1	2.934615	-2.051546	4.012615
1	3.969403	-3.176889	3.091440
77	-2.595669	2.359348	-0.073895
6	-4.425067	2.050237	0.826318
1	-4.420278	2.522037	1.813096
1	-5.205182	2.499254	0.204535
1	-4.590475	0.974043	0.927504
1	-9.285358	-0.813466	-1.589987
7	3.639719	-1.622414	-0.448107
7	4.076710	-2.664074	-0.557486

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**Q-TS(B-C)<sub>Ir(Me)</sub>**  
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 Number of imaginary frequencies: 10    Electronic energy:    HF=-5513.55220876  
 Zero-point correction=                    2.315434 (Hartree/Particle)  
 Thermal correction to Energy=            2.456897  
 Thermal correction to Enthalpy=         2.457841  
 Thermal correction to Gibbs Free Energy= 2.089027  
 Sum of electronic and zero-point Energies= -5511.236775  
 Sum of electronic and thermal Energies= -5511.095312  
 Sum of electronic and thermal Enthalpies= -5511.094368  
 Sum of electronic and thermal Free Energies= -5511.463182  
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Cartesian Coordinates  
 -----

6	0.387948	-5.534413	-1.977818
6	-0.160317	-5.930150	-0.785408
6	-0.107579	-4.773616	0.099157
6	0.611756	-6.346433	-3.219267
6	-0.666090	-7.291542	-0.398223
6	0.384818	-8.165799	0.320779
6	-0.159426	-9.542238	0.714843
8	-7.055188	4.354059	0.284490
8	-5.570589	5.309157	0.456868
8	-3.964231	6.650108	-5.684873
8	-2.996278	5.502461	-4.756645
8	-1.175814	4.098838	5.828413
8	-1.594568	5.817676	5.741403
8	-1.119427	5.100109	7.289611
8	-7.709892	-1.251698	5.593095
8	-6.070685	-1.564244	4.986228
8	-6.326108	-1.235595	6.712023
8	-2.576622	-5.127236	-3.422465
8	-2.966071	-4.534955	-5.046179
8	-3.966655	-4.061866	-3.664129
8	2.015679	8.344811	2.318995
8	3.258414	7.091747	2.115858

8	3.287213	8.541219	1.089727
8	2.905113	-2.019979	5.911030
8	4.131777	-1.020939	6.718444
8	3.104949	-0.315819	5.459676
8	5.167794	5.556901	-3.274917
8	3.752078	6.279873	-2.476126
8	4.335424	4.697588	-1.958483
8	1.296968	2.686375	-4.367120
8	1.918228	3.746591	-5.628021
8	5.526088	-0.892710	-1.744155
8	6.610385	-2.170775	-1.187930
8	9.930748	0.705320	-1.719412
8	10.405352	-0.166201	-0.253908
8	0.605576	-10.143278	1.219344
8	-1.015009	-9.451839	1.395975
8	-0.497067	-10.103443	-0.165473
8	-4.328977	-6.513262	5.052399
8	-2.816665	-7.340928	4.649019
8	-2.956134	-6.445335	6.168483
8	-4.718225	-6.455994	-3.387303
8	-3.651113	-6.950008	-4.691163
8	-4.973067	-5.556587	-6.297336
8	-6.909918	-7.132144	-6.416487
8	-5.411792	-8.001087	-6.038784
8	-6.590256	-7.666193	-4.759062
8	-7.249967	-4.750581	-5.634145
8	-6.915540	-5.176772	-3.948697
8	-5.992955	-3.888231	-4.740110
8	-2.294974	7.679031	-4.150759
8	-3.765421	9.470873	-3.243473
8	-4.237913	9.025659	-4.892824
8	-5.195560	8.447501	-3.524337
8	-2.661409	7.747422	-1.705336
8	-4.084183	6.709211	-1.858194
8	-2.463862	6.073139	-2.239649
8	-4.176024	3.763660	-4.159529
8	-7.044039	3.903132	-4.181136
8	-6.905328	1.470191	-3.595130
8	-5.827736	1.867071	-4.954464
8	-5.162019	1.617314	-3.318787
8	-4.821027	4.384571	-1.640177
8	-5.496741	3.548905	2.102943
8	-4.271197	3.196418	0.887621
8	-4.383212	1.146086	-0.442619
8	-7.698452	2.267823	2.057971
8	-5.435494	-1.050487	-0.849498
8	-8.752172	0.067905	1.651020
8	-7.626932	-1.602883	0.185969
8	-0.612549	3.567950	-5.664662
8	-0.654991	4.245588	-4.017265

8	-0.097588	5.240660	-5.371755
8	3.778302	4.310515	-4.641620
8	1.136617	6.358363	1.072608
8	2.104718	5.971436	-1.032639
8	0.233099	7.544661	-0.940943
8	0.140449	8.577950	0.498967
8	1.421201	8.843387	-0.708357
8	-3.169816	3.676133	7.277435
8	-4.867151	5.464456	7.677525
8	-3.303428	5.914080	8.379391
8	-3.832075	6.644010	6.854627
8	-4.957120	4.024383	5.561614
8	-3.909617	5.144264	4.683467
8	-3.447967	3.442354	4.807828
8	-6.785651	0.745373	4.420401
8	-4.909206	1.712963	5.418211
8	-7.098833	2.448171	6.232714
8	-8.334371	1.186592	6.341619
8	-6.948348	1.171529	7.458426
8	4.139754	-1.845781	3.749948
8	5.156687	-2.563069	4.994549
8	7.057685	-1.287819	5.972267
8	4.628530	0.412397	2.862515
8	8.739317	0.497039	5.639974
8	6.305681	2.193324	2.520305
8	8.369255	2.256491	3.917596
8	6.234308	-1.294509	-4.104706
8	5.508676	-2.731768	-3.368811
8	8.310123	-1.218228	-0.214501
8	8.890361	1.347999	1.097521
8	8.405239	2.149911	-0.395615
8	10.779777	2.891694	-0.754417
8	12.381321	2.823140	1.175597
8	11.252264	1.799828	2.078072
8	12.018291	1.193814	0.599906
8	-0.868457	-5.706967	1.834229
8	0.637494	-0.061265	4.373245
8	3.036555	1.824128	-1.216848
8	1.678592	-3.895867	-3.704627
8	0.481676	-1.758019	6.135211
8	-1.209939	-1.345992	5.851941
8	-0.778370	-2.969547	6.393393
8	-0.890994	-5.010680	5.531747
8	-0.736418	-5.936721	4.056094
8	-3.046478	-5.170367	3.357712
8	-3.188154	-4.285263	4.865012
8	1.898762	3.452575	3.713748
8	0.863882	2.211051	4.444214
8	2.623007	2.077741	4.550088
8	2.640104	3.743141	0.056730



8	4.151426	4.981663	1.420015
8	4.143264	3.667292	2.734880
8	3.774441	0.940024	-4.810636
8	3.484185	1.958948	-3.398864
8	4.865780	0.869002	-3.423186
8	3.926440	-1.340368	-5.404200
8	2.718618	-2.815077	-6.848097
8	1.360785	-3.015529	-5.613154
8	0.169291	-7.342960	-3.128157
8	0.171054	-5.869487	-4.104002
8	1.681265	-6.482014	-3.428034
8	-1.010590	-7.823615	-1.294615
8	-1.550293	-7.192671	0.246471
8	0.744692	-7.636531	1.212493
8	1.257455	-8.282197	-0.334945
8	9.518959	3.788011	1.897152
8	10.713114	4.702234	0.962698
8	9.098139	4.408012	0.292059
6	-1.284142	-1.188729	-0.396691
6	-2.431800	-2.037798	0.065831
6	-2.900477	-3.061546	-0.779210
6	-3.050537	-1.912225	1.337687
6	-3.913373	-3.937393	-0.390652
8	-2.433314	-3.194425	-1.745539
6	-4.094923	-2.767058	1.707324
6	-4.518657	-3.783845	0.853687
8	-4.226347	-4.727025	-1.067122
8	-4.574237	-2.640565	2.670361
8	-5.322584	-4.445132	1.165533
6	-1.560702	-0.653694	-1.800585
8	-2.046389	0.434294	-2.058679
8	-1.232126	-1.551056	-2.741749
6	-1.668967	-1.249057	-4.096431
8	-1.632481	-2.220314	-4.594322
8	-2.706790	-0.906936	-4.050602
6	-0.788547	-0.229276	-4.802154
8	-0.850736	0.741075	-4.304389
8	0.254132	-0.554679	-4.825328
8	-1.136587	-0.115382	-5.836377
8	-2.606477	-0.913093	2.139920
6	-3.383654	-0.515988	3.266797
8	-4.407414	-0.266746	2.972035
8	-3.394010	-1.292178	4.039119
8	-2.891141	0.370425	3.666471
7	-1.548500	0.451772	0.397034
7	-1.077365	1.375817	0.797926
77	0.821901	-1.834659	0.223763
6	2.714782	-2.637950	0.694629
8	2.639856	-3.293547	1.569433
8	3.097718	-3.219744	-0.150588

8 3.418593 -1.826380 0.913124  
8 8.681664 -2.088827 -3.997064

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**Q-C<sub>Ir(Me)</sub>**  
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Number of imaginary frequencies: 7    Electronic energy:    HF=-5513.5999187  
Zero-point correction=                    2.313692 (Hartree/Particle)  
Thermal correction to Energy=            2.459170  
Thermal correction to Enthalpy=         2.460114  
Thermal correction to Gibbs Free Energy= 2.075899  
Sum of electronic and zero-point Energies= -5511.286226  
Sum of electronic and thermal Energies= -5511.140749  
Sum of electronic and thermal Enthalpies= -5511.139805  
Sum of electronic and thermal Free Energies= -5511.524020  
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Cartesian Coordinates  
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6 -0.156739 -5.015137 -4.507374  
6 1.080214 -4.695044 -5.354803  
6 1.393306 -5.714142 -6.469056  
6 2.527645 -5.201067 -7.369016  
6 1.735852 -7.105125 -5.913381  
6 -7.409553 3.466153 -4.003996  
6 -8.034795 2.092810 -3.805072  
8 -9.244593 1.898121 -3.839964  
6 -7.858907 4.527015 -2.964657  
6 -9.326384 4.943459 -3.142577  
6 -7.575721 4.068632 -1.525822  
7 -7.147867 1.069683 -3.563687  
6 -7.604082 -0.306781 -3.418374  
6 -8.052041 -0.672201 -1.987588  
8 -8.688151 -1.699796 -1.786302  
6 -6.531429 -1.296168 -3.887678  
7 -7.659073 0.188567 -1.008049  
6 -7.961551 -0.026420 0.393708  
6 -6.761979 -0.559018 1.208935  
6 -6.240127 -1.895444 0.718471  
6 -4.975172 -2.008278 0.124923  
6 -7.032537 -3.051679 0.820704  
6 -4.518254 -3.236214 -0.364157  
6 -6.578239 -4.279827 0.336919  
6 -5.318717 -4.374921 -0.260786  
6 -1.832967 4.671572 -3.808536  
6 -1.748702 5.535301 -2.568906  
8 -2.445427 5.318894 -1.569053  
6 -3.271766 4.577704 -4.336806  
7 -0.865886 6.552733 -2.647530  
6 -0.623930 7.435938 -1.530034  
6 -3.428810 7.790195 2.944611

6	-3.664564	6.824596	1.782735
8	-2.528401	6.924580	0.922234
6	-4.954678	7.132103	1.017682
6	-5.035687	2.239899	6.994147
6	-4.650463	0.839475	6.489467
6	-4.232517	-0.070295	7.653964
6	-5.788756	0.203945	5.675697
6	-5.244486	-5.310929	5.293446
6	-6.089282	-4.615407	4.231754
8	-5.364446	-3.448732	3.822147
6	-7.480565	-4.237879	4.746164
6	2.955391	0.844428	6.278157
6	4.087068	0.981789	5.241323
6	4.200298	2.380623	4.668514
6	5.081872	3.319229	5.223415
6	3.401018	2.778903	3.587077
6	5.160912	4.619044	4.720194
6	3.470739	4.079220	3.081575
6	4.351535	5.005733	3.648541
6	5.362333	3.495931	-1.122962
6	5.987297	4.881307	-0.991527
8	6.342813	5.542555	-1.967477
6	5.582816	2.880053	-2.503674
16	7.334496	2.449384	-2.880464
7	6.116936	5.336223	0.284285
6	6.660599	6.655873	0.568482
6	5.620041	7.781403	0.451931
6	6.187254	9.197744	0.669725
6	5.133543	10.256804	0.311223
6	6.702081	9.414617	2.102032
6	3.886225	-4.233857	1.074063
6	0.912296	-0.985151	3.091286
6	1.075652	1.656069	-0.969603
6	3.599905	-1.866335	-3.152099
7	2.318136	-2.479035	1.745739
6	3.043524	-3.608909	1.992629
6	2.828632	-4.034403	3.370177
6	1.973828	-3.122479	3.932152
6	1.675854	-2.134962	2.904765
6	1.421135	-3.096589	5.325900
6	3.417907	-5.268412	3.992556
6	2.627223	-6.557308	3.677740
6	3.258645	-7.805784	4.301111
7	1.137486	0.057986	0.881493
6	0.690093	0.042819	2.173176
6	-0.000195	1.286998	2.463427
6	0.074467	2.055615	1.322607
6	0.785582	1.255073	0.331503
6	-0.681230	1.611724	3.757936
6	-0.462948	3.394508	1.081726

6	-0.497131	4.398335	1.973398
7	2.226033	-0.356155	-1.796317
6	1.726559	0.914836	-1.956642
6	1.985269	1.363877	-3.307616
6	2.621782	0.329080	-3.961776
6	2.811465	-0.728882	-2.975677
6	1.572247	2.684904	-3.883811
6	3.025942	0.326677	-5.365512
6	3.052007	-0.724009	-6.200097
7	3.485668	-2.825506	-0.894898
6	3.944624	-2.807066	-2.186304
6	4.882785	-3.899651	-2.382270
6	4.985931	-4.556478	-1.182039
6	4.105237	-3.867030	-0.251388
6	5.596349	-4.187229	-3.669424
6	5.862193	-5.726905	-0.834553
6	7.194044	-5.326199	-0.162811
6	8.066419	-6.534990	0.188837
1	-8.790049	-0.738378	0.427396
1	-8.308683	0.915763	0.834998
1	-7.695443	3.807891	-5.006830
1	-6.314086	3.394420	-3.989887
1	-5.302380	2.904573	6.163497
1	-5.900308	2.187195	7.669126
1	-4.210571	2.706094	7.546040
1	-5.734689	-6.225915	5.643545
1	-4.261103	-5.574474	4.890396
1	-5.094643	-4.647441	6.153189
1	-0.338484	-4.229393	-3.766966
1	-1.052068	-5.105030	-5.136880
1	-0.044414	-5.956468	-3.957861
1	-4.252084	7.739469	3.665667
1	-2.495897	7.544719	3.462298
1	-3.353208	8.818544	2.572437
1	2.917149	-0.175130	6.679863
1	3.102060	1.534195	7.117341
1	1.982071	1.070437	5.828295
1	-0.039950	8.292288	-1.876052
1	-1.564655	7.791374	-1.106385
1	-0.072609	6.931861	-0.727534
1	-1.484219	3.669617	-3.529315
1	-1.161189	5.036041	-4.594646
1	4.279037	3.592763	-0.950425
1	5.741773	2.828437	-0.340745
1	7.471204	6.834737	-0.144877
1	7.096983	6.622441	1.571912
1	9.005136	-6.223523	0.660628
1	7.551286	-7.209175	0.884764
1	8.320307	-7.116343	-0.706376
1	2.677321	-8.705130	4.067686

1	4.279150	-7.963470	3.929928
1	3.315422	-7.720320	5.393524
1	1.957999	-4.601888	-4.697304
1	0.944084	-3.706674	-5.817667
1	0.489685	-5.812880	-7.091326
1	2.734603	-5.898185	-8.189949
1	2.280111	-4.227642	-7.809848
1	3.457662	-5.080520	-6.796629
1	1.957740	-7.808543	-6.724985
1	2.620707	-7.057728	-5.264270
1	0.913622	-7.527602	-5.326140
1	-7.234021	5.410638	-3.159155
1	-9.591168	5.727754	-2.423151
1	-9.503074	5.338738	-4.150153
1	-9.996691	4.092119	-2.998677
1	-7.793626	4.870857	-0.811778
1	-8.205112	3.210648	-1.257475
1	-6.523552	3.784532	-1.391705
1	-6.154402	1.250745	-3.610558
1	-8.503071	-0.416182	-4.031347
1	-6.901913	-2.315768	-3.758700
1	-6.290818	-1.134909	-4.943953
1	-5.613581	-1.195814	-3.294704
1	-7.164005	1.022969	-1.288337
1	-7.082565	-0.635453	2.257610
1	-5.952461	0.181173	1.186556
1	-4.330127	-1.135585	0.053289
1	-8.027638	-2.983524	1.254068
1	-3.530874	-3.302934	-0.811323
1	-7.214641	-5.157347	0.413919
1	-4.964145	-5.328719	-0.641961
1	-3.332683	3.877236	-5.176198
1	-3.938788	4.235234	-3.540648
1	-3.631508	5.553280	-4.682096
1	-0.291704	6.636069	-3.472661
1	-3.728407	5.800069	2.186723
1	-2.632876	6.308085	0.169000
1	-5.082247	6.437121	0.178602
1	-5.833847	7.043360	1.667445
1	-4.922381	8.151033	0.614034
1	-3.782207	0.950889	5.821951
1	-3.926083	-1.060401	7.295713
1	-3.394969	0.359466	8.216978
1	-5.065352	-0.213604	8.355362
1	-5.510222	-0.784356	5.288652
1	-6.685714	0.077717	6.297301
1	-6.065632	0.835714	4.822140
1	-6.200301	-5.293029	3.370121
1	-5.763512	-3.131019	2.994106
1	-8.060966	-3.732230	3.965051

1	-8.042988	-5.125496	5.060187
1	-7.396253	-3.557462	5.601136
1	3.914457	0.265387	4.428828
1	5.038527	0.701197	5.710407
1	5.716295	3.026244	6.057594
1	2.718017	2.065146	3.133963
1	5.851041	5.330385	5.167106
1	2.826820	4.367531	2.254403
1	4.395646	6.023869	3.268931
1	5.221574	3.557658	-3.280411
1	5.032645	1.939068	-2.583424
1	5.752281	4.783159	1.049490
1	4.803096	7.600794	1.167300
1	5.182368	7.719389	-0.551793
1	7.036844	9.324424	-0.019001
1	7.087815	10.433118	2.229013
1	5.893779	9.273902	2.832374
1	7.511874	8.723899	2.362126
1	4.426956	-5.104060	1.429345
1	0.483258	-0.848956	4.078248
1	0.750518	2.652796	-1.246647
1	4.062118	-1.981257	-4.124644
1	1.623674	-2.141337	5.826308
1	0.331872	-3.236566	5.333609
1	1.856146	-3.889309	5.941619
1	3.470439	-5.143101	5.081734
1	4.457019	-5.397650	3.659269
1	2.551143	-6.676908	2.589494
1	1.597535	-6.437770	4.039107
1	-1.440157	2.385532	3.606811
1	-1.173541	0.730205	4.185026
1	0.020813	1.990841	4.513503
1	-0.881151	3.579784	0.092160
1	-0.952750	5.353495	1.724187
1	-0.065035	4.296095	2.965612
1	2.224314	2.978341	-4.713132
1	0.547394	2.655386	-4.278562
1	1.612266	3.484824	-3.136372
1	3.300780	1.300747	-5.771539
1	3.368926	-0.606289	-7.232298
1	2.741553	-1.719200	-5.895987
1	6.171390	-5.115761	-3.607748
1	4.896250	-4.287190	-4.508761
1	6.297224	-3.383767	-3.930828
1	6.084426	-6.301738	-1.742754
1	5.322729	-6.417134	-0.170946
1	6.979503	-4.743409	0.742224
1	7.741162	-4.652435	-0.834660
1	4.255148	10.173044	0.964890
1	5.535098	11.270945	0.424246

1	4.791310	10.143562	-0.724262
6	0.441933	-2.433829	-0.401109
6	0.148666	-3.803416	0.025712
6	0.904512	-4.859719	-0.514864
6	-0.905792	-4.126679	0.927593
6	0.591742	-6.190672	-0.243991
1	1.710758	-4.614919	-1.194557
6	-1.185976	-5.461487	1.237927
6	-0.447096	-6.484821	0.639056
1	1.164457	-6.988140	-0.707904
1	-1.979963	-5.706531	1.933453
1	-0.686031	-7.518245	0.876801
6	-0.738995	-1.707594	-0.962016
8	-1.314967	-0.731487	-0.528582
8	-1.056618	-2.299754	-2.152856
6	-2.041013	-1.637693	-2.978946
1	-2.471684	-2.441716	-3.580781
1	-2.816793	-1.214584	-2.336228
6	-1.403860	-0.568296	-3.854095
1	-0.979766	0.229944	-3.238532
1	-0.604609	-0.991907	-4.469940
1	-2.159655	-0.134096	-4.520382
8	-1.550051	-3.069237	1.472422
6	-2.501497	-3.296560	2.510226
1	-3.352340	-3.886280	2.162247
1	-2.029656	-3.794780	3.366179
1	-2.855484	-2.311394	2.810355
7	-3.971968	1.692390	-1.815903
7	-2.992617	1.982383	-1.393547
77	2.203392	-1.456129	-0.050044
6	3.908072	-0.353955	0.652220
1	3.856179	-0.211617	1.736849
1	4.828391	-0.901985	0.418123
1	3.947333	0.631063	0.172629
1	7.768318	3.725287	-2.948196

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**Qmutated-A<sub>Ir(Me)</sub>**  
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-----Number of imaginary frequencies: 10    Electronic energy:    HF=-4200.06901572  
 Zero-point correction=                            2.034047 (Hartree/Particle)  
 Thermal correction to Energy=                    2.153830  
 Thermal correction to Enthalpy=                2.154774  
 Thermal correction to Gibbs Free Energy=      1.826212  
 Sum of electronic and zero-point Energies=    -4198.034969  
 Sum of electronic and thermal Energies=       -4197.915186  
 Sum of electronic and thermal Enthalpies=     -4197.914241  
 Sum of electronic and thermal Free Energies=   -4198.242803

.....  
 Cartesian Coordinates  
 .....

6	-3.594067	-4.433811	-4.433424
6	-4.291336	-4.717252	-3.097591
6	-5.730941	-4.176575	-2.982964
6	-6.395802	-4.684293	-1.694441
6	-5.791018	-2.642612	-3.051118
6	-3.953519	6.723492	-4.015885
6	-5.263052	6.047987	-3.634160
8	-6.324650	6.651615	-3.531549
6	-3.549298	7.896289	-3.083948
6	-4.448088	9.128993	-3.261693
6	-3.484339	7.455610	-1.613514
7	-5.172561	4.698419	-3.379238
6	-6.356760	3.896482	-3.094954
6	-6.720381	3.821528	-1.599439
8	-7.768018	3.281595	-1.252359
6	-6.212108	2.479743	-3.662413
7	-5.809710	4.348362	-0.742562
6	-5.995072	4.383726	0.695769
6	-4.943849	3.580132	1.476864
6	-4.866818	2.086177	1.202130
6	-3.680238	1.402415	1.515557
6	-5.941365	1.346115	0.688320
6	-3.568671	0.021636	1.336809
6	-5.831602	-0.036894	0.504565
6	-4.651890	-0.705986	0.831626
6	1.152861	4.203187	-4.419311
6	2.101269	4.442536	-3.261496
8	2.074953	3.769914	-2.231174
6	-0.228588	3.733138	-3.954385
7	3.007670	5.434062	-3.453980
6	4.075552	5.643796	-2.501606
6	2.659185	7.718352	2.157388
6	1.495174	7.128567	1.356894
6	-1.513431	4.418438	6.792893
6	-2.313396	3.106392	6.784410
6	-3.326467	3.068572	7.937683
6	-3.009233	2.885207	5.432739
6	-6.534431	-1.385579	5.769155
6	-6.208190	-0.581649	4.515352
8	-4.794575	-0.337386	4.530219
6	-6.989716	0.732213	4.449992
6	3.758653	-1.650664	5.493342
6	4.761659	-1.908904	4.354300
6	5.719173	-0.753106	4.151646
6	6.927340	-0.688410	4.860261
6	5.398650	0.302370	3.286064
6	7.787983	0.401126	4.716987
6	6.255793	1.394632	3.137841
6	7.452887	1.448936	3.856282
6	6.357743	-1.158545	-2.291491



6	7.443137	-0.107243	-2.171466
8	7.427843	0.927811	-2.835114
7	8.434351	-0.396568	-1.279223
6	9.521564	0.529404	-0.998075
6	9.134985	1.661057	-0.032823
6	10.261213	2.684986	0.212700
6	9.718157	3.912563	0.959769
6	11.454564	2.079434	0.969946
6	-1.080551	-5.170194	0.211676
6	-0.096358	-1.112716	2.673522
6	2.429550	0.569608	-1.110540
6	1.493586	-3.517990	-3.547921
7	-0.403734	-3.003759	1.140046
6	-1.080897	-4.198711	1.208382
6	-1.777346	-4.299086	2.481788
6	-1.494501	-3.154201	3.180880
6	-0.624462	-2.353039	2.335032
6	-1.987186	-2.747720	4.538579
6	-2.669574	-5.436551	2.890785
6	-4.111741	-5.318951	2.350335
6	-5.003327	-6.488246	2.779061
7	1.095289	-0.587050	0.591731
6	0.696177	-0.288824	1.875512
6	1.197091	1.014932	2.260263
6	1.910493	1.499298	1.183509
6	1.834200	0.480639	0.143114
6	0.915953	1.692222	3.567418
6	2.586420	2.784893	1.019598
6	3.194798	3.486041	1.991524
7	1.734634	-1.591363	-2.056398
6	2.377326	-0.373926	-2.133516
6	2.976183	-0.215551	-3.442138
6	2.672720	-1.353092	-4.158620
6	1.916264	-2.221887	-3.263568
6	3.738921	0.990784	-3.906425
6	3.044906	-1.602528	-5.550623
6	2.343211	-2.270919	-6.479594
7	0.286528	-4.030064	-1.472704
6	0.741104	-4.352711	-2.730221
6	0.286600	-5.685082	-3.090224
6	-0.454270	-6.151347	-2.035354
6	-0.442213	-5.105495	-1.022856
6	0.601004	-6.367824	-4.388235
6	-1.126923	-7.487190	-1.886569
6	-0.293312	-8.518652	-1.094909
6	-1.004230	-9.867462	-0.948607
1	-7.004660	4.013504	0.886725
1	-5.962551	5.425438	1.040672
1	-4.070615	7.105225	-5.038325
1	-3.137611	5.988686	-4.040669

1	-0.764020	4.434629	5.992069
1	-2.176852	5.281176	6.645228
1	-0.989772	4.561484	7.745947
1	-7.601016	-1.632955	5.803654
1	-5.958618	-2.316623	5.790018
1	-6.282649	-0.808254	6.666493
1	-2.597115	-4.888145	-4.451090
1	-4.167051	-4.843681	-5.275274
1	-3.465995	-3.359960	-4.609136
1	2.599433	7.435539	3.214703
1	3.625735	7.366370	1.777291
1	2.665764	8.813593	2.108509
1	3.081776	-2.503493	5.620350
1	4.277554	-1.480962	6.443693
1	3.150337	-0.763408	5.283155
1	4.602680	6.567855	-2.751818
1	3.660023	5.733563	-1.494811
1	4.792508	4.813420	-2.500485
1	1.607571	3.427875	-5.052300
1	1.070169	5.103309	-5.041881
1	5.436377	-0.791405	-1.826996
1	6.621178	-2.114070	-1.825851
1	9.834167	0.960639	-1.954920
1	10.359286	-0.057975	-0.608226
1	-0.391356	-10.581646	-0.387042
1	-1.958863	-9.758725	-0.418672
1	-1.220039	-10.311595	-1.928404
1	-6.019497	-6.379757	2.383372
1	-4.605515	-7.445089	2.418090
1	-5.075859	-6.552310	3.871881
1	-3.687128	-4.304545	-2.276114
1	-4.316140	-5.804825	-2.937692
1	-6.304204	-4.574653	-3.835403
1	-7.432066	-4.334338	-1.613626
1	-6.407542	-5.780386	-1.655266
1	-5.854565	-4.326332	-0.807956
1	-6.825540	-2.287117	-2.970738
1	-5.219847	-2.190714	-2.228958
1	-5.382889	-2.256325	-3.991343
1	-2.531520	8.177627	-3.391150
1	-4.100866	9.950771	-2.623838
1	-4.430998	9.480638	-4.300393
1	-5.485180	8.897941	-3.005865
1	-3.095193	8.261802	-0.981624
1	-4.483110	7.199035	-1.238487
1	-2.827317	6.585860	-1.479864
1	-4.310893	4.216267	-3.596869
1	-7.205268	4.399915	-3.568457
1	-7.106484	1.902697	-3.418105
1	-6.092145	2.508720	-4.750409

1	-5.348306	1.963159	-3.225171
1	-4.999237	4.796341	-1.146936
1	-5.146065	3.739924	2.546839
1	-3.953134	4.022358	1.301792
1	-2.828529	1.959885	1.900297
1	-6.863462	1.840839	0.399995
1	-2.637791	-0.481405	1.581827
1	-6.675767	-0.587932	0.098277
1	-4.567913	-1.780315	0.691711
1	-0.853371	3.463856	-4.812635
1	-0.129199	2.861992	-3.301862
1	-0.739529	4.519777	-3.386475
1	3.054220	5.888887	-4.353775
1	1.491554	6.034004	1.407552
1	-1.603251	2.279157	6.935049
1	-3.876198	2.120089	7.952688
1	-2.831428	3.187490	8.909287
1	-4.061698	3.878411	7.838008
1	-3.549681	1.931535	5.404364
1	-3.733302	3.688071	5.234838
1	-2.282503	2.887878	4.609945
1	-6.459175	-1.187531	3.630063
1	-4.550423	0.038303	3.667080
1	-6.737130	1.288735	3.540527
1	-8.070817	0.547470	4.439583
1	-6.751908	1.357771	5.318235
1	4.208463	-2.098879	3.426009
1	5.328125	-2.822852	4.575019
1	7.195304	-1.501922	5.531829
1	4.468665	0.270395	2.722100
1	8.719543	0.431521	5.276867
1	5.983479	2.199795	2.460712
1	8.117843	2.301974	3.748175
1	8.327978	-1.207518	-0.687464
1	8.806485	1.234670	0.925975
1	8.268444	2.174847	-0.465793
1	10.621365	3.026485	-0.770394
1	12.234251	2.831850	1.138621
1	11.140522	1.700500	1.951589
1	11.915644	1.248737	0.423863
1	-1.640113	-6.075751	0.419789
1	-0.340112	-0.740358	3.662707
1	2.972373	1.482066	-1.324032
1	1.784157	-3.917260	-4.512002
1	-1.187492	-2.301472	5.142002
1	-2.804358	-2.015151	4.484377
1	-2.366852	-3.612297	5.092803
1	-2.709398	-5.494288	3.986131
1	-2.241500	-6.392085	2.556952
1	-4.081176	-5.256151	1.254354

1	-4.543734	-4.372008	2.699621
1	0.986784	2.779395	3.460639
1	-0.086446	1.452747	3.940082
1	1.629278	1.397254	4.349796
1	2.582838	3.197759	0.011547
1	3.656896	4.445944	1.777203
1	3.279152	3.126020	3.012571
1	3.730738	1.061881	-4.998879
1	3.297922	1.908225	-3.505137
1	4.791035	0.972311	-3.588714
1	3.990637	-1.157040	-5.860169
1	2.725776	-2.384603	-7.489945
1	1.364951	-2.697306	-6.279364
1	0.092276	-7.333257	-4.464802
1	0.292597	-5.763191	-5.250769
1	1.677440	-6.554677	-4.497696
1	-1.347156	-7.900615	-2.879111
1	-2.101534	-7.363521	-1.394180
1	-0.060410	-8.109479	-0.103331
1	0.671366	-8.657180	-1.600299
1	9.336448	3.631200	1.950055
1	10.500815	4.666313	1.108449
1	8.896123	4.383389	0.407909
77	0.737217	-2.332456	-0.422476
6	2.471479	-3.173629	0.313234
1	2.257190	-3.642591	1.278093
1	2.829985	-3.923429	-0.398002
1	3.219984	-2.384958	0.435142
1	6.142522	-1.328340	-3.349377
1	1.555196	7.411865	0.299213
1	0.530502	7.482795	1.738880

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**Qmutated-BIr(Me)**  
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-----Number of imaginary frequencies: 8    Electronic energy:    HF=-4961.5739089  
 Zero-point correction=                    2.254257 (Hartree/Particle)  
 Thermal correction to Energy=            2.393912  
 Thermal correction to Enthalpy=         2.394856  
 Thermal correction to Gibbs Free Energy=    2.018552  
 Sum of electronic and zero-point Energies=    -4959.319652  
 Sum of electronic and thermal Energies=    -4959.179997  
 Sum of electronic and thermal Enthalpies=    -4959.179053  
 Sum of electronic and thermal Free Energies=   -4959.555357

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 Cartesian Coordinates  
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6	0.193144	6.641628	-0.667274
6	1.457731	6.157701	0.052171
6	2.773328	6.803253	-0.427823
6	3.938712	6.403052	0.490068

6	3.097134	6.458806	-1.889745
6	5.500112	-1.620498	-5.992652
6	6.399735	-0.567810	-5.356016
8	7.588245	-0.459096	-5.646216
6	5.880533	-3.079386	-5.626177
6	7.214151	-3.515410	-6.250520
6	5.871954	-3.302575	-4.106013
7	5.800140	0.257055	-4.436838
6	6.569006	1.295951	-3.763741
6	7.345003	0.806839	-2.520290
8	8.392192	1.345432	-2.188156
6	5.684669	2.493700	-3.394687
7	6.758394	-0.208003	-1.815296
6	7.460523	-0.907981	-0.749498
6	7.103335	-0.475538	0.689905
6	7.530992	0.923501	1.085273
6	6.584549	1.929821	1.313962
6	8.887974	1.235208	1.256653
6	6.980397	3.213349	1.701613
6	9.287694	2.513459	1.642646
6	8.333178	3.509549	1.867786
6	-0.102003	-2.181783	-5.047708
6	-0.345548	-3.410177	-4.201093
8	0.171657	-3.563661	-3.095822
6	1.392739	-1.987023	-5.343779
7	-1.179196	-4.325203	-4.767702
6	-1.484239	-5.578118	-4.127086
6	1.858819	-8.430612	-1.177088
6	1.916190	-7.553268	-2.431235
6	5.211796	-5.886520	4.486528
6	5.106917	-7.049559	3.488986
6	4.376807	-8.247606	4.113121
6	4.424364	-6.602310	2.188121
6	6.720440	1.419692	6.554380
6	6.546676	0.472161	5.366204
8	5.510103	-0.490120	5.634428
6	7.848872	-0.222436	4.969100
6	-2.321478	-3.512457	6.468144
6	-3.761187	-3.612483	5.931645
6	-3.936182	-4.752520	4.950165
6	-4.278298	-6.037218	5.395178
6	-3.711757	-4.561928	3.579508
6	-4.384970	-7.103170	4.500429
6	-3.815814	-5.624331	2.679164
6	-4.150386	-6.900475	3.138627
6	-6.373049	-1.796143	-0.477286
6	-6.826453	-3.176066	-0.910843
8	-6.572437	-3.634584	-2.024043
7	-7.541451	-3.871839	0.019905
6	-8.017420	-5.225809	-0.219295

6	-6.955859	-6.307753	0.033406
6	-7.430349	-7.738602	-0.290438
6	-6.249525	-8.720079	-0.242162
6	-8.559325	-8.211823	0.640020
6	-3.478212	5.303251	1.192445
6	-1.360329	1.205961	2.681558
6	-2.744779	-1.003239	-1.403971
6	-4.921248	3.078978	-2.865717
7	-2.513576	3.088216	1.610500
6	-2.761907	4.393175	1.965118
6	-2.178822	4.669337	3.269924
6	-1.586358	3.506843	3.688844
6	-1.805486	2.521436	2.645117
6	-0.838627	3.240202	4.960914
6	-2.219118	5.998109	3.971591
6	-1.126515	6.986562	3.508954
6	-1.196644	8.331088	4.239503
7	-2.193728	0.428078	0.508892
6	-1.521962	0.236335	1.695831
6	-0.993500	-1.111779	1.754623
6	-1.357208	-1.733438	0.579822
6	-2.124487	-0.757321	-0.183945
6	-0.157417	-1.661045	2.869070
6	-0.999611	-3.063329	0.088679
6	-0.839347	-4.166763	0.836605
7	-3.696231	1.221179	-1.841418
6	-3.487766	-0.102791	-2.164462
6	-4.137266	-0.412388	-3.419648
6	-4.699312	0.760191	-3.876711
6	-4.437779	1.773463	-2.859576
6	-4.195117	-1.773397	-4.047247
6	-5.426134	0.922930	-5.135777
6	-5.427798	1.994255	-5.944100
7	-4.006191	3.882517	-0.733839
6	-4.715745	4.056805	-1.898636
6	-5.222164	5.416621	-1.966764
6	-4.809702	6.052598	-0.825125
6	-4.056805	5.075708	-0.052831
6	-6.035132	5.964557	-3.101517
6	-5.090847	7.464033	-0.391795
6	-6.303507	7.594262	0.555890
6	-6.563557	9.040002	0.989847
1	8.531944	-0.760134	-0.917027
1	7.245515	-1.977449	-0.852637
1	5.578902	-1.492165	-7.079137
1	4.452555	-1.445692	-5.716732
1	5.764277	-5.041259	4.058012
1	4.213966	-5.526453	4.771830
1	5.727901	-6.192414	5.404764
1	7.440810	2.212558	6.323230

1	5.764706	1.884275	6.817823
1	7.092622	0.877054	7.434593
1	-0.703657	6.185170	-0.233336
1	0.087089	7.731286	-0.586954
1	0.204457	6.389916	-1.733840
1	2.261409	-9.431859	-1.370832
1	2.441196	-7.992174	-0.358234
1	0.829162	-8.552418	-0.820208
1	-2.222624	-2.681523	7.176480
1	-2.029417	-4.435284	6.982090
1	-1.609486	-3.349642	5.650835
1	-1.034427	-6.426441	-4.659271
1	-1.071002	-5.540966	-3.118721
1	-2.567038	-5.736571	-4.066233
1	-0.479677	-1.319224	-4.483381
1	-0.674725	-2.222355	-5.982735
1	-5.285070	-1.789675	-0.356561
1	-6.831103	-1.457853	0.457687
1	-8.341793	-5.272432	-1.263907
1	-8.899194	-5.380652	0.411148
1	-7.429861	9.105551	1.657860
1	-5.699699	9.457292	1.522436
1	-6.760254	9.685442	0.124704
1	-0.410259	9.012647	3.895963
1	-2.162070	8.824820	4.071857
1	-1.076363	8.201994	5.322389
1	1.540163	5.064372	-0.049698
1	1.345703	6.352514	1.128281
1	2.650363	7.895731	-0.358376
1	4.874991	6.881231	0.178762
1	3.744007	6.690949	1.530558
1	4.099961	5.316826	0.468750
1	4.034093	6.931925	-2.206575
1	3.217014	5.374015	-2.016381
1	2.310787	6.791662	-2.575827
1	5.087310	-3.707685	-6.057773
1	7.429705	-4.562245	-6.003131
1	7.184934	-3.426919	-7.343352
1	8.037738	-2.892059	-5.891963
1	6.025423	-4.361298	-3.867004
1	6.678040	-2.736055	-3.623243
1	4.919963	-2.993388	-3.656830
1	4.829274	0.114869	-4.178692
1	7.349515	1.613503	-4.458414
1	6.291229	3.257731	-2.900206
1	5.232702	2.928395	-4.292902
1	4.883733	2.200068	-2.705897
1	5.963194	-0.665086	-2.240689
1	7.588875	-1.203136	1.357157
1	6.025863	-0.590481	0.847529

1	5.527708	1.709961	1.190221
1	9.640189	0.469576	1.079775
1	6.227127	3.978382	1.873444
1	10.345149	2.734546	1.763621
1	8.643971	4.507073	2.167793
1	1.552807	-1.076450	-5.931535
1	1.957166	-1.901520	-4.412243
1	1.792840	-2.831872	-5.916516
1	-1.541589	-4.146661	-5.692174
1	2.946421	-7.436363	-2.787108
1	6.129410	-7.370692	3.239706
1	4.329407	-9.092769	3.416090
1	4.879950	-8.591864	5.024830
1	3.346132	-7.980453	4.381895
1	4.376130	-7.421433	1.460409
1	3.395407	-6.269796	2.380293
1	4.961945	-5.770399	1.716933
1	6.167050	1.033693	4.506391
1	5.803407	-1.029281	6.387478
1	7.673662	-0.915464	4.140168
1	8.601712	0.506281	4.649730
1	8.262746	-0.791069	5.813897
1	-4.031972	-2.664653	5.449320
1	-4.450662	-3.742188	6.775677
1	-4.462956	-6.202661	6.454879
1	-3.452617	-3.571039	3.211329
1	-4.651729	-8.091411	4.866669
1	-3.629329	-5.452682	1.622584
1	-4.225619	-7.729826	2.440476
1	-7.635797	-3.483313	0.946706
1	-6.618238	-6.257972	1.078780
1	-6.088469	-6.065721	-0.592804
1	-7.818900	-7.734973	-1.320773
1	-8.864134	-9.236330	0.395329
1	-8.229200	-8.204962	1.687360
1	-9.451615	-7.580049	0.566871
1	-3.602475	6.297344	1.608348
1	-0.811342	0.908162	3.567923
1	-2.646835	-2.007821	-1.801100
1	-5.538861	3.357552	-3.710749
1	-1.296298	2.425673	5.537561
1	0.200089	2.946190	4.761504
1	-0.814246	4.124868	5.603944
1	-2.117437	5.843599	5.053450
1	-3.203341	6.466454	3.831310
1	-1.217417	7.144821	2.426600
1	-0.142337	6.526097	3.667242
1	0.516058	-2.437085	2.491034
1	0.452583	-0.880882	3.335462
1	-0.769450	-2.117232	3.660035



1	-0.816098	-3.145856	-0.982342
1	-0.526638	-5.101626	0.379623
1	-1.026423	-4.188150	1.906027
1	-4.545492	-1.716048	-5.082057
1	-3.213127	-2.261571	-4.061433
1	-4.880170	-2.432288	-3.495026
1	-6.000880	0.052500	-5.452326
1	-6.006114	1.996584	-6.863625
1	-4.840400	2.883911	-5.737270
1	-6.234157	7.032279	-2.970582
1	-5.523691	5.839674	-4.064567
1	-7.005827	5.458472	-3.187216
1	-5.266272	8.091567	-1.275092
1	-4.205737	7.888528	0.102051
1	-6.140783	6.962566	1.438851
1	-7.191204	7.189259	0.052834
1	-5.822502	-8.767920	0.768313
1	-6.563910	-9.734244	-0.516553
1	-5.450305	-8.417333	-0.928906
6	3.079968	-0.295429	-0.420084
6	2.939693	0.423659	0.866206
6	2.625543	1.793075	0.897305
6	3.185498	-0.219788	2.108894
6	2.555096	2.502117	2.096481
1	2.432171	2.309154	-0.032418
6	3.142040	0.497217	3.308781
6	2.825327	1.857382	3.300697
1	2.303111	3.557878	2.076198
1	3.389318	0.008654	4.243897
1	2.803931	2.405118	4.238976
6	2.726234	0.146381	-1.781902
8	3.217708	-0.348693	-2.794592
8	1.810827	1.125314	-1.809231
6	1.398228	1.588783	-3.120951
1	2.267437	2.020352	-3.627881
1	1.061796	0.725821	-3.701653
6	0.290806	2.604721	-2.917069
1	-0.567109	2.152831	-2.409228
1	0.638678	3.456881	-2.324333
1	-0.045020	2.978852	-3.890463
8	3.477757	-1.549634	2.043110
6	3.727809	-2.268123	3.249487
1	4.566158	-1.841060	3.809897
1	2.835300	-2.279258	3.887600
1	3.961091	-3.287168	2.936710
77	-3.155621	2.136893	-0.084777
6	-4.928870	1.601683	0.824496
1	-5.216056	2.390211	1.526008
1	-5.698844	1.485236	0.056428
1	-4.781711	0.658573	1.358742

7	3.729593	-1.446667	-0.494995
7	4.260419	-2.435127	-0.665752
1	-6.610411	-1.080296	-1.268984
1	1.334132	-7.993616	-3.250016
1	1.518605	-6.549048	-2.243769

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**Q<sub>mutated</sub>-TS(B-C)<sub>Ir(Me)</sub>**  
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Number of imaginary frequencies: 12    Electronic energy:    HF=-4961.52424788  
 Zero-point correction=                    2.251588 (Hartree/Particle)  
 Thermal correction to Energy=            2.387470  
 Thermal correction to Enthalpy=         2.388414  
 Thermal correction to Gibbs Free Energy= 2.029536  
 Sum of electronic and zero-point Energies= -4959.272660  
 Sum of electronic and thermal Energies= -4959.136778  
 Sum of electronic and thermal Enthalpies= -4959.135834  
 Sum of electronic and thermal Free Energies= -4959.494712

.....  
 Cartesian Coordinates  
 .....

6	-3.859231	-4.293849	-4.432443
6	-4.774232	-5.506741	-4.643457
6	-6.166742	-5.179657	-5.219520
6	-6.924195	-6.471345	-5.562889
6	-7.001400	-4.300417	-4.275573
6	-4.026869	6.859658	-3.836662
6	-5.291913	6.189823	-3.317680
8	-6.315480	6.808609	-3.049143
6	-3.462470	7.960700	-2.900561
6	-4.343976	9.218077	-2.869657
6	-3.200822	7.422508	-1.485475
7	-5.209488	4.828276	-3.141534
6	-6.379315	4.050384	-2.746574
6	-6.656109	4.066084	-1.228362
8	-7.747063	3.711769	-0.800264
6	-6.256809	2.601870	-3.233125
7	-5.611062	4.449026	-0.443345
6	-5.681045	4.478081	1.004114
6	-4.932310	3.306593	1.680577
6	-5.519300	1.949302	1.358004
6	-4.945000	1.122626	0.383256
6	-6.682780	1.508033	2.005774
6	-5.519875	-0.110207	0.061623
6	-7.259272	0.277904	1.688251
6	-6.678178	-0.536018	0.712821
6	0.989327	4.281734	-4.719278
6	1.960390	4.617671	-3.603089
8	1.830462	4.196023	-2.454553

6	-0.440457	4.085013	-4.207021
7	3.008202	5.399406	-3.971743
6	4.088003	5.657553	-3.045846
6	3.113021	7.682086	1.746394
6	2.025813	7.530371	0.679070
6	-0.683655	4.368300	6.685223
6	-2.089117	3.960067	7.149519
6	-2.615939	4.917482	8.228162
6	-3.060664	3.881269	5.962140
6	-5.854491	-1.356691	6.028060
6	-5.674975	0.145538	5.845892
8	-4.261500	0.389189	5.875030
6	-6.390817	0.953401	6.930483
6	4.370480	-1.747141	4.848379
6	5.498848	-1.873977	3.808286
6	6.396946	-0.654783	3.770823
6	7.502744	-0.549181	4.626773
6	6.122150	0.415054	2.906755
6	8.307261	0.591501	4.627201
6	6.925277	1.557941	2.900775
6	8.019578	1.651407	3.764237
6	6.285785	-1.175279	-3.126893
6	7.354589	-0.105362	-3.026116
8	7.212305	1.010786	-3.522852
7	8.484157	-0.475118	-2.354919
6	9.573589	0.453870	-2.093203
6	9.339177	1.338738	-0.858781
6	10.461443	2.361882	-0.593486
6	10.027090	3.360547	0.490031
6	11.790003	1.692297	-0.205117
6	-0.079320	-4.808013	1.124601
6	1.188751	-0.562562	3.080499
6	2.561807	1.041684	-1.286975
6	1.436813	-3.265879	-3.209450
7	0.560393	-2.525525	1.754185
6	0.120524	-3.789522	2.051415
6	-0.058374	-3.921527	3.493173
6	0.293933	-2.717379	4.042471
6	0.696197	-1.855019	2.940868
6	0.301828	-2.315271	5.487712
6	-0.529063	-5.163375	4.198221
6	-2.063713	-5.320249	4.254561
6	-2.499673	-6.611930	4.953169
7	1.675756	-0.045239	0.728734
6	1.665717	0.269979	2.068325
6	2.246158	1.581792	2.270780
6	2.621068	2.046261	1.027724
6	2.264321	1.007882	0.070126
6	2.357030	2.278838	3.592760
6	3.229995	3.320576	0.653490

6	4.097895	4.028251	1.395493
7	1.756121	-1.180047	-1.964061
6	2.363193	0.023934	-2.220011
6	2.828724	0.057659	-3.590194
6	2.493900	-1.156748	-4.153534
6	1.840607	-1.935694	-3.104189
6	3.551605	1.206781	-4.229723
6	2.774229	-1.542539	-5.535306
6	2.072576	-2.365433	-6.332369
7	0.630187	-3.667870	-0.925163
6	0.871317	-4.059415	-2.216071
6	0.496858	-5.455239	-2.379433
6	0.053195	-5.891933	-1.158375
6	0.171504	-4.762490	-0.246095
6	0.612846	-6.225706	-3.661364
6	-0.414534	-7.267762	-0.774527
6	0.695402	-8.160723	-0.177894
6	0.189726	-9.552222	0.214866
1	-6.741968	4.447824	1.265242
1	-5.267766	5.428839	1.363888
1	-4.272697	7.308998	-4.807477
1	-3.244865	6.110594	-4.019142
1	-0.289904	3.670940	5.935773
1	-0.696115	5.369012	6.233659
1	0.020884	4.391158	7.524956
1	-6.914895	-1.627943	5.987181
1	-5.327277	-1.905313	5.240933
1	-5.449769	-1.673018	6.996281
1	-2.866125	-4.608621	-4.090275
1	-3.728358	-3.734878	-5.368227
1	-4.259861	-3.601841	-3.684037
1	2.996767	8.617784	2.306083
1	3.079617	6.855772	2.464882
1	4.114506	7.689466	1.299343
1	3.737349	-2.641776	4.845526
1	4.778452	-1.615626	5.857651
1	3.735395	-0.883982	4.624696
1	4.756495	6.407746	-3.475637
1	3.685613	6.039908	-2.104059
1	4.666547	4.751403	-2.826824
1	1.341307	3.351783	-5.187269
1	1.021685	5.053633	-5.499134
1	5.412972	-0.877736	-2.536890
1	6.616594	-2.160753	-2.783198
1	9.675521	1.085183	-2.981429
1	10.492288	-0.133805	-1.993542
1	0.996105	-10.166373	0.631698
1	-0.604575	-9.488618	0.969313
1	-0.221229	-10.085345	-0.651697
1	-3.591824	-6.698255	4.987829

1	-2.112382	-7.495953	4.431081
1	-2.129661	-6.650839	5.985396
1	-4.901023	-6.041416	-3.689698
1	-4.274275	-6.213219	-5.320845
1	-6.014244	-4.620023	-6.156077
1	-7.900747	-6.253494	-6.011509
1	-6.359781	-7.090552	-6.270625
1	-7.100618	-7.073143	-4.661460
1	-7.986846	-4.087922	-4.706867
1	-7.162837	-4.805538	-3.313734
1	-6.518121	-3.339261	-4.070050
1	-2.491459	8.243972	-3.332444
1	-3.887531	9.989803	-2.237942
1	-4.465761	9.637166	-3.875915
1	-5.340033	8.988727	-2.482738
1	-2.708190	8.180290	-0.865798
1	-4.142044	7.153491	-0.989959
1	-2.551323	6.537478	-1.502581
1	-4.399405	4.334651	-3.491315
1	-7.259806	4.519920	-3.194876
1	-7.132903	2.037731	-2.904876
1	-6.199889	2.563898	-4.326714
1	-5.367111	2.115526	-2.814587
1	-4.766166	4.752647	-0.906212
1	-4.959543	3.482974	2.765024
1	-3.875754	3.338195	1.384685
1	-4.039545	1.436790	-0.130462
1	-7.150275	2.142684	2.756226
1	-5.052417	-0.741256	-0.688788
1	-8.164908	-0.041622	2.197635
1	-7.121422	-1.496680	0.465307
1	-1.098110	3.756051	-5.018892
1	-0.459105	3.336357	-3.410562
1	-0.840570	5.019532	-3.796347
1	3.127099	5.636165	-4.945570
1	1.025272	7.547178	1.126900
1	-2.021093	2.955602	7.593230
1	-3.605217	4.610173	8.588368
1	-1.941075	4.953067	9.091522
1	-2.706603	5.938496	7.834489
1	-4.063480	3.577268	6.291476
1	-3.163131	4.857048	5.469685
1	-2.708676	3.168940	5.204205
1	-6.076250	0.432450	4.860305
1	-4.123564	1.341864	5.755379
1	-6.243578	2.031190	6.782102
1	-7.470547	0.763768	6.917552
1	-6.001825	0.689227	7.920463
1	5.053592	-2.037102	2.819383
1	6.098174	-2.765359	4.035290

1	7.736003	-1.372724	5.299146
1	5.271282	0.352919	2.231776
1	9.159967	0.651421	5.299187
1	6.695474	2.370838	2.216963
1	8.642291	2.542358	3.764610
1	8.486901	-1.363589	-1.875258
1	9.203119	0.705853	0.030415
1	8.393122	1.871491	-1.013758
1	10.625651	2.927069	-1.524320
1	12.565422	2.443721	-0.013900
1	11.672336	1.096849	0.709992
1	12.166871	1.027409	-0.990524
1	-0.433675	-5.754581	1.517395
1	1.243665	-0.174104	4.091708
1	3.037935	1.943164	-1.651095
1	1.625805	-3.751350	-4.158694
1	1.287421	-1.949246	5.801948
1	-0.419179	-1.512500	5.691848
1	0.041748	-3.157136	6.136389
1	-0.138105	-5.171710	5.224017
1	-0.100932	-6.050987	3.712292
1	-2.468283	-5.288351	3.235351
1	-2.489013	-4.453113	4.777670
1	2.382912	3.364298	3.453356
1	1.509276	2.042155	4.246231
1	3.272362	1.998442	4.132065
1	2.939745	3.714044	-0.320518
1	4.488719	4.977170	1.039781
1	4.464307	3.683072	2.357851
1	3.427775	1.196527	-5.317598
1	3.170502	2.163161	-3.859461
1	4.631133	1.187633	-4.021371
1	3.651348	-1.062201	-5.969877
1	2.395958	-2.558799	-7.351200
1	1.155481	-2.852222	-6.015766
1	0.178852	-7.225620	-3.565679
1	0.098595	-5.720514	-4.489153
1	1.660148	-6.352206	-3.966733
1	-0.833944	-7.771824	-1.655255
1	-1.240205	-7.194356	-0.053335
1	1.129278	-7.659751	0.697058
1	1.508977	-8.251090	-0.909398
1	9.826701	2.843809	1.437386
1	10.805947	4.110310	0.675041
1	9.111748	3.889502	0.199184
6	-1.067880	-1.178643	-0.544786
6	-2.170133	-2.070084	-0.049855
6	-2.686253	-3.055565	-0.912759
6	-2.696377	-2.022846	1.268297
6	-3.661541	-3.963581	-0.501996

1	-2.286010	-3.132254	-1.914512
6	-3.705471	-2.908558	1.663226
6	-4.180443	-3.883085	0.787268
1	-4.012621	-4.721525	-1.195985
1	-4.115136	-2.840729	2.663639
1	-4.954473	-4.570237	1.118472
6	-1.446992	-0.569579	-1.894398
8	-1.939160	0.533405	-2.058728
8	-1.205718	-1.421604	-2.902254
6	-1.765698	-1.061361	-4.196436
1	-1.790581	-2.012690	-4.731911
1	-2.789673	-0.711582	-4.037186
6	-0.945146	-0.024219	-4.946137
1	-0.942683	0.926623	-4.409367
1	0.085027	-0.359280	-5.086031
1	-1.393801	0.133474	-5.935050
8	-2.202332	-1.065357	2.091144
6	-2.878655	-0.760258	3.307078
1	-3.929633	-0.515854	3.124309
1	-2.803025	-1.585481	4.023005
1	-2.367137	0.109463	3.718802
7	-1.293758	0.411035	0.355339
7	-0.805606	1.318918	0.772608
77	1.077837	-1.816317	-0.112685
6	3.018936	-2.594213	0.169219
1	3.735990	-1.770473	0.266282
1	3.052154	-3.208737	1.076030
1	3.305985	-3.212333	-0.688114
1	5.961099	-1.256219	-4.167797
1	2.070970	8.343048	-0.055956
1	2.124363	6.581897	0.138545

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**Q<sub>mutated</sub>-C<sub>Ir</sub>(Me)**

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Number of imaginary frequencies: 11    Electronic energy:    HF=-4961.56752721  
Zero-point correction=                    2.250725 (Hartree/Particle)  
Thermal correction to Energy=            2.388618  
Thermal correction to Enthalpy=         2.389562  
Thermal correction to Gibbs Free Energy=    2.026673  
Sum of electronic and zero-point Energies=    -4959.316803  
Sum of electronic and thermal Energies=    -4959.178909  
Sum of electronic and thermal Enthalpies=    -4959.177965  
Sum of electronic and thermal Free Energies=    -4959.540854

.....  
Cartesian Coordinates

.....  
6    2.449730    5.007372    -4.461189  
6    3.002234    6.309939    -5.053494  
6    4.378538    6.738907    -4.505202  
6    4.952868    7.899014    -5.332643

6	4.323633	7.117135	-3.016828
6	6.657689	-5.286618	-3.418721
6	7.600391	-4.178979	-2.967792
8	8.794876	-4.358445	-2.758308
6	6.671675	-6.544151	-2.510997
6	7.969984	-7.354336	-2.643228
6	6.376985	-6.189130	-1.045473
7	7.014717	-2.947852	-2.791567
6	7.802685	-1.776463	-2.428196
6	7.992408	-1.595609	-0.907065
8	8.800679	-0.776575	-0.484965
6	7.197000	-0.499467	-3.022102
7	7.197469	-2.365969	-0.115184
6	7.232993	-2.298034	1.332363
6	5.993892	-1.620681	1.954609
6	5.773788	-0.195828	1.487402
6	4.656007	0.143561	0.714241
6	6.700703	0.814785	1.795598
6	4.462027	1.450294	0.258418
6	6.510837	2.122838	1.344125
6	5.389213	2.444696	0.574521
6	1.066481	-4.751217	-4.436288
6	0.182215	-5.289784	-3.331237
8	-0.042723	-4.652655	-2.302418
6	2.251241	-3.943683	-3.898708
7	-0.361002	-6.507039	-3.591658
6	-1.350339	-7.109960	-2.732019
6	0.191158	-8.462131	2.150094
6	1.476633	-7.631641	2.195042
6	2.450643	-3.824129	6.989173
6	2.978284	-2.380485	6.950515
6	4.076507	-2.166180	8.002252
6	3.477997	-2.003908	5.546987
6	5.165712	3.373406	6.121434
6	5.844274	2.421744	5.141957
8	4.809721	1.634809	4.539878
6	6.882821	1.526179	5.822426
6	-4.482869	-0.041675	4.863727
6	-5.607260	-0.488887	3.911155
6	-5.744594	-1.995654	3.837021
6	-6.626079	-2.682973	4.683061
6	-4.962944	-2.743687	2.944137
6	-6.723006	-4.075385	4.644661
6	-5.056549	-4.136076	2.899823
6	-5.936257	-4.807689	3.752956
6	-5.885805	-1.550759	-3.094978
6	-6.496582	-2.933089	-2.968753
8	-5.945784	-3.935128	-3.420602
7	-7.700154	-2.977644	-2.323452
6	-8.376606	-4.230083	-2.016710



6	-7.863865	-4.899567	-0.731758
6	-8.545844	-6.241865	-0.400866
6	-7.788119	-6.961070	0.725694
6	-10.028205	-6.072699	-0.029267
6	-2.632335	4.804515	0.866697
6	-1.266616	0.684884	3.018855
6	-1.722674	-1.678382	-1.198153
6	-2.979196	2.472094	-3.373941
7	-1.891041	2.586130	1.606476
6	-2.197568	3.901990	1.832653
6	-2.039572	4.202092	3.250779
6	-1.654301	3.035673	3.857361
6	-1.576326	2.024602	2.813121
6	-1.370632	2.785130	5.308946
6	-2.243518	5.553830	3.874852
6	-1.012816	6.480507	3.765788
6	-1.256624	7.861827	4.381087
7	-1.527072	-0.172007	0.731617
6	-1.261122	-0.334354	2.066570
6	-1.018622	-1.734303	2.348617
6	-1.163614	-2.411412	1.155180
6	-1.474434	-1.408765	0.143874
6	-0.653513	-2.290216	3.691373
6	-1.036426	-3.840109	0.877383
6	-1.343640	-4.834982	1.726661
7	-2.192664	0.594299	-2.007759
6	-2.069735	-0.759509	-2.189432
6	-2.383952	-1.095511	-3.562429
6	-2.684796	0.089023	-4.202185
6	-2.599223	1.141941	-3.194103
6	-2.389840	-2.482886	-4.132956
6	-3.022576	0.222580	-5.618295
6	-2.736504	1.249704	-6.434981
7	-2.642284	3.351021	-1.105205
6	-3.009176	3.483709	-2.417074
6	-3.459889	4.845258	-2.652485
6	-3.359381	5.510493	-1.456449
6	-2.852455	4.550239	-0.487334
6	-3.943602	5.366175	-3.973200
6	-3.736482	6.932025	-1.146932
6	-5.159219	7.085311	-0.565802
6	-5.516448	8.540849	-0.249797
1	8.139738	-1.744683	1.588600
1	7.332768	-3.311793	1.740987
1	6.959135	-5.577183	-4.433849
1	5.629829	-4.906221	-3.488857
1	1.642101	-3.973170	6.263294
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1	2.062831	-4.081193	7.982370
1	5.902345	4.021695	6.608509

1	4.436123	4.002466	5.601153
1	4.636909	2.806371	6.896570
1	1.489338	4.746067	-4.921585
1	3.141960	4.174179	-4.638159
1	2.286412	5.077270	-3.381478
1	0.389715	-9.520166	2.358059
1	-0.536254	-8.111473	2.891310
1	-0.286974	-8.404962	1.164678
1	-4.408420	1.051649	4.889648
1	-4.666090	-0.399968	5.883771
1	-3.517178	-0.437051	4.533540
1	-1.062423	-8.131176	-2.456609
1	-1.418362	-6.502776	-1.828920
1	-2.337052	-7.138720	-3.210701
1	0.436875	-4.102191	-5.061219
1	1.415415	-5.563605	-5.086664
1	-5.008862	-1.478322	-2.444076
1	-6.575374	-0.741234	-2.834106
1	-8.213086	-4.897643	-2.868325
1	-9.449980	-4.020889	-1.956678
1	-6.530375	8.622385	0.158063
1	-4.825482	8.969273	0.487146
1	-5.467898	9.166783	-1.149678
1	-0.367883	8.497791	4.297616
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1	-1.512127	7.784540	5.445375
1	2.283154	7.126016	-4.885523
1	3.080785	6.196770	-6.144086
1	5.060225	5.880214	-4.611566
1	5.944976	8.194407	-4.970625
1	5.048507	7.627407	-6.390933
1	4.302302	8.781793	-5.273282
1	5.317827	7.394534	-2.646180
1	3.660880	7.979537	-2.861587
1	3.953778	6.297401	-2.391928
1	5.846685	-7.175758	-2.872117
1	7.918675	-8.261889	-2.029497
1	8.136636	-7.662025	-3.682863
1	8.833180	-6.763133	-2.328057
1	6.296930	-7.095207	-0.434141
1	7.182232	-5.576110	-0.622399
1	5.433042	-5.637746	-0.945486
1	6.051420	-2.815193	-3.068081
1	8.810559	-1.930099	-2.823937
1	7.805597	0.357309	-2.724290
1	7.169405	-0.555147	-4.115643
1	6.178771	-0.332835	-2.648449
1	6.578327	-3.022944	-0.568267
1	6.116565	-1.651550	3.046644
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1	3.920456	-0.616496	0.463420
1	7.593412	0.570654	2.366846
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1	1.897578	-3.159851	-3.224294
1	2.939965	-4.584225	-3.335650
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1	1.953857	-7.691682	3.180113
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1	4.433484	-1.129126	7.999393
1	3.714798	-2.395177	9.012151
1	4.939542	-2.815578	7.803163
1	3.820328	-0.962468	5.501839
1	4.318875	-2.646606	5.251014
1	2.687375	-2.131292	4.797006
1	6.345102	3.018039	4.362721
1	5.185106	1.211361	3.748592
1	7.346345	0.846454	5.097412
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1	6.407127	0.918670	6.601030
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1	-6.556780	-0.049592	4.243318
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1	-7.983762	-4.210406	0.117092
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1	-3.340877	2.735766	-4.360070
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1	-0.327972	2.483561	5.474932
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1	-2.502643	5.434782	4.934813
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1	-0.729072	6.582473	2.710765
1	-0.160983	5.996001	4.260909
1	-0.091852	-3.223302	3.580240
1	-0.035123	-1.589310	4.263318
1	-1.540139	-2.515454	4.300018

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1	-2.241848	-2.464705	-5.217728
1	-1.596134	-3.094173	-3.693030
1	-3.341871	-2.998458	-3.938999
1	-3.531255	-0.637778	-6.053995
1	-3.034203	1.229541	-7.479485
1	-2.184733	2.123980	-6.102983
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1	-3.014696	7.366426	-0.441535
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1	-5.880882	6.669644	-1.281013
1	-7.778850	-6.354243	1.640193
1	-8.254061	-7.924535	0.966024
1	-6.745697	-7.151237	0.443798
6	-0.085328	2.144120	-0.704383
6	0.606316	3.379969	-0.263867
6	0.575557	4.521475	-1.079576
6	1.287568	3.445661	0.976541
6	1.144635	5.725624	-0.658049
1	0.067563	4.465352	-2.036668
6	1.883181	4.646690	1.381269
6	1.799379	5.781930	0.570742
1	1.079874	6.605328	-1.291508
1	2.415008	4.698300	2.323895
1	2.261131	6.707568	0.904161
6	0.724537	1.472297	-1.756846
8	1.566083	0.650901	-1.431491
8	0.505243	1.885594	-3.015030
6	1.432041	1.398221	-4.026046
1	1.385407	2.158819	-4.807646
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1	1.754048	-0.261370	-5.348023
8	1.354223	2.286386	1.675559
6	2.037952	2.277950	2.924142
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1	1.572730	2.973183	3.634513
1	1.948382	1.259925	3.302691
7	2.542580	-3.749013	0.183726
7	3.431542	-3.560839	-0.445486
77	-1.960134	1.603240	-0.208717
6	-4.056089	1.237747	0.117165
1	-4.195235	0.220537	0.505116

1	-4.467482	1.952820	0.839186
1	-4.614045	1.327730	-0.821881
1	-5.543095	-1.405516	-4.122222
1	2.203989	-7.983350	1.453747
1	1.273229	-6.574988	1.987836

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**Q-<sup>5</sup>A<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 8    Electronic energy:    HF=-4730.3868925  
Zero-point correction=                    2.046588 (Hartree/Particle)  
Thermal correction to Energy=            2.169481  
Thermal correction to Enthalpy=         2.170425  
Thermal correction to Gibbs Free Energy= 1.842507  
Sum of electronic and zero-point Energies= -4728.340304  
Sum of electronic and thermal Energies= -4728.217412  
Sum of electronic and thermal Enthalpies= -4728.216468  
Sum of electronic and thermal Free Energies= -4728.544385

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Cartesian Coordinates

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6	-4.000396	-6.261679	4.760397
6	-4.766631	-6.147920	3.436758
6	-4.831229	-4.726994	2.840743
6	-5.449686	-4.758341	1.434498
6	-5.597597	-3.747047	3.742647
6	-6.876632	-1.430399	-4.892552
6	-7.862781	-0.900305	-3.867448
8	-8.489250	0.153995	-4.038126
6	-5.510864	-0.695618	-4.955829
6	-5.645094	0.779210	-5.358638
6	-4.709267	-0.857846	-3.659100
7	-8.041563	-1.661570	-2.751959
6	-9.041880	-1.363702	-1.722801
6	-8.537653	-0.313304	-0.697698
8	-8.482098	-0.561032	0.506039
6	-9.475174	-2.649115	-1.024287
7	-8.193908	0.872349	-1.259220
6	-7.706984	2.010692	-0.498027
6	-6.283394	2.458978	-0.858520
6	-5.135244	1.523534	-0.510769
6	-3.863406	1.802210	-1.038519
6	-5.272100	0.416418	0.337487
6	-2.757723	1.013082	-0.723120
6	-4.166095	-0.384353	0.642014
6	-2.905599	-0.090466	0.121953
6	-1.419038	-2.931268	-4.149160
6	-0.797611	-1.769435	-4.900962
8	-1.462148	-0.955814	-5.544983

6	-1.416958	-2.739135	-2.620968
7	0.556483	-1.720381	-4.822424
6	1.309862	-0.671990	-5.470664
6	0.054020	4.460991	-5.179622
6	0.648752	3.558182	-4.104749
8	1.739803	2.860581	-4.715962
6	-0.375404	2.580971	-3.521776
6	-2.619308	7.504282	0.598519
6	-2.578129	5.972317	0.671267
6	-3.985385	5.392973	0.874791
6	-1.906539	5.376358	-0.573822
6	-6.248765	4.381636	6.682971
6	-5.987895	3.207752	5.743792
8	-5.483725	2.146321	6.558748
6	-5.008201	3.560886	4.622609
6	3.705822	3.765449	4.109955
6	5.245728	3.739778	4.134392
6	5.866204	4.497962	2.978547
6	6.276208	5.830011	3.132040
6	6.013482	3.892769	1.720747
6	6.818831	6.544914	2.062284
6	6.555025	4.605261	0.648746
6	6.959823	5.932786	0.814939
6	3.962688	-1.284535	3.405567
6	4.459720	-2.727595	3.357042
8	4.138365	-3.544829	4.227341
6	4.833614	-0.166662	2.812827
16	5.043942	-0.151906	0.971266
7	5.231994	-3.064034	2.296200
6	5.624823	-4.441303	2.063215
6	6.274255	-4.580243	0.682154
6	6.582459	-6.028456	0.257373
6	7.061419	-6.066455	-1.202421
6	7.605556	-6.711490	1.178981
26	2.823927	-0.073562	-0.089379
6	0.485702	-1.523617	2.068256
6	1.613264	3.045476	0.900850
6	4.199016	1.450504	-2.877781
6	2.977526	-3.115628	-1.781143
7	1.273240	0.635882	1.222408
6	0.573429	-0.125083	2.114655
6	-0.072894	0.729721	3.110233
6	0.232818	2.021494	2.761840
6	1.077689	1.942407	1.574642
6	-0.197004	3.292789	3.432079
6	-0.899554	0.264934	4.278143
6	-2.376530	-0.027579	3.942003
6	-3.209374	-0.369946	5.181955
7	2.809988	1.911931	-0.911633
6	2.417737	3.038889	-0.247326

6	2.953984	4.225646	-0.898897
6	3.681384	3.775639	-1.982361
6	3.576274	2.313443	-1.965004
6	2.719186	5.640953	-0.467317
6	4.369223	4.545281	-3.016340
6	5.030840	5.701598	-2.848688
7	3.403351	-0.725073	-2.058005
6	4.121334	0.050209	-2.924774
6	4.768676	-0.782652	-3.921204
6	4.384714	-2.084827	-3.656362
6	3.534374	-2.020172	-2.460626
6	5.638914	-0.277880	-5.033957
6	4.785426	-3.256317	-4.431139
6	4.099200	-4.391620	-4.645282
7	1.824072	-1.970343	0.065088
6	2.183076	-3.093223	-0.627191
6	1.618256	-4.278491	0.010843
6	0.914774	-3.836971	1.102751
6	1.054671	-2.381197	1.116250
6	1.802071	-5.690678	-0.461589
6	0.199092	-4.664808	2.133549
6	1.128636	-5.184192	3.253161
6	0.373233	-5.952919	4.341181
1	3.322679	3.315279	3.188989
1	3.292047	3.207655	4.958689
1	3.332756	4.795994	4.163105
1	3.788491	-1.078694	4.470040
1	2.977768	-1.267579	2.925986
1	4.740064	-5.090601	2.136103
1	6.308298	-4.767877	2.858296
1	1.059145	-6.320471	5.112965
1	-0.161853	-6.818285	3.926966
1	-0.369128	-5.313064	4.836730
1	-4.240195	-0.631207	4.907611
1	-3.242948	0.474382	5.883077
1	-2.789983	-1.227204	5.723507
1	-3.948600	-7.304809	5.094139
1	-2.971124	-5.898021	4.653764
1	-4.476413	-5.685089	5.561424
1	-1.612860	7.926592	0.490522
1	-3.213271	7.837559	-0.263371
1	-3.070455	7.937116	1.500257
1	-0.885618	-3.857769	-4.402290
1	-2.445200	-3.032140	-4.514162
1	2.367959	-0.939580	-5.451968
1	0.977872	-0.576125	-6.508991
1	1.184093	0.305618	-4.993361
1	-0.335880	3.858459	-6.008637
1	-0.766103	5.062768	-4.771415
1	0.819716	5.135977	-5.576767

1	-5.793055	-6.522384	3.572073
1	-4.296022	-6.812894	2.698797
1	-3.797028	-4.361219	2.743948
1	-5.460636	-3.759049	0.982931
1	-4.888787	-5.423451	0.766557
1	-6.487109	-5.118033	1.471868
1	-5.642296	-2.749495	3.289440
1	-6.631598	-4.084985	3.895746
1	-5.129932	-3.641679	4.727504
1	-6.694412	-2.499701	-4.722380
1	-4.946823	-1.202224	-5.751143
1	-4.651141	1.224558	-5.475825
1	-6.181768	0.886964	-6.308940
1	-6.195338	1.353075	-4.605711
1	-3.695527	-0.470176	-3.795949
1	-5.169889	-0.324521	-2.819811
1	-4.619061	-1.915502	-3.377321
1	-7.430077	-2.451392	-2.596347
1	-9.889631	-0.916227	-2.255638
1	-10.242204	-2.430818	-0.277850
1	-9.875452	-3.361803	-1.752948
1	-8.634655	-3.107974	-0.492753
1	-8.315338	0.958708	-2.268116
1	-7.784756	1.743553	0.558194
1	-6.118776	3.423626	-0.355413
1	-6.246660	2.685082	-1.933825
1	-3.739933	2.650873	-1.708528
1	-6.239880	0.155585	0.754628
1	-1.782337	1.253035	-1.136058
1	-4.296403	-1.242864	1.297084
1	-2.044136	-0.702776	0.372332
1	-1.911384	-3.583797	-2.127515
1	-0.401720	-2.669248	-2.216208
1	-1.950691	-1.825876	-2.339314
1	1.036747	-2.305870	-4.152585
1	1.035036	4.189781	-3.289862
1	2.205196	2.372313	-4.014992
1	0.090786	1.959574	-2.747446
1	-1.211035	3.122356	-3.059434
1	-0.773145	1.919702	-4.300748
1	-1.971297	5.692841	1.545819
1	-3.959274	4.299525	0.943462
1	-4.448113	5.781152	1.791035
1	-4.639588	5.660548	0.033326
1	-1.833404	4.285607	-0.503184
1	-2.479878	5.618530	-1.479315
1	-0.892386	5.771135	-0.708747
1	-6.933782	4.083206	7.483272
1	-6.947181	2.901860	5.291285
1	-5.293011	1.391155	5.980603



1	-4.835652	2.701091	3.962969
1	-5.392387	4.379323	4.002077
1	-4.043345	3.866223	5.043610
1	5.581559	2.696028	4.109621
1	5.600714	4.163260	5.083509
1	6.172533	6.310164	4.103884
1	5.708697	2.857755	1.571978
1	7.135210	7.576016	2.204839
1	6.657137	4.119549	-0.317586
1	7.387806	6.482500	-0.020159
1	5.839219	-0.209678	3.248903
1	4.392264	0.788349	3.116859
1	5.351713	-2.364843	1.557380
1	7.200411	-3.987167	0.652103
1	5.599344	-4.133052	-0.060330
1	5.642353	-6.600105	0.316790
1	7.242326	-7.096521	-1.535398
1	6.325290	-5.615528	-1.878435
1	8.001059	-5.509971	-1.318253
1	7.816511	-7.734565	0.842446
1	8.555234	-6.159491	1.180262
1	7.252787	-6.768624	2.214271
1	-0.086878	-1.995050	2.861208
1	1.378554	4.020223	1.317600
1	4.820321	1.920753	-3.634300
1	3.213025	-4.096598	-2.177537
1	0.659098	3.935341	3.673365
1	-0.868675	3.880942	2.791357
1	-0.732634	3.093496	4.365928
1	-0.867285	1.026666	5.068846
1	-0.451336	-0.636952	4.717956
1	-2.425387	-0.852373	3.220857
1	-2.808022	0.841778	3.430314
1	2.822691	6.327751	-1.314449
1	1.717184	5.772657	-0.042222
1	3.442457	5.955322	0.297436
1	4.308654	4.130026	-4.022699
1	5.484321	6.211960	-3.694603
1	5.162663	6.158305	-1.872337
1	6.101281	-1.097987	-5.591783
1	5.067445	0.322760	-5.754895
1	6.444657	0.361624	-4.652446
1	5.759626	-3.171899	-4.915073
1	4.521001	-5.190022	-5.249533
1	3.099387	-4.556204	-4.255877
1	1.154081	-6.381912	0.087441
1	1.569689	-5.797104	-1.529380
1	2.836280	-6.035908	-0.325564
1	-0.287240	-5.524998	1.650447
1	-0.614776	-4.081292	2.585723

1	1.684372	-4.351087	3.697651
1	1.891224	-5.834123	2.804369
1	-6.690345	5.223880	6.138867
1	-5.310716	4.714622	7.141919
1	-8.382849	2.860508	-0.666063
1	-7.376240	-1.336637	-5.864391

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**Q-10SS<sup>TS</sup>(B-C)<sub>Fe(cys)</sub>**  
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Number of imaginary frequencies: 11    Electronic energy:    HF=-5491.80824563  
 Zero-point correction=                    2.265324 (Hartree/Particle)  
 Thermal correction to Energy=            2.402938  
 Thermal correction to Enthalpy=         2.403882  
 Thermal correction to Gibbs Free Energy= 2.045853  
 Sum of electronic and zero-point Energies= -5489.542921  
 Sum of electronic and thermal Energies= -5489.405307  
 Sum of electronic and thermal Enthalpies= -5489.404363  
 Sum of electronic and thermal Free Energies= -5489.762393

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 Cartesian Coordinates  
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6	2.883618	6.174956	-3.592629
6	2.403954	7.134862	-2.497617
6	3.079378	8.521092	-2.500475
6	2.387667	9.459463	-1.499752
6	4.586052	8.440334	-2.209683
6	5.764044	-4.589314	-4.368581
6	6.873251	-3.679795	-3.856523
8	8.025243	-4.063367	-3.679917
6	5.415026	-5.770359	-3.423693
6	6.548913	-6.801503	-3.325468
6	4.973086	-5.280997	-2.036664
7	6.507981	-2.381462	-3.581164
6	7.517451	-1.388000	-3.222710
6	8.032636	-1.527988	-1.774343
8	9.149622	-1.126965	-1.473997
6	6.978236	0.029246	-3.447368
7	7.141393	-2.052609	-0.886543
6	7.472619	-2.309301	0.503427
6	6.857883	-1.300784	1.499670
6	7.433496	0.096120	1.404490
6	6.750751	1.115163	0.728950
6	8.673587	0.396592	1.986991
6	7.292512	2.399836	0.635144
6	9.218896	1.676753	1.894966
6	8.528536	2.685039	1.216734
6	0.214582	-3.280739	-4.355689
6	-0.216304	-4.443876	-3.466607
8	0.568734	-5.190265	-2.876801
6	1.732079	-3.158382	-4.478497

7	-1.572662	-4.604881	-3.427191
6	-2.208783	-5.530948	-2.517361
6	-0.120284	-7.664696	1.852803
6	-0.030681	-6.563783	0.787316
8	0.237342	-7.191544	-0.466225
6	1.038986	-5.520828	1.120474
6	3.438198	-3.958550	6.689452
6	2.594860	-5.213273	6.959039
6	1.568065	-5.441366	5.840073
6	3.487899	-6.448062	7.149701
6	6.962933	2.913040	6.141160
6	6.173359	2.262610	5.008260
8	4.926099	2.961057	4.938409
6	5.956955	0.764922	5.237585
6	-3.125356	0.835890	6.191515
6	-3.922824	2.106452	5.841073
6	-5.339214	1.812119	5.386336
6	-6.382307	1.710901	6.318232
6	-5.633095	1.608972	4.030124
6	-7.683438	1.413100	5.909000
6	-6.933510	1.312102	3.613894
6	-7.961688	1.213504	4.554614
6	-5.949617	0.514201	-1.523539
6	-7.151445	0.017495	-0.726787
8	-7.908554	0.756736	-0.100868
6	-5.237725	1.723969	-0.908054
16	-4.074084	1.330311	0.456172
7	-7.384301	-1.328712	-0.844621
6	-8.580058	-1.971078	-0.325253
6	-9.712235	-2.056310	-1.362401
6	-11.027715	-2.655242	-0.827623
6	-12.154015	-2.485267	-1.858739
6	-10.884169	-4.132842	-0.427773
26	-1.941830	0.786278	-0.378414
6	-1.314036	4.109206	-0.090594
6	-0.974361	0.319328	2.873129
6	-3.218828	-2.353174	-0.464321
6	-2.759370	1.219561	-3.684822
7	-1.217459	1.967772	1.086991
6	-1.060690	3.322828	1.025581
6	-0.563144	3.840797	2.295423
6	-0.406796	2.757702	3.114654
6	-0.852235	1.598974	2.352066
6	0.138314	2.714196	4.510195
6	-0.270414	5.284544	2.594506
6	1.108667	5.771984	2.101637
6	1.370012	7.242939	2.440479
7	-1.977028	-0.759076	0.917689
6	-1.542786	-0.768923	2.214516
6	-1.841491	-2.036656	2.849244

6	-2.522983	-2.784635	1.913771
6	-2.591953	-1.962076	0.709415
6	-1.451144	-2.428414	4.242232
6	-3.052874	-4.137848	2.016951
6	-3.437425	-4.784046	3.131372
7	-2.698740	-0.393347	-1.845492
6	-3.252181	-1.635656	-1.658733
6	-3.868479	-2.100087	-2.883440
6	-3.600999	-1.142655	-3.844273
6	-2.928070	-0.057022	-3.151800
6	-4.729656	-3.320902	-3.063328
6	-3.988389	-1.220263	-5.249441
6	-3.314415	-0.726762	-6.301219
7	-1.987524	2.347517	-1.652263
6	-2.365486	2.340956	-2.969886
6	-2.345454	3.689078	-3.513446
6	-1.957174	4.512022	-2.490448
6	-1.736479	3.651920	-1.334718
6	-2.712309	4.051592	-4.922223
6	-1.824005	6.008658	-2.497505
6	-3.061196	6.745853	-1.940163
6	-2.896290	8.268878	-1.943387
1	8.563455	-2.289233	0.576716
1	7.132052	-3.319774	0.761985
1	6.104456	-4.992150	-5.330916
1	4.850792	-4.012805	-4.562999
1	4.150260	-3.772150	7.502819
1	4.014427	-4.067927	5.761127
1	2.806787	-3.068062	6.585202
1	7.960150	2.466859	6.224683
1	7.074377	3.986710	5.957915
1	6.437872	2.781652	7.094658
1	2.318422	5.236784	-3.560506
1	2.747961	6.613085	-4.590040
1	3.943886	5.921253	-3.482305
1	-0.409444	-7.237358	2.819251
1	-0.864865	-8.414324	1.563246
1	0.847039	-8.169553	1.963035
1	-2.120021	1.087523	6.551612
1	-3.630810	0.258882	6.975449
1	-3.023286	0.192194	5.311726
1	-3.115163	-5.946160	-2.970315
1	-1.517664	-6.346566	-2.301351
1	-2.472500	-5.052730	-1.564841
1	-0.183071	-2.350244	-3.936251
1	-0.248460	-3.412315	-5.343462
1	-6.359356	0.807503	-2.504812
1	-5.249334	-0.297193	-1.706176
1	-8.910999	-1.377568	0.532438
1	-8.304239	-2.966004	0.041810

1	-3.786710	8.768079	-1.543559
1	-2.039023	8.576881	-1.330976
1	-2.728445	8.649243	-2.959400
1	2.354445	7.567195	2.081811
1	0.616096	7.897142	1.983675
1	1.339779	7.412951	3.524350
1	2.551612	6.669031	-1.511751
1	1.319541	7.276455	-2.604701
1	2.952452	8.950234	-3.507426
1	2.835292	10.460937	-1.514962
1	1.319228	9.564830	-1.724127
1	2.474357	9.072372	-0.475854
1	5.041724	9.438214	-2.215756
1	4.767903	7.998505	-1.220845
1	5.116084	7.830658	-2.949389
1	4.549093	-6.265507	-3.884875
1	6.241959	-7.645624	-2.695897
1	6.809501	-7.197010	-4.315061
1	7.452863	-6.356095	-2.900928
1	4.644795	-6.122693	-1.416749
1	5.801343	-4.787464	-1.510901
1	4.131551	-4.581606	-2.106134
1	5.589762	-2.060700	-3.858210
1	8.402947	-1.554068	-3.843598
1	7.739790	0.757282	-3.156032
1	6.726142	0.188070	-4.502124
1	6.083693	0.215126	-2.841071
1	6.279249	-2.424900	-1.260626
1	7.024426	-1.701112	2.509509
1	5.771362	-1.267393	1.349148
1	5.778208	0.910309	0.290863
1	9.218433	-0.382829	2.516390
1	6.739924	3.176751	0.113070
1	10.182128	1.888149	2.352869
1	8.950042	3.684584	1.146361
1	1.989031	-2.313185	-5.126682
1	2.173070	-2.982066	-3.492789
1	2.177466	-4.070607	-4.891401
1	-2.115500	-3.799617	-3.714546
1	-1.006938	-6.051237	0.747509
1	0.386701	-6.497502	-1.139582
1	1.056757	-4.731582	0.359641
1	0.838593	-5.050649	2.091515
1	2.028735	-5.993174	1.156224
1	2.041063	-5.050854	7.896353
1	0.941892	-6.318153	6.044952
1	0.904888	-4.575839	5.723516
1	2.067783	-5.608932	4.876940
1	2.892053	-7.340645	7.376247
1	4.064728	-6.656564	6.238902

1	4.201955	-6.302763	7.969830
1	6.729365	2.397392	4.067015
1	4.388795	2.551895	4.241673
1	5.384121	0.322801	4.412395
1	6.913309	0.231603	5.295494
1	5.403001	0.597240	6.168817
1	-3.390930	2.652131	5.052107
1	-3.949291	2.765936	6.719372
1	-6.172454	1.873037	7.374749
1	-4.847189	1.685952	3.281944
1	-8.479951	1.343720	6.647137
1	-7.138866	1.165859	2.556081
1	-8.975401	0.987561	4.232173
1	-5.993445	2.397951	-0.490440
1	-4.699087	2.266100	-1.689086
1	-6.693604	-1.890445	-1.320134
1	-9.371869	-2.641004	-2.231148
1	-9.901661	-1.037920	-1.724820
1	-11.309077	-2.087047	0.072437
1	-11.837245	-4.534769	-0.062408
1	-10.576386	-4.741231	-1.289137
1	-10.141809	-4.277060	0.364624
1	-1.152097	5.176399	0.013029
1	-0.669515	0.174427	3.903359
1	-3.717129	-3.315190	-0.454753
1	-3.052360	1.364529	-4.717220
1	-0.511779	2.150434	5.189791
1	1.126912	2.235519	4.536270
1	0.254843	3.720565	4.924818
1	-0.331289	5.450422	3.678502
1	-1.050251	5.921506	2.153540
1	1.177233	5.619792	1.017066
1	1.888677	5.139715	2.543124
1	-1.263772	-3.506967	4.301342
1	-0.542919	-1.910479	4.569103
1	-2.235584	-2.197686	4.976692
1	-3.142697	-4.679233	1.075480
1	-3.800047	-5.807031	3.081237
1	-3.431837	-4.318595	4.111516
1	-4.451792	-3.905603	-3.948774
1	-4.686008	-3.992780	-2.202799
1	-5.784897	-3.040615	-3.203749
1	-4.904983	-1.777827	-5.451389
1	-3.690684	-0.847928	-7.313488
1	-2.363779	-0.214530	-6.186869
1	-2.521183	5.110548	-5.124132
1	-2.140531	3.467238	-5.654816
1	-3.775238	3.866282	-5.127703
1	-1.639641	6.358324	-3.522529
1	-0.941298	6.310532	-1.916224

1	-3.259839	6.392640	-0.920653
1	-3.939635	6.463552	-2.535086
1	-11.922133	-3.027956	-2.785061
1	-13.106349	-2.873533	-1.476577
1	-12.299773	-1.430197	-2.118948
6	0.345353	0.347984	-1.041137
6	1.390656	0.951305	-0.151295
6	1.871025	2.264377	-0.339559
6	1.942942	0.265403	0.975523
6	2.857990	2.846243	0.457564
1	1.451291	2.850107	-1.141368
6	2.949469	0.838970	1.763455
6	3.417860	2.129961	1.508311
1	3.183484	3.861508	0.245104
1	3.362746	0.277995	2.594348
1	4.209788	2.559038	2.118098
6	0.423743	0.606853	-2.501916
8	0.190212	-0.214220	-3.381046
8	0.768869	1.888817	-2.851071
6	0.878726	2.164201	-4.256083
1	0.083894	1.638150	-4.789177
1	0.712985	3.242524	-4.336836
6	2.248829	1.773261	-4.798209
1	3.046320	2.270978	-4.235406
1	2.387329	0.690951	-4.723898
1	2.337111	2.063626	-5.852870
8	1.441435	-0.970709	1.265771
6	2.008649	-1.728946	2.308646
1	3.077336	-1.925684	2.136498
1	1.891602	-1.237470	3.285228
1	1.465310	-2.675150	2.315322
7	0.673431	-1.359872	-1.073445
7	-0.085208	-2.217015	-1.166670

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**W-1C<sup>SSS</sup>TS(C-D)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2835.7237206  
Zero-point correction=                    0.893707 (Hartree/Particle)  
Thermal correction to Energy=            0.950916  
Thermal correction to Enthalpy=         0.951861  
Thermal correction to Gibbs Free Energy= 0.801880  
Sum of electronic and zero-point Energies= -2834.815587  
Sum of electronic and thermal Energies= -2834.758378  
Sum of electronic and thermal Enthalpies= -2834.757433  
Sum of electronic and thermal Free Energies= -2834.907414

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Cartesian Coordinates  
.....

6	3.555716	-3.237684	-0.959380
6	2.257595	-2.703115	-0.598801
7	2.255939	-1.339812	-0.672671
6	3.500641	-0.983396	-1.094508
6	4.336310	-2.161418	-1.280416
6	1.167638	-3.484589	-0.252024
6	-0.097010	-3.021763	0.086882
7	-0.468589	-1.715271	0.145888
6	-1.781811	-1.708482	0.510108
6	-2.261099	-3.065111	0.704714
6	-1.206622	-3.886008	0.434867
6	-2.567973	-0.569334	0.610936
6	-2.168120	0.725533	0.304754
7	-0.905108	1.087097	-0.051298
6	-0.940509	2.425726	-0.281457
6	-2.275881	2.945147	-0.075857
6	-3.046101	1.881907	0.288098
6	0.148786	3.218047	-0.619440
6	1.445967	2.777553	-0.812516
7	1.829201	1.470940	-0.811962
6	3.143288	1.461162	-1.164775
6	3.632999	2.808511	-1.369968
6	2.579695	3.640175	-1.124306
6	3.923065	0.320529	-1.315694
1	-0.031137	4.280296	-0.739534
1	4.945919	0.465305	-1.647933
1	1.309636	-4.560981	-0.257157
1	-3.598563	-0.707232	0.919957
6	-4.534729	1.862134	0.449418
1	-4.857515	1.032757	1.087196
1	-4.876973	2.782508	0.936859
6	-5.204731	1.743247	-0.940820
1	-4.916826	0.788664	-1.397931
1	-4.866169	2.558153	-1.583639
6	-6.702162	1.819978	-0.864554
8	-7.412471	2.716758	-1.237888
8	-7.229926	0.710176	-0.267974
1	-8.193186	0.827699	-0.240545
6	-3.662074	-3.475748	1.040855
1	-4.111951	-2.799085	1.775007
1	-3.642276	-4.463593	1.512165
6	-4.581692	-3.565401	-0.202830
1	-4.045525	-4.021452	-1.037542
1	-5.453201	-4.182957	0.040895
6	-5.097794	-2.217370	-0.643042
8	-4.805122	-1.641455	-1.670189
8	-5.941113	-1.712864	0.267362
1	-6.294320	-0.855119	-0.046132
6	-1.143894	-5.381292	0.462302
1	-2.091939	-5.819866	0.786985



1	-0.913939	-5.790938	-0.528626
1	-0.364247	-5.736176	1.147702
6	-2.677980	4.374575	-0.259860
1	-2.533373	4.702755	-1.296041
1	-3.730735	4.532166	-0.006298
1	-2.079500	5.038095	0.376076
6	3.931846	-4.684845	-0.928852
1	3.453810	-5.203312	-0.090866
1	3.633188	-5.203689	-1.848600
1	5.015274	-4.798842	-0.823764
6	5.044633	3.164411	-1.712639
1	5.733801	2.848305	-0.920147
1	5.368448	2.678500	-2.640917
1	5.163623	4.243934	-1.839678
6	5.736692	-2.128800	-1.698256
6	6.349151	-3.044694	-2.455016
1	6.320878	-1.274652	-1.355699
1	7.402460	-2.953510	-2.702576
1	5.818859	-3.897338	-2.869179
6	2.595591	5.104158	-1.141314
6	1.971293	5.898728	-0.266680
1	3.198591	5.566641	-1.922829
1	2.040023	6.979807	-0.346056
1	1.398745	5.494837	0.563862
6	1.194394	0.164832	1.668847
6	1.230559	1.533839	2.237979
6	0.719001	-0.905745	2.581948
6	0.087049	2.228713	2.628164
6	2.459792	2.192893	2.327922
8	-0.330409	-0.815290	3.179911
8	1.521790	-1.979586	2.606210
6	0.184555	3.549722	3.060362
1	-0.873826	1.731054	2.578193
6	2.575604	3.507692	2.738296
8	3.581125	1.487456	1.943195
6	1.417731	4.192919	3.102231
1	-0.715843	4.076268	3.361197
1	3.553782	3.974237	2.771468
6	3.384857	0.139612	2.034859
1	1.488060	5.225245	3.431282
1	3.271529	-0.247739	3.048879
1	4.114283	-0.402526	1.432245
1	2.402922	-0.166278	1.325216
7	0.097282	-0.339323	-2.252220
6	-1.110487	-0.667231	-2.658792
6	0.860212	-0.169955	-3.381893
7	-1.156834	-0.715346	-4.009105
1	-1.961238	-0.875124	-2.026555
6	0.095687	-0.400389	-4.488670
1	1.901553	0.104518	-3.312117

1	-1.972243	-0.943377	-4.554066
1	0.320024	-0.370303	-5.542719
6	0.999195	-3.150391	3.251894
1	-0.069551	-3.219746	3.033696
1	1.516837	-3.977789	2.761518
6	1.264843	-3.122414	4.745641
1	0.726699	-2.293081	5.211650
1	0.923628	-4.057376	5.202615
1	2.335228	-3.011905	4.947235
26	0.684607	-0.116797	-0.298173

\*w-TS(C-D)<sub>Fe</sub> for wB97XD

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**W-<sup>10SS</sup>TS(C-D)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2835.7000511  
Zero-point correction=                    0.890104 (Hartree/Particle)  
Thermal correction to Energy=            0.947841  
Thermal correction to Enthalpy=         0.948785  
Thermal correction to Gibbs Free Energy= 0.797305  
Sum of electronic and zero-point Energies= -2834.809947  
Sum of electronic and thermal Energies= -2834.752210  
Sum of electronic and thermal Enthalpies= -2834.751266  
Sum of electronic and thermal Free Energies= -2834.902746

.....  
Cartesian Coordinates

.....  

6	3.541019	-3.271398	-0.891451
6	2.234481	-2.736966	-0.577602
7	2.235690	-1.370852	-0.657866
6	3.497210	-1.018745	-1.031391
6	4.333225	-2.196680	-1.184611
6	1.141480	-3.519894	-0.265974
6	-0.119871	-3.045466	0.059221
7	-0.471159	-1.734117	0.131567
6	-1.785719	-1.715858	0.495016
6	-2.282722	-3.064480	0.670898
6	-1.238927	-3.896474	0.390618
6	-2.556330	-0.570960	0.604917
6	-2.137177	0.713775	0.298276
7	-0.871651	1.064750	-0.074348
6	-0.899445	2.406640	-0.298664
6	-2.223307	2.932993	-0.079949
6	-2.999483	1.874860	0.290137
6	0.185188	3.198880	-0.645301
6	1.474772	2.748051	-0.825660
7	1.847370	1.436707	-0.802732
6	3.166392	1.415980	-1.131272
6	3.667312	2.756453	-1.346375
6	2.616369	3.597539	-1.132223

6	3.939641	0.273604	-1.258653
1	0.008579	4.260850	-0.766115
1	4.971998	0.404692	-1.563728
1	1.280040	-4.595989	-0.271525
1	-3.586407	-0.694357	0.919338
6	-4.485993	1.874444	0.470273
1	-4.815191	1.037418	1.094125
1	-4.805728	2.789500	0.981887
6	-5.172970	1.797330	-0.914733
1	-4.906591	0.848419	-1.395706
1	-4.827762	2.620857	-1.542926
6	-6.667673	1.901457	-0.814509
8	-7.360914	2.834446	-1.125085
8	-7.211333	0.771108	-0.274713
1	-8.170946	0.907773	-0.219776
6	-3.688215	-3.460517	1.004558
1	-4.130496	-2.782475	1.741891
1	-3.678755	-4.450125	1.472002
6	-4.606695	-3.534651	-0.240904
1	-4.075561	-3.997501	-1.075172
1	-5.488100	-4.138564	0.000196
6	-5.097023	-2.175809	-0.676907
8	-4.772133	-1.590513	-1.689365
8	-5.951868	-1.671813	0.221838
1	-6.289872	-0.805679	-0.085208
6	-1.194399	-5.392373	0.404924
1	-2.158259	-5.821777	0.692536
1	-0.935609	-5.795517	-0.581319
1	-0.443740	-5.761292	1.114490
6	-2.611282	4.368599	-0.242919
1	-2.451199	4.715807	-1.270373
1	-3.665570	4.529603	0.000905
1	-2.015096	5.011662	0.415512
6	3.914289	-4.718576	-0.842161
1	3.428905	-5.226099	-0.002051
1	3.623041	-5.246075	-1.759217
1	4.996311	-4.831447	-0.725833
6	5.089360	3.098274	-1.654967
1	5.746366	2.806441	-0.826993
1	5.443557	2.582661	-2.555473
1	5.214258	4.173144	-1.811162
6	5.750085	-2.167450	-1.545938
6	6.376959	-3.070610	-2.305321
1	6.330612	-1.332936	-1.153270
1	7.440223	-2.990051	-2.510009
1	5.849479	-3.902927	-2.762519
6	2.636589	5.061612	-1.175372
6	2.017753	5.870234	-0.310448
1	3.237453	5.507730	-1.967761
1	2.089622	6.949678	-0.406918

1	1.452016	5.480083	0.531336
6	1.190314	0.125182	1.616537
6	1.219879	1.511111	2.171819
6	0.601034	-0.887526	2.533685
6	0.075449	2.189098	2.604430
6	2.440310	2.205843	2.240821
8	-0.409806	-0.752854	3.193178
8	1.339345	-2.018738	2.552773
6	0.131384	3.513227	3.026013
1	-0.869157	1.657984	2.593845
6	2.508020	3.534505	2.642385
8	3.622686	1.609080	1.869949
6	1.346476	4.194227	3.027982
1	-0.777726	4.012039	3.349100
1	3.474017	4.028447	2.650652
6	3.679542	0.250122	2.081605
1	1.397672	5.231489	3.347319
1	3.621559	-0.053413	3.131026
1	4.466155	-0.206695	1.488206
1	2.407969	-0.162141	1.566502
7	0.091152	-0.359221	-2.297663
6	-1.103365	-0.727466	-2.708175
6	0.840815	-0.121878	-3.423260
7	-1.154096	-0.735872	-4.058517
1	-1.943867	-0.984898	-2.079744
6	0.081245	-0.352452	-4.533419
1	1.869944	0.194886	-3.348000
1	-1.962905	-0.977680	-4.607993
1	0.298276	-0.282169	-5.587105
6	0.791481	-3.124448	3.272088
1	-0.291284	-3.147176	3.120144
1	1.235779	-4.004398	2.798580
6	1.137286	-3.053830	4.749312
1	0.669325	-2.176718	5.203036
1	0.774131	-3.949442	5.265333
1	2.221378	-2.990560	4.888083
26	0.708602	-0.135990	-0.259461

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**W-<sup>3</sup>TS(C-D)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2835.6866358  
Zero-point correction=                    0.890068 (Hartree/Particle)  
Thermal correction to Energy=            0.947954  
Thermal correction to Enthalpy=         0.948898  
Thermal correction to Gibbs Free Energy= 0.795684  
Sum of electronic and zero-point Energies= -2834.801235  
Sum of electronic and thermal Energies= -2834.743349  
Sum of electronic and thermal Enthalpies= -2834.742405  
Sum of electronic and thermal Free Energies= -2834.895619

.....  
 Cartesian Coordinates  
 .....

6	3.650053	-3.178894	-0.830303
6	2.327836	-2.665568	-0.541958
7	2.306698	-1.303411	-0.621261
6	3.564988	-0.930492	-0.976134
6	4.427948	-2.090431	-1.110057
6	1.240341	-3.466843	-0.252903
6	-0.035154	-3.022027	0.054084
7	-0.434206	-1.719881	0.113555
6	-1.750092	-1.743968	0.476341
6	-2.199889	-3.104319	0.659962
6	-1.127969	-3.903686	0.386437
6	-2.560394	-0.626189	0.581048
6	-2.171768	0.664655	0.269707
7	-0.911067	1.033666	-0.098854
6	-0.959786	2.374440	-0.322628
6	-2.294667	2.880164	-0.107061
6	-3.054282	1.810840	0.260742
6	0.109968	3.183503	-0.668082
6	1.412580	2.761483	-0.841311
7	1.826889	1.463468	-0.809849
6	3.155289	1.484149	-1.117580
6	3.610794	2.836190	-1.337363
6	2.528589	3.643251	-1.142653
6	3.971306	0.371185	-1.216863
1	-0.086389	4.241080	-0.794501
1	5.003752	0.534126	-1.505910
1	1.399427	-4.540038	-0.253252
1	-3.586050	-0.779691	0.895609
6	-4.539788	1.781307	0.445366
1	-4.847886	0.945593	1.081833
1	-4.877313	2.695825	0.946182
6	-5.230867	1.670488	-0.935128
1	-4.940091	0.724933	-1.408540
1	-4.912909	2.497655	-1.572918
6	-6.727552	1.731424	-0.827451
8	-7.449377	2.641660	-1.140144
8	-7.234641	0.588994	-0.277551
1	-8.197510	0.698013	-0.217567
6	-3.592406	-3.542597	0.996181
1	-4.052740	-2.877654	1.734287
1	-3.552155	-4.530708	1.464844
6	-4.511260	-3.645200	-0.247010
1	-3.969123	-4.092964	-1.082446
1	-5.373249	-4.275285	-0.002684
6	-5.044458	-2.302585	-0.684097
8	-4.743578	-1.711497	-1.700458
8	-5.907993	-1.820823	0.218701

1	-6.272226	-0.965443	-0.088674
6	-1.035677	-5.397111	0.416329
1	-1.990521	-5.854416	0.690152
1	-0.745400	-5.800665	-0.560793
1	-0.287200	-5.733724	1.143912
6	-2.700153	4.311382	-0.259923
1	-2.527169	4.673606	-1.279969
1	-3.760318	4.455227	-0.031653
1	-2.122110	4.951373	0.417480
6	4.048098	-4.618845	-0.769360
1	3.556946	-5.132223	0.063873
1	3.783271	-5.154780	-1.689565
1	5.129669	-4.711537	-0.632830
6	5.024557	3.226247	-1.626637
1	5.673996	2.983178	-0.777341
1	5.418124	2.703085	-2.506027
1	5.109880	4.300953	-1.808145
6	5.850133	-2.032155	-1.445433
6	6.509957	-2.924335	-2.189705
1	6.405008	-1.184375	-1.044136
1	7.575010	-2.822435	-2.374498
1	6.008727	-3.769464	-2.652965
6	2.504406	5.107072	-1.200251
6	1.860696	5.906992	-0.345565
1	3.094348	5.561664	-1.996015
1	1.903085	6.986827	-0.454187
1	1.304728	5.510855	0.499943
6	1.216707	0.158984	1.663908
6	1.071325	1.540482	2.201500
6	0.684889	-0.913565	2.538858
6	-0.143647	2.083681	2.636592
6	2.203572	2.378113	2.248366
8	-0.332910	-0.872957	3.203175
8	1.493316	-1.998121	2.522022
6	-0.249843	3.412231	3.031497
1	-1.015814	1.440668	2.642594
6	2.105123	3.712667	2.631577
8	3.449297	1.936724	1.888820
6	0.874156	4.235390	3.010423
1	-1.212055	3.803013	3.349771
1	3.004740	4.319645	2.627132
6	3.684993	0.580125	2.105995
1	0.801270	5.277263	3.310962
1	3.769050	0.322319	3.167956
1	4.517745	0.246019	1.491472
1	2.531142	0.025322	1.692219
7	0.167239	-0.386963	-2.322646
6	-1.031054	-0.720112	-2.753323
6	0.964883	-0.248586	-3.431724
7	-1.037527	-0.801345	-4.100932

1	-1.899287	-0.910637	-2.138658
6	0.230504	-0.503040	-4.552877
1	2.005220	0.023110	-3.336343
1	-1.837095	-1.040207	-4.665301
1	0.483092	-0.499720	-5.600928
6	1.024998	-3.151252	3.220227
1	-0.055617	-3.242439	3.076522
1	1.522451	-3.990668	2.725653
6	1.377245	-3.090578	4.696577
1	0.855743	-2.256530	5.172544
1	1.078700	-4.019479	5.195053
1	2.455692	-2.957494	4.828951
26	0.709960	-0.116683	-0.283452

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**W-1CSSS<sup>TS</sup>(C-D)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3047.6562772  
Zero-point correction=                    0.856948 (Hartree/Particle)  
Thermal correction to Energy=            0.913370  
Thermal correction to Enthalpy=         0.914315  
Thermal correction to Gibbs Free Energy= 0.767098  
Sum of electronic and zero-point Energies= -3046.799329  
Sum of electronic and thermal Energies= -3046.742907  
Sum of electronic and thermal Enthalpies= -3046.741963  
Sum of electronic and thermal Free Energies= -3046.889180

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Cartesian Coordinates

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6	2.837535	1.314420	3.375408
6	1.969579	2.289501	2.893990
6	0.747406	1.938185	2.325318
6	0.366979	0.599768	2.257100
6	1.224753	-0.353266	2.812473
6	2.456523	-0.025711	3.348918
6	-0.858063	0.139609	1.565961
8	0.818289	-1.669850	2.769724
6	-0.538814	-1.778765	2.611480
26	-0.836760	-0.083056	-0.521854
7	-2.464796	1.092183	-0.679055
6	-2.480103	2.442317	-0.768722
6	-3.848639	2.936516	-0.826463
6	-4.655071	1.832151	-0.773038
6	-3.765335	0.691131	-0.695083
6	-1.350731	3.251736	-0.831579
6	-0.036266	2.819958	-0.806925
7	0.364255	1.530043	-0.660557
6	1.718766	1.551843	-0.659003
6	2.217461	2.910833	-0.827079

6	1.116213	3.705128	-0.907964
6	-4.195499	-0.628326	-0.656235
6	-3.385290	-1.751334	-0.584128
7	-2.032190	-1.724106	-0.454409
6	-1.626879	-3.021368	-0.391644
6	-2.760582	-3.916641	-0.442668
6	-3.867849	-3.127222	-0.586858
6	2.525278	0.439235	-0.475542
6	2.083843	-0.865123	-0.319221
7	0.789076	-1.268661	-0.361709
6	0.811548	-2.626928	-0.264313
6	2.174897	-3.107566	-0.115296
6	2.967829	-2.003001	-0.135013
6	-0.304915	-3.447287	-0.286496
6	-2.137398	0.602623	2.150629
8	-3.031882	-0.382502	2.342864
8	-2.364310	1.771159	2.381860
1	-0.134306	-4.518717	-0.223982
1	-5.265836	-0.798272	-0.686768
1	-1.513769	4.319679	-0.941197
1	3.595742	0.597096	-0.480679
1	0.089320	2.690997	1.908739
1	2.248549	3.338524	2.938839
1	3.099465	-0.811401	3.730808
1	3.814770	1.587016	3.759076
1	-1.130477	-1.490911	3.482344
1	-0.874719	-1.145360	1.574522
1	-0.803570	-2.752458	2.197405
6	0.848436	-0.506862	-3.436203
1	1.272057	-1.427912	-3.016558
1	0.877570	-0.587364	-4.529788
1	1.496432	0.327093	-3.140705
16	-0.874765	-0.243667	-2.900632
6	1.025184	5.188792	-1.083123
1	2.015010	5.654833	-1.114688
1	0.504030	5.448905	-2.012524
1	0.468558	5.652880	-0.259199
6	2.562812	-4.544050	0.041017
1	2.253410	-5.137268	-0.828420
1	3.646284	-4.658921	0.149485
1	2.090253	-4.992004	0.924108
6	-2.678739	-5.410903	-0.414213
1	-2.123019	-5.768375	0.461945
1	-3.673545	-5.866444	-0.389341
1	-2.164027	-5.796392	-1.303152
6	-6.149454	1.766618	-0.746487
1	-6.571320	1.607711	-1.747771
1	-6.502590	0.945366	-0.112191
1	-6.569027	2.700607	-0.357240
6	-4.222791	4.345636	-0.878162



6	-5.300472	4.860047	-1.481974
1	-3.550322	5.033418	-0.364903
1	-5.508931	5.925775	-1.443655
1	-5.989146	4.244492	-2.053482
6	-5.248002	-3.594221	-0.719225
6	-6.197278	-3.080514	-1.509238
1	-5.506461	-4.470286	-0.121575
1	-7.196817	-3.506340	-1.530475
1	-6.000422	-2.244416	-2.173583
6	4.455575	-1.916665	0.000739
6	5.151211	-1.766703	-1.375957
1	4.839132	-2.819626	0.490350
1	4.735848	-1.068342	0.636893
1	4.861802	-2.596635	-2.024562
1	4.841048	-0.828216	-1.843001
6	3.660575	3.313356	-0.936360
6	4.496284	3.151805	0.357685
1	3.701131	4.363915	-1.241415
1	4.144469	2.750833	-1.741580
1	5.183106	4.003739	0.455236
1	3.857670	3.148646	1.242106
6	6.638813	-1.750291	-1.194945
8	7.311899	-0.789462	-0.863824
8	7.210252	-2.950829	-1.373303
1	8.153836	-2.833455	-1.175088
6	5.378588	1.924357	0.449405
8	5.632661	1.338039	1.480528
8	5.904158	1.575119	-0.731628
1	6.458398	0.767999	-0.615135
6	-4.356176	0.038362	2.679782
6	-5.221993	-1.203596	2.722038
1	-4.699575	0.746517	1.920325
1	-4.334821	0.557689	3.644276
1	-6.253164	-0.930436	2.971285
1	-5.214094	-1.703422	1.749414
1	-4.857386	-1.907715	3.477421

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**W-<sup>10SS</sup>TS(C-D) Fe(his)**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3047.667639  
Zero-point correction=                    0.853726 (Hartree/Particle)  
Thermal correction to Energy=            0.910506  
Thermal correction to Enthalpy=         0.911450  
Thermal correction to Gibbs Free Energy= 0.763415  
Sum of electronic and zero-point Energies= -3046.813913  
Sum of electronic and thermal Energies= -3046.757133  
Sum of electronic and thermal Enthalpies= -3046.756189  
Sum of electronic and thermal Free Energies= -3046.904224

Cartesian Coordinates

6	2.893530	1.209769	3.285518
6	1.975238	2.185974	2.904511
6	0.743329	1.819527	2.372858
6	0.379692	0.476738	2.218844
6	1.287056	-0.486147	2.702876
6	2.537095	-0.131069	3.198942
6	-0.868033	0.036696	1.543124
8	0.998083	-1.828776	2.674332
6	-0.354071	-2.139495	2.737158
26	-0.850694	-0.092395	-0.524793
7	-2.498563	1.065127	-0.654205
6	-2.519723	2.417152	-0.686954
6	-3.886998	2.904480	-0.747892
6	-4.688817	1.795156	-0.759454
6	-3.798293	0.658208	-0.708985
6	-1.399426	3.239486	-0.709643
6	-0.085002	2.817161	-0.710377
7	0.336731	1.526780	-0.630527
6	1.692752	1.568788	-0.642801
6	2.166773	2.938182	-0.762051
6	1.053775	3.718956	-0.787752
6	-4.221078	-0.659198	-0.710558
6	-3.395349	-1.767698	-0.626624
7	-2.043560	-1.721450	-0.493553
6	-1.619603	-3.009376	-0.408210
6	-2.739660	-3.917877	-0.449214
6	-3.856708	-3.145648	-0.612038
6	2.519019	0.468553	-0.511196
6	2.082527	-0.837772	-0.373675
7	0.790086	-1.244090	-0.415175
6	0.812567	-2.601172	-0.304053
6	2.176279	-3.075740	-0.154890
6	2.967542	-1.971080	-0.186353
6	-0.295605	-3.424506	-0.311330
6	-2.101521	0.609771	2.107088
8	-3.084693	-0.322676	2.217541
8	-2.288214	1.763148	2.453845
1	-0.119463	-4.493146	-0.229554
1	-5.288175	-0.840566	-0.759485
1	-1.572074	4.309124	-0.766812
1	3.586569	0.638565	-0.518264
1	0.039523	2.575444	2.044401
1	2.223478	3.240408	3.000765
1	3.212595	-0.919978	3.515834
1	3.881002	1.484443	3.643760
1	-0.812986	-1.916068	3.707135
1	-0.901381	-1.204388	1.865887
1	-0.527651	-3.144850	2.362079

6	0.815395	-0.145790	-3.451890
1	1.422571	-0.953590	-3.028599
1	0.816750	-0.245707	-4.543114
1	1.286071	0.808473	-3.191157
16	-0.903468	-0.223953	-2.863241
6	0.940138	5.208226	-0.879356
1	1.923376	5.687369	-0.907231
1	0.394119	5.513371	-1.780241
1	0.398636	5.615591	-0.016795
6	2.563679	-4.506554	0.042704
1	2.207259	-5.135906	-0.781801
1	3.650386	-4.623685	0.101536
1	2.133944	-4.905254	0.969750
6	-2.641209	-5.409653	-0.381181
1	-2.115851	-5.736705	0.524697
1	-3.631765	-5.874542	-0.381578
1	-2.090042	-5.812071	-1.240204
6	-6.182780	1.720729	-0.753570
1	-6.590485	1.570365	-1.761798
1	-6.536756	0.891627	-0.130656
1	-6.611129	2.648021	-0.359041
6	-4.268308	4.313380	-0.740123
6	-5.323490	4.848269	-1.364290
1	-3.626331	4.975836	-0.159492
1	-5.547340	5.908053	-1.279492
1	-5.979544	4.255274	-1.995221
6	-5.233157	-3.627461	-0.736605
6	-6.172642	-3.152717	-1.561062
1	-5.494493	-4.475027	-0.101129
1	-7.171558	-3.579920	-1.575789
1	-5.969079	-2.344775	-2.257852
6	4.452754	-1.874498	-0.029340
6	5.167676	-1.710155	-1.394049
1	4.835330	-2.776630	0.460753
1	4.712905	-1.028117	0.617731
1	4.904406	-2.549690	-2.042880
1	4.849724	-0.780228	-1.871505
6	3.604664	3.359866	-0.871063
6	4.460414	3.115774	0.395818
1	3.631741	4.427729	-1.109546
1	4.074405	2.853437	-1.720459
1	5.091935	3.993198	0.589469
1	3.830270	2.976349	1.276017
6	6.653900	-1.669519	-1.199661
8	7.333791	-0.673099	-1.028650
8	7.213859	-2.888428	-1.175014
1	8.155341	-2.750747	-0.980523
6	5.416149	1.941079	0.361597
8	5.778390	1.331692	1.345379
8	5.867620	1.661091	-0.868911

1	6.466575	0.879677	-0.815121
6	-4.353592	0.163246	2.631530
6	-5.297929	-1.022864	2.673143
1	-4.696932	0.926469	1.924287
1	-4.263848	0.642012	3.613478
1	-6.298164	-0.699746	2.983913
1	-5.368342	-1.491213	1.686981
1	-4.939225	-1.776021	3.382554

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**W-<sup>3</sup>TS(C-D)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3047.6628451  
Zero-point correction=                    0.853385 (Hartree/Particle)  
Thermal correction to Energy=            0.910306  
Thermal correction to Enthalpy=         0.911250  
Thermal correction to Gibbs Free Energy= 0.761755  
Sum of electronic and zero-point Energies= -3046.809460  
Sum of electronic and thermal Energies= -3046.752539  
Sum of electronic and thermal Enthalpies= -3046.751595  
Sum of electronic and thermal Free Energies= -3046.901090

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Cartesian Coordinates

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6	2.923589	1.150956	3.257636
6	1.998860	2.132573	2.906924
6	0.755869	1.773233	2.396432
6	0.387053	0.432286	2.232170
6	1.303437	-0.538702	2.686748
6	2.563310	-0.188497	3.162288
6	-0.868964	-0.001463	1.575576
8	1.015859	-1.880211	2.652768
6	-0.340671	-2.198130	2.731334
26	-0.854581	-0.086453	-0.558900
7	-2.496290	1.073143	-0.647625
6	-2.518413	2.425604	-0.660444
6	-3.885978	2.912887	-0.708543
6	-4.688101	1.804438	-0.733980
6	-3.798891	0.666203	-0.703223
6	-1.400327	3.250627	-0.679311
6	-0.086797	2.825874	-0.689068
7	0.331166	1.534099	-0.627237
6	1.689843	1.574942	-0.640761
6	2.165200	2.945160	-0.746088
6	1.053592	3.727334	-0.758402
6	-4.225402	-0.647344	-0.721110
6	-3.401784	-1.760524	-0.649119
7	-2.051487	-1.714929	-0.520637
6	-1.628112	-3.003270	-0.436591
6	-2.748103	-3.910829	-0.475984

6	-3.865348	-3.137175	-0.635719
6	2.514766	0.475887	-0.521042
6	2.076009	-0.832780	-0.389765
7	0.784705	-1.236549	-0.436995
6	0.804233	-2.595186	-0.324673
6	2.165935	-3.070054	-0.168020
6	2.958789	-1.966034	-0.197947
6	-0.303797	-3.416864	-0.337148
6	-2.094281	0.588889	2.127659
8	-3.095154	-0.330202	2.217468
8	-2.272468	1.742305	2.483285
1	-0.127682	-4.485441	-0.253748
1	-5.293221	-0.824510	-0.768263
1	-1.573846	4.320639	-0.721441
1	3.582424	0.644851	-0.526198
1	0.046143	2.533497	2.091292
1	2.250155	3.185726	3.010552
1	3.243788	-0.981698	3.457646
1	3.918327	1.420187	3.599929
1	-0.766023	-2.021449	3.727045
1	-0.899066	-1.274284	1.925779
1	-0.505608	-3.201150	2.343790
6	0.784094	0.063748	-3.475065
1	1.510185	-0.638821	-3.051784
1	0.790645	-0.043702	-4.565361
1	1.103650	1.080367	-3.222914
16	-0.895401	-0.277978	-2.869829
6	0.940977	5.217683	-0.829429
1	1.924459	5.696298	-0.856351
1	0.389927	5.535534	-1.722863
1	0.404594	5.613242	0.041728
6	2.550865	-4.499650	0.041967
1	2.186405	-5.137486	-0.772343
1	3.637636	-4.619054	0.093819
1	2.127179	-4.885120	0.977327
6	-2.651030	-5.402641	-0.406508
1	-2.126877	-5.729005	0.500285
1	-3.642002	-5.866606	-0.407079
1	-2.099652	-5.806665	-1.264631
6	-6.182025	1.730707	-0.721001
1	-6.594796	1.587201	-1.728110
1	-6.532710	0.897590	-0.101648
1	-6.607632	2.655455	-0.317884
6	-4.267031	4.321705	-0.676910
6	-5.321233	4.866476	-1.293943
1	-3.626038	4.973733	-0.083629
1	-5.546100	5.924482	-1.191627
1	-5.975963	4.283459	-1.935547
6	-5.242825	-3.616544	-0.755781
6	-6.186492	-3.135650	-1.571962

1	-5.501876	-4.467364	-0.123778
1	-7.186157	-3.561149	-1.583213
1	-5.986083	-2.323829	-2.265193
6	4.442555	-1.869469	-0.027167
6	5.170413	-1.704209	-1.384679
1	4.820650	-2.771493	0.466198
1	4.695411	-1.023393	0.623234
1	4.915959	-2.546504	-2.033928
1	4.854306	-0.776919	-1.868212
6	3.603724	3.364726	-0.855296
6	4.463784	3.098376	0.404001
1	3.632985	4.435752	-1.078810
1	4.067342	2.868726	-1.714135
1	5.085245	3.977331	0.621237
1	3.836100	2.928969	1.280780
6	6.655448	-1.659325	-1.180924
8	7.339599	-0.658983	-1.056520
8	7.209097	-2.878228	-1.093675
1	8.149732	-2.735913	-0.898636
6	5.431769	1.934983	0.340624
8	5.814491	1.318474	1.312214
8	5.867517	1.671977	-0.899272
1	6.473186	0.894774	-0.860260
6	-4.357660	0.170307	2.630426
6	-5.320358	-1.001680	2.655934
1	-4.687594	0.946431	1.930638
1	-4.266416	0.637624	3.617860
1	-6.317189	-0.666852	2.965523
1	-5.393448	-1.459712	1.665050
1	-4.976074	-1.767250	3.359169

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**W-<sup>1</sup>CSSS\*TS(C-D)<sub>Fe</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2609.5220952  
Zero-point correction=                    0.816893 (Hartree/Particle)  
Thermal correction to Energy=            0.870382  
Thermal correction to Enthalpy=         0.871326  
Thermal correction to Gibbs Free Energy= 0.727229  
Sum of electronic and zero-point Energies= -2608.705202  
Sum of electronic and thermal Energies= -2608.651714  
Sum of electronic and thermal Enthalpies= -2608.650769  
Sum of electronic and thermal Free Energies= -2608.794866

.....  
Cartesian Coordinates

.....  
6        3.523039   -3.268377   -1.318352  
6        2.218931   -2.729475   -0.997993  
7        2.227748   -1.362450   -1.052084

6	3.497173	-1.013352	-1.414893
6	4.324436	-2.194487	-1.591576
6	1.115325	-3.508466	-0.696353
6	-0.158468	-3.035742	-0.424249
7	-0.525977	-1.721368	-0.408337
6	-1.847269	-1.706257	-0.060279
6	-2.334348	-3.051472	0.155270
6	-1.278653	-3.883296	-0.085528
6	-2.614440	-0.561473	0.068996
6	-2.169932	0.730399	-0.151498
7	-0.882700	1.080331	-0.446220
6	-0.881109	2.440528	-0.557363
6	-2.208373	2.973971	-0.342141
6	-3.013722	1.906184	-0.085540
6	0.229178	3.231337	-0.798628
6	1.515580	2.767772	-1.009345
7	1.859950	1.450414	-1.094975
6	3.188712	1.429053	-1.408164
6	3.713402	2.767675	-1.516829
6	2.674268	3.611873	-1.241465
6	3.950911	0.283931	-1.577907
1	0.078318	4.303600	-0.836077
1	4.987749	0.420228	-1.866103
1	1.253322	-4.584783	-0.689111
1	-3.648896	-0.686579	0.366126
6	-4.500602	1.901328	0.094412
1	-4.812872	1.090871	0.761054
1	-4.821219	2.834398	0.571646
6	-5.208097	1.756506	-1.271603
1	-4.952424	0.787362	-1.718006
1	-4.880586	2.546286	-1.950522
6	-6.704267	1.843683	-1.170510
8	-7.427854	2.650293	-1.693101
8	-7.217252	0.863514	-0.366659
1	-8.181787	0.975428	-0.368217
6	-3.725539	-3.441562	0.559274
1	-4.099893	-2.780249	1.347582
1	-3.691612	-4.442939	0.999419
6	-4.743895	-3.471045	-0.605158
1	-4.284221	-3.860719	-1.515435
1	-5.575840	-4.129028	-0.326960
6	-5.349590	-2.124595	-0.924180
8	-5.317482	-1.572267	-2.000618
8	-5.963731	-1.598506	0.149057
1	-6.376302	-0.748961	-0.113451
6	-1.219061	-5.377417	-0.017905
1	-2.179743	-5.807126	0.278522
1	-0.952085	-5.808911	-0.989697
1	-0.467312	-5.715614	0.705899
6	-2.564029	4.425288	-0.409225

1	-2.376666	4.836882	-1.407724
1	-3.619740	4.590817	-0.175992
1	-1.968446	5.010851	0.301517
6	3.883491	-4.719523	-1.301921
1	3.385294	-5.245598	-0.480610
1	3.596320	-5.220361	-2.234899
1	4.963327	-4.845475	-1.178514
6	5.140451	3.109492	-1.805619
1	5.800958	2.737916	-1.013051
1	5.476799	2.666534	-2.750327
1	5.284357	4.191222	-1.871623
6	5.740362	-2.170787	-1.957443
6	6.359345	-3.069013	-2.728956
1	6.328111	-1.343790	-1.559448
1	7.422015	-2.991144	-2.937495
1	5.825656	-3.891942	-3.195535
6	2.728674	5.074428	-1.179922
6	2.117952	5.839050	-0.270326
1	3.349753	5.559169	-1.932939
1	2.216011	6.920381	-0.294150
1	1.527983	5.409434	0.534564
6	1.137947	0.021040	1.499913
6	1.234924	1.358337	2.096716
6	0.612677	-1.084192	2.318782
6	0.081738	2.054136	2.473663
6	2.468688	2.023677	2.167798
8	-0.516179	-1.015519	2.761496
8	1.408051	-2.154466	2.385436
6	0.164892	3.377818	2.896409
1	-0.876477	1.552188	2.404357
6	2.555791	3.339939	2.589384
8	3.616424	1.377291	1.787446
6	1.395808	4.022696	2.948792
1	-0.742021	3.899897	3.184807
1	3.530723	3.813378	2.626259
6	3.541966	-0.003987	1.866499
1	1.462990	5.054758	3.279307
1	3.521455	-0.381989	2.894386
1	4.343648	-0.443385	1.271782
1	2.592648	-0.367854	1.310359
6	0.814903	-3.355207	2.911225
1	-0.220724	-3.410004	2.566013
1	1.389747	-4.158737	2.445937
6	0.903985	-3.398266	4.424977
1	0.310519	-2.592591	4.864704
1	0.516079	-4.353985	4.792699
1	1.942401	-3.297575	4.755583
26	0.705185	-0.129092	-0.574509

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W-<sup>10</sup>STS(C-D)<sub>Fe</sub>



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Number of imaginary frequencies: 1	Electronic energy:	HF=-2609.5261606
Zero-point correction=	0.815680 (Hartree/Particle)	
Thermal correction to Energy=	0.868501	
Thermal correction to Enthalpy=	0.869446	
Thermal correction to Gibbs Free Energy=	0.729096	
Sum of electronic and zero-point Energies=	-2608.710480	
Sum of electronic and thermal Energies=	-2608.657659	
Sum of electronic and thermal Enthalpies=	-2608.656715	
Sum of electronic and thermal Free Energies=	-2608.797065	

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Cartesian Coordinates

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6	3.617337	-3.228950	-1.236606
6	2.294691	-2.717997	-0.974040
7	2.279494	-1.345276	-0.986243
6	3.568475	-0.975173	-1.258201
6	4.418717	-2.136223	-1.420155
6	1.196903	-3.520872	-0.741852
6	-0.071295	-3.060818	-0.449631
7	-0.431284	-1.743473	-0.371897
6	-1.750910	-1.753065	-0.010263
6	-2.230027	-3.105383	0.172733
6	-1.182081	-3.923787	-0.127089
6	-2.536464	-0.624635	0.107500
6	-2.123247	0.661123	-0.184429
7	-0.845889	1.023331	-0.524926
6	-0.884393	2.383945	-0.674055
6	-2.217202	2.890796	-0.471909
6	-2.991882	1.814967	-0.158259
6	0.206570	3.200182	-0.900954
6	1.507392	2.761599	-1.021409
7	1.880323	1.445967	-1.025231
6	3.223941	1.452058	-1.277376
6	3.722864	2.798989	-1.414154
6	2.654300	3.625676	-1.228676
6	4.014069	0.325713	-1.394211
1	0.029907	4.266185	-0.976179
1	5.062053	0.476144	-1.629541
1	1.343278	-4.595179	-0.775325
1	-3.564292	-0.760702	0.421876
6	-4.474296	1.792442	0.054094
1	-4.763585	0.981760	0.730048
1	-4.793747	2.723348	0.536148
6	-5.208030	1.636752	-1.296526
1	-4.950888	0.668993	-1.745001
1	-4.904302	2.428500	-1.984186
6	-6.702795	1.707160	-1.163812
8	-7.446341	2.502493	-1.675185

8	-7.185747	0.724391	-0.345261
1	-8.151451	0.823837	-0.324218
6	-3.608688	-3.514603	0.598769
1	-3.982594	-2.854361	1.388018
1	-3.549768	-4.511763	1.045852
6	-4.641594	-3.571638	-0.551368
1	-4.189833	-3.972224	-1.460911
1	-5.464608	-4.230885	-0.251249
6	-5.257871	-2.233258	-0.882050
8	-5.222790	-1.686215	-1.961274
8	-5.881351	-1.706931	0.185231
1	-6.307451	-0.866152	-0.083567
6	-1.118080	-5.418793	-0.118742
1	-0.833957	-5.811070	-1.102099
1	-0.378597	-5.782832	0.605133
1	-2.083008	-5.860906	0.143537
6	-2.605065	4.331579	-0.573447
1	-2.383057	4.738457	-1.566484
1	-3.673891	4.472547	-0.389760
1	-2.056774	4.935804	0.159573
6	3.996445	-4.675479	-1.247349
1	3.478287	-5.229938	-0.457858
1	3.749238	-5.153767	-2.203256
1	5.072662	-4.790030	-1.088597
6	5.154799	3.162679	-1.641343
1	5.776922	2.842042	-0.797262
1	5.552910	2.688628	-2.546029
1	5.276549	4.243926	-1.746172
6	5.855048	-2.083370	-1.694071
6	6.524711	-2.933698	-2.476893
1	6.410544	-1.279870	-1.211074
1	7.597596	-2.842133	-2.615560
1	6.024277	-3.730363	-3.019899
6	2.663917	5.091075	-1.224395
6	1.999142	5.867416	-0.364225
1	3.295871	5.566094	-1.974380
1	2.065806	6.949709	-0.423513
1	1.396652	5.448103	0.437268
6	1.126295	0.062357	1.374349
6	0.989410	1.420797	1.966214
6	0.570530	-1.061287	2.178361
6	-0.238101	1.971339	2.353318
6	2.132383	2.226728	2.112394
8	-0.461102	-1.031430	2.817359
8	1.371678	-2.142994	2.120964
6	-0.332360	3.276662	2.818714
1	-1.125367	1.354987	2.268528
6	2.048566	3.540258	2.562579
8	3.381243	1.769641	1.773124
6	0.811329	4.068697	2.909240

1	-1.300720	3.676008	3.104642
1	2.959587	4.125049	2.633720
6	3.578735	0.414329	1.928731
1	0.745038	5.092963	3.265200
1	3.534440	0.065367	2.965061
1	4.428923	0.075804	1.343465
1	2.385702	-0.104069	1.378189
6	0.885887	-3.329920	2.755410
1	-0.190302	-3.411102	2.579371
1	1.395459	-4.143644	2.232780
6	1.204145	-3.336123	4.240041
1	0.672634	-2.524881	4.743622
1	0.892345	-4.286388	4.686761
1	2.279498	-3.213811	4.403923
26	0.763286	-0.133274	-0.515074

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**W-<sup>3</sup>TS(C-D)<sub>Fe</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2609.5256022  
Zero-point correction=                    0.819583 (Hartree/Particle)  
Thermal correction to Energy=            0.871791  
Thermal correction to Enthalpy=         0.872735  
Thermal correction to Gibbs Free Energy= 0.734230  
Sum of electronic and zero-point Energies= -2608.706020  
Sum of electronic and thermal Energies= -2608.653811  
Sum of electronic and thermal Enthalpies= -2608.652867  
Sum of electronic and thermal Free Energies= -2608.791372

.....  
Cartesian Coordinates

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6	3.570455	-3.236820	-1.305048
6	2.262710	-2.711920	-0.982309
7	2.262414	-1.342123	-1.004746
6	3.535824	-0.980295	-1.350073
6	4.370486	-2.152680	-1.543746
6	1.160152	-3.500727	-0.702566
6	-0.108992	-3.036630	-0.402897
7	-0.472691	-1.721938	-0.338984
6	-1.792584	-1.722201	0.013790
6	-2.275826	-3.076564	0.204031
6	-1.225396	-3.898346	-0.075860
6	-2.573342	-0.586809	0.134223
6	-2.156131	0.706622	-0.134358
7	-0.877338	1.067169	-0.449655
6	-0.903255	2.423289	-0.605959
6	-2.239703	2.940371	-0.412530
6	-3.023271	1.868110	-0.110585
6	0.200412	3.225482	-0.840809
6	1.499742	2.779068	-0.995059
7	1.865700	1.464063	-1.035525

6	3.199286	1.460631	-1.332057
6	3.706725	2.807509	-1.457427
6	2.650780	3.639182	-1.220445
6	3.978342	0.324908	-1.488188
1	0.033721	4.293982	-0.912336
1	5.017116	0.474804	-1.763282
1	1.298651	-4.576895	-0.729096
1	-3.605198	-0.723318	0.436988
6	-4.509678	1.846362	0.072921
1	-4.810897	1.038114	0.747100
1	-4.841479	2.779575	0.542540
6	-5.217425	1.680864	-1.290507
1	-4.948647	0.711446	-1.728476
1	-4.901871	2.469215	-1.976719
6	-6.714467	1.747211	-1.188948
8	-7.451105	2.533984	-1.723655
8	-7.211831	0.771953	-0.369423
1	-8.178006	0.868306	-0.372639
6	-3.661293	-3.480980	0.612871
1	-4.043137	-2.820165	1.397998
1	-3.614054	-4.479697	1.058301
6	-4.680582	-3.530578	-0.549833
1	-4.218171	-3.927244	-1.455708
1	-5.508114	-4.190680	-0.263599
6	-5.293946	-2.191428	-0.883077
8	-5.258527	-1.646979	-1.963524
8	-5.920231	-1.662609	0.181719
1	-6.340632	-0.820178	-0.090755
6	-1.163616	-5.393648	-0.057296
1	-2.121597	-5.833528	0.233449
1	-0.905100	-5.793732	-1.044801
1	-0.405271	-5.755263	0.648411
6	-2.624522	4.380733	-0.536258
1	-2.437576	4.759180	-1.547917
1	-3.685394	4.532904	-0.317191
1	-2.047599	5.005661	0.156341
6	3.937607	-4.686533	-1.322662
1	3.428486	-5.237560	-0.524745
1	3.668486	-5.162969	-2.273680
1	5.015888	-4.811607	-1.184770
6	5.132207	3.164374	-1.735857
1	5.793727	2.797578	-0.941721
1	5.478420	2.726878	-2.679747
1	5.265447	4.247691	-1.798961
6	5.789307	-2.113695	-1.896550
6	6.422608	-2.994509	-2.676628
1	6.367351	-1.288470	-1.480857
1	7.486410	-2.904471	-2.874323
1	5.900102	-3.814219	-3.161092
6	2.678175	5.103142	-1.181916

6	2.030735	5.869542	-0.299303
1	3.309723	5.588754	-1.925633
1	2.109639	6.952093	-0.335781
1	1.426345	5.440751	0.495563
6	1.167630	0.063008	1.413426
6	1.124204	1.421444	2.010432
6	0.632742	-1.053899	2.236080
6	-0.045322	2.089811	2.360370
6	2.338267	2.086868	2.183342
8	-0.431782	-0.988623	2.807165
8	1.430940	-2.131810	2.222167
6	0.021058	3.395092	2.844925
1	-0.998318	1.588189	2.241980
6	2.428892	3.385885	2.642574
8	3.469763	1.381613	1.815578
6	1.245233	4.044922	2.973462
1	-0.897053	3.906317	3.116644
1	3.398730	3.860619	2.738578
6	3.244315	0.043475	1.865658
1	1.287601	5.064976	3.342773
1	3.078535	-0.378532	2.856984
1	3.968081	-0.505011	1.260375
1	2.293207	-0.239460	1.009693
6	0.892611	-3.332997	2.798431
1	-0.170640	-3.389133	2.552289
1	1.421448	-4.136003	2.280604
6	1.124234	-3.376826	4.297180
1	0.575738	-2.570712	4.791068
1	0.771857	-4.332098	4.700090
1	2.189820	-3.278998	4.528482
26	0.723750	-0.119478	-0.546925

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**1CSSS<sup>+</sup>TS(C-D)<sub>Fe</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2610.2775955  
 Zero-point correction=                    0.807751 (Hartree/Particle)  
 Thermal correction to Energy=            0.861551  
 Thermal correction to Enthalpy=         0.862495  
 Thermal correction to Gibbs Free Energy= 0.718544  
 Sum of electronic and zero-point Energies= -2609.469844  
 Sum of electronic and thermal Energies= -2609.416045  
 Sum of electronic and thermal Enthalpies= -2609.415101  
 Sum of electronic and thermal Free Energies= -2609.559052

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 Cartesian Coordinates  
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6	3.523516	-3.254025	-1.432751
6	2.238254	-2.722375	-1.034162
7	2.249962	-1.344155	-1.028091

6	3.515079	-0.986913	-1.432735
6	4.331067	-2.166788	-1.690377
6	1.132037	-3.505482	-0.726846
6	-0.129843	-3.037747	-0.390112
7	-0.483603	-1.713045	-0.287858
6	-1.815716	-1.713448	0.048009
6	-2.314774	-3.073754	0.189726
6	-1.260578	-3.900121	-0.098564
6	-2.595980	-0.571357	0.170405
6	-2.174184	0.727257	-0.088496
7	-0.881059	1.089057	-0.381220
6	-0.911763	2.449624	-0.572796
6	-2.258655	2.964756	-0.416498
6	-3.049068	1.889625	-0.109132
6	0.188985	3.247645	-0.853977
6	1.488799	2.800662	-1.045595
7	1.860026	1.479441	-1.044350
6	3.179397	1.465563	-1.434634
6	3.666919	2.807897	-1.668904
6	2.619463	3.655445	-1.396914
6	3.949901	0.321528	-1.605460
1	0.014009	4.310194	-0.968689
1	4.968775	0.466134	-1.946836
1	1.257039	-4.581215	-0.785309
1	-3.635602	-0.709841	0.442500
6	-4.540891	1.878563	0.068043
1	-4.850940	1.069196	0.737027
1	-4.862718	2.812251	0.545471
6	-5.282883	1.733328	-1.291770
1	-5.035383	0.767300	-1.747274
1	-4.975162	2.529264	-1.973220
6	-6.779357	1.827902	-1.143117
8	-7.504352	2.705666	-1.544358
8	-7.292379	0.761847	-0.437241
1	-8.257135	0.902008	-0.386384
6	-3.708933	-3.490865	0.571336
1	-4.118977	-2.828554	1.341213
1	-3.656285	-4.484565	1.029424
6	-4.725039	-3.578394	-0.605206
1	-4.250571	-3.984971	-1.500828
1	-5.539875	-4.250142	-0.307262
6	-5.359120	-2.252742	-0.968757
8	-5.271919	-1.693591	-2.043328
8	-6.062703	-1.748055	0.070593
1	-6.474060	-0.899910	-0.211918
6	-1.226193	-5.399493	-0.140479
1	-2.157264	-5.834249	0.235589
1	-1.083132	-5.773414	-1.163097
1	-0.406525	-5.806535	0.465330
6	-2.657408	4.400407	-0.587884

1	-2.533890	4.736126	-1.625892
1	-3.705124	4.561047	-0.315518
1	-2.049083	5.066429	0.036975
6	3.875523	-4.708902	-1.506426
1	3.328359	-5.295858	-0.760796
1	3.646412	-5.141835	-2.490289
1	4.946159	-4.856965	-1.330613
6	5.063415	3.158207	-2.086858
1	5.799646	2.863276	-1.327231
1	5.345521	2.655218	-3.020683
1	5.174641	4.234946	-2.243071
6	5.728174	-2.124169	-2.110497
6	6.383546	-3.042872	-2.838003
1	6.289387	-1.244509	-1.794709
1	7.435422	-2.915414	-3.077343
1	5.898922	-3.927621	-3.238204
6	2.648868	5.116366	-1.456863
6	2.016972	5.967996	-0.634626
1	3.282980	5.540954	-2.235974
1	2.112488	7.042456	-0.764176
1	1.415530	5.626779	0.202846
6	1.242673	0.055576	1.509919
6	1.227240	1.405140	2.144560
6	0.685066	-1.050632	2.341506
6	0.077557	2.086454	2.554570
6	2.461967	2.027126	2.381504
8	-0.365753	-0.962342	2.944392
8	1.473219	-2.152386	2.343206
6	0.183575	3.341209	3.163844
1	-0.890695	1.627246	2.402161
6	2.594548	3.274567	2.966934
8	3.583864	1.321955	1.941929
6	1.428844	3.939553	3.360988
1	-0.719569	3.851324	3.486307
1	3.580690	3.700323	3.119196
6	3.355151	-0.011838	1.952236
1	1.501363	4.915215	3.832710
1	3.178619	-0.478366	2.919833
1	4.021572	-0.550450	1.279643
1	2.260008	-0.242772	1.004828
6	0.958062	-3.314776	3.038716
1	-0.120659	-3.365401	2.877844
1	1.438354	-4.158357	2.537842
6	1.299624	-3.272110	4.520716
1	0.802966	-2.427316	5.006133
1	0.961641	-4.194742	5.006928
1	2.381341	-3.184867	4.671695
26	0.728487	-0.106354	-0.487098

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<sup>10</sup>SS<sup>TS(C-D)</sup><sub>Fe</sub>

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Number of imaginary frequencies: 1	Electronic energy:	HF=-2610.2859227
Zero-point correction=	0.804937 (Hartree/Particle)	
Thermal correction to Energy=	0.858994	
Thermal correction to Enthalpy=	0.859938	
Thermal correction to Gibbs Free Energy=	0.715324	
Sum of electronic and zero-point Energies=	-2609.480985	
Sum of electronic and thermal Energies=	-2609.426928	
Sum of electronic and thermal Enthalpies=	-2609.425984	
Sum of electronic and thermal Free Energies=	-2609.570599	

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Cartesian Coordinates

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6	3.534460	-3.257397	-1.395760
6	2.240246	-2.732047	-1.028691
7	2.240864	-1.351677	-1.026565
6	3.517459	-0.992229	-1.391833
6	4.342197	-2.166444	-1.631378
6	1.141352	-3.523821	-0.733978
6	-0.116489	-3.055411	-0.395168
7	-0.466779	-1.728151	-0.299550
6	-1.797021	-1.729672	0.048835
6	-2.292769	-3.086308	0.206751
6	-1.241411	-3.914344	-0.087781
6	-2.579316	-0.591085	0.156221
6	-2.158187	0.699485	-0.130708
7	-0.865525	1.059745	-0.442674
6	-0.902067	2.424333	-0.628691
6	-2.245882	2.933301	-0.472179
6	-3.032600	1.856643	-0.156677
6	0.193687	3.231293	-0.891361
6	1.494653	2.786175	-1.051009
7	1.863808	1.462831	-1.038926
6	3.191526	1.451645	-1.397361
6	3.683450	2.792968	-1.620595
6	2.630381	3.639937	-1.373629
6	3.961932	0.310440	-1.558583
1	0.016874	4.293686	-1.001298
1	4.987895	0.451180	-1.878470
1	1.272706	-4.598592	-0.786049
1	-3.616093	-0.724813	0.439322
6	-4.522923	1.845327	0.032636
1	-4.827085	1.041359	0.710385
1	-4.840105	2.782280	0.506167
6	-5.274319	1.689784	-1.320559
1	-5.032229	0.719155	-1.769286
1	-4.970584	2.479106	-2.011443
6	-6.769912	1.788227	-1.161915
8	-7.495979	2.661426	-1.570313
8	-7.278161	0.731945	-0.438721



1	-8.242492	0.872959	-0.381353
6	-3.681342	-3.500294	0.610716
1	-4.083261	-2.826915	1.375066
1	-3.619728	-4.485989	1.084290
6	-4.709906	-3.609512	-0.553029
1	-4.245624	-4.034550	-1.445436
1	-5.522411	-4.273351	-0.232642
6	-5.342942	-2.288442	-0.934590
8	-5.250973	-1.741636	-2.015195
8	-6.047109	-1.770570	0.097435
1	-6.459604	-0.926421	-0.195372
6	-1.204613	-5.413754	-0.116467
1	-2.135636	-5.845606	0.262438
1	-1.059963	-5.796234	-1.135538
1	-0.385561	-5.812664	0.495096
6	-2.646434	4.368884	-0.638362
1	-2.489439	4.718660	-1.666841
1	-3.703381	4.520077	-0.399553
1	-2.063194	5.027349	0.017470
6	3.895278	-4.710498	-1.457725
1	3.350541	-5.294801	-0.708433
1	3.671436	-5.151784	-2.438960
1	4.966111	-4.849075	-1.277441
6	5.090411	3.144487	-1.998378
1	5.799423	2.869812	-1.206305
1	5.407881	2.626078	-2.911953
1	5.198865	4.218930	-2.170781
6	5.750690	-2.119448	-2.013058
6	6.414791	-3.023893	-2.749664
1	6.309796	-1.254184	-1.657142
1	7.473349	-2.901137	-2.959964
1	5.930966	-3.892535	-3.184945
6	2.654312	5.101654	-1.432881
6	2.017965	5.944262	-0.605517
1	3.285203	5.530799	-2.211954
1	2.106606	7.019985	-0.729078
1	1.423448	5.593633	0.233156
6	1.197145	0.051515	1.428576
6	1.119270	1.391601	2.089314
6	0.662233	-1.069762	2.269433
6	-0.080963	1.955490	2.556685
6	2.296864	2.146665	2.286580
8	-0.375261	-1.039943	2.905814
8	1.499305	-2.139108	2.268491
6	-0.110796	3.210995	3.161017
1	-0.993327	1.383299	2.444287
6	2.277307	3.410269	2.875918
8	3.528384	1.675816	1.867049
6	1.067609	3.947592	3.310685
1	-1.055690	3.612855	3.516375

1	3.215363	3.943297	2.995024
6	3.688529	0.307351	1.938489
1	1.050092	4.927789	3.779703
1	3.647726	-0.111975	2.947755
1	4.503126	-0.029031	1.303919
1	2.440617	-0.143279	1.374279
6	1.076208	-3.288948	3.033816
1	-0.005017	-3.404684	2.928302
1	1.579473	-4.132429	2.554121
6	1.476627	-3.161923	4.497100
1	0.955579	-2.322035	4.964924
1	1.211238	-4.077478	5.039064
1	2.556935	-3.008056	4.593675
26	0.750030	-0.116457	-0.458405

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**<sup>3</sup>TS(C-D)<sub>Fe</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2610.2645737  
Zero-point correction=                    0.805572 (Hartree/Particle)  
Thermal correction to Energy=            0.860170  
Thermal correction to Enthalpy=         0.861114  
Thermal correction to Gibbs Free Energy=    0.712814  
Sum of electronic and zero-point Energies=    -2609.459001  
Sum of electronic and thermal Energies=    -2609.404404  
Sum of electronic and thermal Enthalpies=    -2609.403460  
Sum of electronic and thermal Free Energies=   -2609.551760

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Cartesian Coordinates

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6	3.376195	-3.358799	-1.514735
6	2.112888	-2.789519	-1.096903
7	2.158203	-1.414591	-1.132474
6	3.416772	-1.091610	-1.572168
6	4.197558	-2.296505	-1.825508
6	1.000262	-3.535652	-0.729511
6	-0.244460	-3.028025	-0.386228
7	-0.575874	-1.695342	-0.327007
6	-1.906468	-1.651583	0.010956
6	-2.431213	-2.995886	0.192335
6	-1.392582	-3.853104	-0.061906
6	-2.658303	-0.489792	0.121235
6	-2.196135	0.797679	-0.115402
7	-0.892737	1.126690	-0.396646
6	-0.869588	2.491626	-0.547852
6	-2.197613	3.046816	-0.371481
6	-3.026681	1.990645	-0.102217
6	0.257549	3.253040	-0.822301
6	1.532322	2.758145	-1.057477
7	1.854544	1.425667	-1.108245
6	3.159315	1.367337	-1.538120

6	3.689739	2.696846	-1.747702
6	2.686654	3.575504	-1.415920
6	3.883735	0.202722	-1.756492
1	0.126271	4.324873	-0.899840
1	4.896024	0.320183	-2.125258
1	1.100295	-4.614912	-0.749354
1	-3.700762	-0.599773	0.392987
6	-4.517840	2.022070	0.075599
1	-4.849580	1.222817	0.746504
1	-4.812564	2.965149	0.551440
6	-5.264090	1.894724	-1.283783
1	-5.043022	0.922069	-1.738728
1	-4.935371	2.681463	-1.966162
6	-6.757433	2.030352	-1.133179
8	-7.456684	2.932461	-1.525654
8	-7.300050	0.973083	-0.436590
1	-8.260224	1.140832	-0.382075
6	-3.835606	-3.369536	0.581535
1	-4.224922	-2.687579	1.344980
1	-3.809246	-4.359023	1.050417
6	-4.856376	-3.440988	-0.592220
1	-4.394764	-3.866636	-1.485702
1	-5.686680	-4.089967	-0.286738
6	-5.458974	-2.102912	-0.965037
8	-5.363664	-1.555843	-2.044959
8	-6.142897	-1.570806	0.073837
1	-6.532701	-0.714038	-0.213337
6	-1.386397	-5.353369	-0.048570
1	-2.325243	-5.755901	0.343323
1	-1.251464	-5.767200	-1.056727
1	-0.574176	-5.752220	0.572204
6	-2.542136	4.501369	-0.492176
1	-2.408827	4.867230	-1.518640
1	-3.582311	4.691246	-0.210384
1	-1.907610	5.121564	0.153185
6	3.695589	-4.822325	-1.552955
1	3.161544	-5.373359	-0.771290
1	3.425398	-5.280734	-2.514524
1	4.768179	-4.987159	-1.406956
6	5.087045	3.006164	-2.193762
1	5.829639	2.666880	-1.459538
1	5.327048	2.516593	-3.146185
1	5.232536	4.081826	-2.327218
6	5.583334	-2.295350	-2.283668
6	6.195353	-3.245606	-3.008195
1	6.173210	-1.422822	-2.002886
1	7.242727	-3.149466	-3.279556
1	5.678244	-4.126677	-3.374532
6	2.770134	5.035817	-1.428853
6	2.209398	5.876967	-0.546828

1	3.382327	5.464474	-2.223030
1	2.338193	6.951585	-0.641777
1	1.638678	5.524094	0.307214
6	1.269706	-0.005021	1.602898
6	1.518082	1.308196	2.230496
6	0.615399	-1.011554	2.460892
6	0.473189	2.138461	2.667750
6	2.834036	1.798899	2.360883
8	-0.512800	-0.818928	2.884349
8	1.316973	-2.152645	2.638289
6	0.741143	3.400279	3.205311
1	-0.545291	1.780765	2.579756
6	3.109171	3.048574	2.896546
8	3.887440	1.019674	1.907566
6	2.052173	3.861479	3.316647
1	-0.086225	4.016642	3.545919
1	4.143367	3.365632	2.984025
6	3.621439	-0.336335	1.929143
1	2.260638	4.839265	3.741048
1	3.558351	-0.773389	2.930379
1	4.301994	-0.865067	1.260193
1	2.559539	-0.509147	1.377636
6	0.638375	-3.221640	3.344501
1	-0.411519	-3.225242	3.043793
1	1.122201	-4.130332	2.978186
6	0.787880	-3.075614	4.851435
1	0.289483	-2.167250	5.201206
1	0.330997	-3.935136	5.355845
1	1.844415	-3.033250	5.137411
26	0.674634	-0.130375	-0.576284

**Optimised geometries where cyclohexene is used as a substrate for intermolecular C-H insertion**

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**1C5SS<sup>+</sup>TS(C-D)<sub>Fe(his)</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2110.173879  
 Zero-point correction=                    0.670953 (Hartree/Particle)  
 Thermal correction to Energy=            0.711705  
 Thermal correction to Enthalpy=         0.712649  
 Thermal correction to Gibbs Free Energy= 0.598901  
 Sum of electronic and zero-point Energies= -2109.502926  
 Sum of electronic and thermal Energies= -2109.462174  
 Sum of electronic and thermal Enthalpies= -2109.461230  
 Sum of electronic and thermal Free Energies= -2109.574978

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 Cartesian Coordinates  
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26	0.935767	-0.190751	0.176390
7	1.600767	-0.339301	-1.732500

6	2.231993	0.637117	-2.454719
6	1.532816	-1.435266	-2.550750
6	2.562676	0.148775	-3.778163
6	2.116341	-1.133836	-3.843216
1	3.060343	0.729198	-4.545352
1	2.178796	-1.829020	-4.671568
7	0.577772	-2.189954	0.181832
6	0.250082	-2.959266	1.267260
6	0.670814	-3.050280	-0.879847
6	0.120710	-4.348433	0.878269
6	0.370727	-4.403192	-0.458768
1	-0.132744	-5.159649	1.550149
1	0.368528	-5.268696	-1.110135
7	0.415879	-0.083483	2.126426
6	0.409707	1.035466	2.922316
6	0.110214	-1.139472	2.949436
6	0.051733	0.682339	4.279233
6	-0.123454	-0.670134	4.297940
1	-0.027580	1.382543	5.102127
1	-0.379607	-1.303304	5.138919
7	1.471066	1.761217	0.223120
6	1.311299	2.639676	1.261473
6	2.140464	2.445063	-0.757742
6	1.872908	3.930455	0.918545
6	2.399786	3.805259	-0.331407
1	1.882405	4.796162	1.569991
1	2.920960	4.550585	-0.920137
6	-1.077942	0.281380	-0.682973
6	2.507420	1.922616	-1.996930
6	0.779066	2.316206	2.509315
6	1.071763	-2.693164	-2.166832
6	0.036069	-2.474883	2.555713
1	0.728933	3.110074	3.249957
1	3.027724	2.589185	-2.679512
1	1.088104	-3.478481	-2.917646
1	-0.217644	-3.201893	3.322825
1	-1.649371	0.718413	0.382965
6	-1.941809	-0.824730	-1.166059
6	-2.389948	-0.957577	-2.501587
6	-2.372195	-1.803533	-0.239636
6	-3.216588	-2.013548	-2.880371
1	-2.062040	-0.240158	-3.242012
6	-3.216569	-2.842807	-0.617542
1	-2.037901	-1.737005	0.786486
6	-3.643668	-2.957181	-1.943179
1	-3.533351	-2.095289	-3.917410
1	-3.528699	-3.574946	0.122880
1	-4.293671	-3.775412	-2.243205
6	-0.960111	1.447554	-1.609421
8	-1.140120	2.657178	-1.013739

8	-0.686505	1.361697	-2.795606
6	-0.987675	3.806229	-1.874424
1	0.042627	3.836449	-2.238502
1	-1.646046	3.691638	-2.742018
6	-1.330356	5.039633	-1.058361
1	-1.226281	5.935820	-1.680795
1	-2.361269	4.997876	-0.689946
1	-0.655493	5.133029	-0.202332
6	-2.643940	1.385390	1.098932
6	-3.804015	1.872933	0.248912
6	-2.989296	0.455671	2.165676
6	-4.883840	0.805639	0.016595
1	-3.444522	2.280775	-0.697128
1	-4.242533	2.725806	0.794570
6	-4.221674	-0.089321	2.280417
1	-2.230624	0.225876	2.905456
6	-5.356862	0.182755	1.336885
1	-5.732676	1.250310	-0.516159
1	-4.482057	0.017950	-0.626582
1	-4.431258	-0.728255	3.137683
1	-6.073477	0.850260	1.845546
1	-5.911470	-0.745892	1.146001
1	-1.925816	2.158808	1.371576
7	2.871393	-0.642115	0.786173
6	3.610017	-0.031240	1.778911
6	3.639408	-1.586576	0.275235
6	4.842589	-0.620133	1.865222
1	3.202640	0.784092	2.355017
1	3.363491	-2.253843	-0.526059
1	5.692327	-0.433802	2.503211
1	5.604597	-2.239868	0.689201
7	4.845371	-1.609836	0.899868

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<sup>10SS</sup>TS(C-D) Fe(his)  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2110.1737557  
 Zero-point correction=                    0.670112 (Hartree/Particle)  
 Thermal correction to Energy=            0.711145  
 Thermal correction to Enthalpy=         0.712089  
 Thermal correction to Gibbs Free Energy= 0.596093  
 Sum of electronic and zero-point Energies= -2109.503644  
 Sum of electronic and thermal Energies= -2109.462610  
 Sum of electronic and thermal Enthalpies= -2109.461666  
 Sum of electronic and thermal Free Energies= -2109.577663

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 Cartesian Coordinates  
 .....

26	0.844535	-0.144978	0.208331
7	1.229724	-1.695893	-1.034939
6	1.747981	-1.628482	-2.303602

6	0.972391	-3.021631	-0.798890
6	1.798137	-2.947731	-2.892498
6	1.324087	-3.813054	-1.954955
1	2.161204	-3.164818	-3.889433
1	1.212733	-4.887918	-2.023623
7	0.149366	-1.432039	1.595138
6	-0.319885	-1.119877	2.844619
6	0.088162	-2.799549	1.496394
6	-0.714987	-2.321017	3.545769
6	-0.454025	-3.364079	2.710234
1	-1.122457	-2.345639	4.548938
1	-0.608098	-4.421820	2.883805
7	0.707585	1.362716	1.531526
6	1.183760	2.643287	1.388266
6	0.131723	1.309857	2.777443
6	0.859989	3.429452	2.555352
6	0.199766	2.604707	3.415013
1	1.121275	4.471910	2.689228
1	-0.191153	2.829950	4.399573
7	1.855574	1.088840	-1.067417
6	2.228957	2.387495	-0.834337
6	2.345450	0.769367	-2.307971
6	2.972072	2.904770	-1.961053
6	3.033971	1.902568	-2.881816
1	3.382410	3.905162	-2.024438
1	3.503980	1.910550	-3.857394
6	-0.936593	0.151332	-0.703980
6	2.254025	-0.481734	-2.908790
6	1.915274	3.118055	0.306046
6	0.464473	-3.543622	0.385323
6	-0.358004	0.160267	3.390447
1	2.262267	4.146429	0.352370
1	2.658364	-0.584780	-3.911390
1	0.331707	-4.620055	0.438258
1	-0.755823	0.262824	4.396186
1	-1.805488	0.733825	0.202908
6	-1.710584	-1.062725	-1.136843
6	-1.781657	-1.514967	-2.473003
6	-2.430549	-1.800244	-0.174545
6	-2.532456	-2.639794	-2.815697
1	-1.244800	-0.974665	-3.239720
6	-3.189287	-2.917091	-0.521241
1	-2.410076	-1.482211	0.859669
6	-3.245455	-3.348299	-1.847522
1	-2.560249	-2.960103	-3.854857
1	-3.737405	-3.449981	0.252454
1	-3.834599	-4.220187	-2.121541
6	-0.826596	1.240082	-1.733631
8	-0.878647	2.485650	-1.187542
8	-0.704784	1.091150	-2.938972

6	-0.797904	3.581305	-2.120200
1	0.191978	3.577901	-2.586770
1	-1.537738	3.431362	-2.913241
6	-1.053716	4.863461	-1.347222
1	-0.986978	5.724883	-2.021807
1	-2.051612	4.857613	-0.895957
1	-0.317244	4.989766	-0.547692
6	-2.835551	1.493208	0.763752
6	-3.832376	1.886378	-0.320874
6	-3.422646	0.781102	1.896635
6	-4.916607	0.821769	-0.547364
1	-3.320366	2.108503	-1.260853
1	-4.309725	2.829987	-0.007163
6	-4.693690	0.319115	1.912634
1	-2.799694	0.641473	2.775174
6	-5.646255	0.469713	0.757666
1	-5.634544	1.173397	-1.298545
1	-4.450030	-0.083028	-0.949898
1	-5.072482	-0.160868	2.814441
1	-6.386485	1.249691	1.005564
1	-6.229065	-0.453213	0.629602
1	-2.152900	2.295855	1.047018
7	2.858084	-0.557910	1.078281
6	3.222315	-0.529132	2.408063
6	3.942016	-0.886922	0.402615
6	4.548510	-0.846330	2.532494
1	2.506551	-0.284308	3.177081
1	4.004533	-0.997142	-0.669071
1	5.198097	-0.930860	3.389785
1	5.930378	-1.328749	0.969527
7	4.993616	-1.071683	1.243260

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**<sup>3</sup>TS(C-D) Fe(his)**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2110.173677  
Zero-point correction=                    0.668646 (Hartree/Particle)  
Thermal correction to Energy=            0.711449  
Thermal correction to Enthalpy=         0.712393  
Thermal correction to Gibbs Free Energy= 0.584425  
Sum of electronic and zero-point Energies= -2109.505030  
Sum of electronic and thermal Energies= -2109.462228  
Sum of electronic and thermal Enthalpies= -2109.461284  
Sum of electronic and thermal Free Energies= -2109.589252

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Cartesian Coordinates

.....

26	1.362397	-0.149713	0.079491
7	1.698138	0.545207	-1.783198
6	1.925088	1.844422	-2.162779
6	1.774861	-0.201025	-2.930869



6	2.159586	1.919833	-3.587549
6	2.063888	0.650120	-4.064495
1	2.354739	2.833586	-4.134743
1	2.167330	0.304344	-5.085556
7	1.168954	-2.031329	-0.635387
6	0.901612	-3.176369	0.076515
6	1.319713	-2.424464	-1.940632
6	0.884988	-4.322196	-0.803821
6	1.143168	-3.854092	-2.056594
1	0.694888	-5.341532	-0.490677
1	1.207647	-4.411222	-2.983172
7	0.903004	-0.832793	1.929863
6	0.815751	-0.083422	3.077168
6	0.678325	-2.135169	2.309069
6	0.528003	-0.934079	4.208699
6	0.443259	-2.209154	3.732313
1	0.407483	-0.587966	5.228030
1	0.239646	-3.120881	4.280556
7	1.422443	1.745305	0.778061
6	1.250091	2.142728	2.080470
6	1.687308	2.887898	0.064919
6	1.407454	3.575480	2.191314
6	1.681801	4.038808	0.939750
1	1.321795	4.137560	3.113308
1	1.867488	5.057982	0.623728
6	-1.854482	0.348051	-0.757934
6	1.933464	2.938713	-1.304577
6	0.973216	1.298343	3.151106
6	1.605013	-1.578645	-3.008860
6	0.679418	-3.231296	1.449453
1	0.871087	1.756775	4.130819
1	2.135169	3.913273	-1.740247
1	1.693375	-2.034028	-3.991104
1	0.484056	-4.207253	1.885374
1	-2.321208	0.509273	0.660309
6	-2.639166	-0.724845	-1.322902
6	-3.470831	-0.577239	-2.465423
6	-2.558175	-2.007237	-0.722923
6	-4.173344	-1.659473	-2.978450
1	-3.518316	0.388239	-2.957382
6	-3.291983	-3.079658	-1.220782
1	-1.901402	-2.135995	0.129605
6	-4.096930	-2.910251	-2.350653
1	-4.791827	-1.534201	-3.863520
1	-3.219617	-4.053586	-0.744475
1	-4.656483	-3.752128	-2.750824
6	-1.846924	1.660210	-1.369818
8	-2.097071	2.705846	-0.536694
8	-1.499376	1.811567	-2.539182
6	-1.896255	4.015507	-1.106134

1	-0.877153	4.077608	-1.498056
1	-2.585816	4.152153	-1.946951
6	-2.137519	5.032028	-0.004435
1	-2.003963	6.046385	-0.397937
1	-3.155052	4.950145	0.392770
1	-1.429450	4.882809	0.816899
6	-2.936855	0.745996	1.673004
6	-4.306256	1.366405	1.405583
6	-2.981445	-0.535699	2.414436
6	-5.354372	0.308089	1.029492
1	-4.222452	2.132523	0.629575
1	-4.627472	1.883874	2.323181
6	-4.119198	-1.225930	2.611871
1	-2.043032	-0.918374	2.808142
6	-5.467115	-0.778259	2.110311
1	-6.330386	0.782451	0.869082
1	-5.070292	-0.160124	0.080108
1	-4.087052	-2.146179	3.194681
1	-6.057809	-0.406661	2.964380
1	-6.025726	-1.642312	1.724730
1	-2.229263	1.459626	2.108834
7	3.709969	-0.459293	0.476160
6	4.757265	0.375766	0.151786
6	4.246905	-1.509741	1.062055
6	5.943961	-0.182273	0.549710
1	4.581577	1.318378	-0.345515
1	3.702702	-2.362096	1.442652
1	6.967902	0.151030	0.478156
1	6.238803	-2.061260	1.532582
7	5.601439	-1.389419	1.131148

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**W-<sup>1</sup>CSST<sub>S</sub>(C-D) Fe<sub>(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2109.5647421  
Zero-point correction=                    0.681971 (Hartree/Particle)  
Thermal correction to Energy=            0.721340  
Thermal correction to Enthalpy=         0.722284  
Thermal correction to Gibbs Free Energy= 0.612859  
Sum of electronic and zero-point Energies= -2108.882771  
Sum of electronic and thermal Energies= -2108.843402  
Sum of electronic and thermal Enthalpies= -2108.842458  
Sum of electronic and thermal Free Energies= -2108.951883

.....  
Cartesian Coordinates

.....  
26      0.905774 -0.285140 0.160558  
7        1.495199 -0.405386 -1.758941  
6        2.207010 0.527441 -2.447612  
6        1.248087 -1.419647 -2.633228

6	2.416272	0.093260	-3.811936
6	1.805915	-1.109028	-3.932400
1	2.948411	0.657900	-4.566826
1	1.738059	-1.747229	-4.804279
7	0.334177	-2.219853	0.080297
6	-0.049122	-2.998374	1.130680
6	0.261641	-3.010221	-1.024819
6	-0.378963	-4.330279	0.674743
6	-0.201893	-4.332560	-0.669172
1	-0.714335	-5.139116	1.311747
1	-0.356088	-5.144269	-1.368662
7	0.404846	-0.206554	2.110561
6	0.502429	0.869162	2.944234
6	0.012143	-1.257766	2.887286
6	0.120527	0.498575	4.286814
6	-0.173779	-0.827382	4.252952
1	0.106343	1.169896	5.136257
1	-0.482486	-1.468576	5.069087
7	1.631943	1.587488	0.286853
6	1.546952	2.436531	1.347783
6	2.348392	2.238740	-0.669048
6	2.218312	3.682261	1.048584
6	2.729085	3.553653	-0.201094
1	2.299527	4.522901	1.726567
1	3.308255	4.270845	-0.769256
6	-1.037948	0.427841	-0.626265
6	2.635807	1.744207	-1.936373
6	0.984697	2.122963	2.579189
6	0.643486	-2.626072	-2.305496
6	-0.187028	-2.559790	2.440512
1	1.003805	2.891507	3.347132
1	3.205085	2.388033	-2.601187
1	0.515301	-3.352585	-3.102739
1	-0.504911	-3.291605	3.178240
1	-1.399578	0.864211	0.471810
6	-2.007078	-0.595734	-1.063340
6	-2.481070	-0.715260	-2.381655
6	-2.490035	-1.507884	-0.107629
6	-3.408402	-1.696040	-2.714289
1	-2.100360	-0.047718	-3.143468
6	-3.433180	-2.469767	-0.438381
1	-2.111381	-1.458127	0.903619
6	-3.901156	-2.568345	-1.746389
1	-3.752445	-1.775228	-3.741919
1	-3.784230	-3.158356	0.324926
1	-4.630348	-3.328296	-2.013122
6	-0.809533	1.578845	-1.537080
8	-0.744232	2.766259	-0.901973
8	-0.645479	1.489977	-2.738148
6	-0.475193	3.905091	-1.721912

1	0.540919	3.820635	-2.118012
1	-1.168502	3.911444	-2.569105
6	-0.637331	5.128911	-0.845304
1	-0.435105	6.034754	-1.426012
1	-1.656910	5.192206	-0.450426
1	0.063561	5.087513	-0.006947
6	-2.359324	1.632891	1.085001
6	-3.462012	2.225511	0.233184
6	-2.802201	0.735024	2.145366
6	-4.613317	1.257700	-0.053225
1	-3.059901	2.640128	-0.691670
1	-3.839215	3.085417	0.809405
6	-4.060393	0.265370	2.201685
1	-2.085212	0.452969	2.907712
6	-5.143502	0.604314	1.224357
1	-5.420461	1.797582	-0.559577
1	-4.274516	0.480341	-0.740499
1	-4.338245	-0.368824	3.041811
1	-5.857463	1.269601	1.735000
1	-5.706523	-0.303895	0.976889
1	-1.580687	2.342338	1.369140
7	2.749729	-0.952146	0.716321
6	3.547327	-0.481517	1.730411
6	3.408334	-1.932047	0.140720
6	4.709729	-1.195047	1.764265
1	3.224275	0.335403	2.357159
1	3.053349	-2.514651	-0.695893
1	5.577801	-1.135668	2.400754
1	5.292672	-2.804474	0.486784
7	4.605106	-2.115901	0.744237

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**W-<sup>10SS</sup>TS(C-D) Fe(his)**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2109.5620107  
Zero-point correction=                    0.679451 (Hartree/Particle)  
Thermal correction to Energy=            0.719362  
Thermal correction to Enthalpy=         0.720306  
Thermal correction to Gibbs Free Energy= 0.608629  
Sum of electronic and zero-point Energies= -2108.882560  
Sum of electronic and thermal Energies= -2108.842648  
Sum of electronic and thermal Enthalpies= -2108.841704  
Sum of electronic and thermal Free Energies= -2108.953382

.....  
Cartesian Coordinates

.....

26	0.817721	-0.210980	0.232695
7	1.067981	-1.804211	-0.966440
6	1.572182	-1.804143	-2.234152
6	0.651159	-3.080422	-0.724609
6	1.458797	-3.118375	-2.816777

6	0.895019	-3.912970	-1.874985
1	1.779164	-3.378818	-3.817250
1	0.646991	-4.964321	-1.937926
7	-0.049859	-1.379254	1.605745
6	-0.565621	-0.982998	2.803223
6	-0.262890	-2.723542	1.527154
6	-1.143065	-2.107414	3.496781
6	-0.946379	-3.191384	2.705892
1	-1.623887	-2.055752	4.465142
1	-1.237277	-4.218507	2.883555
7	0.777957	1.327399	1.498982
6	1.374501	2.545032	1.343851
6	0.124076	1.375785	2.697105
6	1.051498	3.403642	2.454098
6	0.265804	2.680646	3.291202
1	1.395538	4.423888	2.565327
1	-0.170320	2.980365	4.235384
7	1.964787	0.881415	-1.036099
6	2.469677	2.128814	-0.814460
6	2.415001	0.504495	-2.266839
6	3.267427	2.553869	-1.938454
6	3.218965	1.550156	-2.849422
1	3.777411	3.506100	-2.009186
1	3.682738	1.500970	-3.826057
6	-0.874959	0.220122	-0.690403
6	2.190659	-0.729638	-2.855782
6	2.202708	2.911508	0.295258
6	0.063872	-3.525846	0.446919
6	-0.507689	0.305908	3.311160
1	2.647745	3.901481	0.331330
1	2.570188	-0.883197	-3.861018
1	-0.205878	-4.575551	0.503427
1	-0.961785	0.483145	4.281672
1	-1.669429	0.925680	0.184150
6	-1.737832	-0.941443	-1.074087
6	-1.756079	-1.495580	-2.364201
6	-2.565336	-1.530875	-0.107145
6	-2.561741	-2.590039	-2.661302
1	-1.128480	-1.063425	-3.131897
6	-3.380049	-2.615482	-0.407611
1	-2.579828	-1.126150	0.896835
6	-3.381159	-3.157227	-1.689486
1	-2.545400	-3.001554	-3.667106
1	-4.010210	-3.039104	0.370088
1	-4.012335	-4.008827	-1.928791
6	-0.655051	1.251724	-1.746551
8	-0.501243	2.481889	-1.212675
8	-0.613247	1.077197	-2.949377
6	-0.295792	3.548985	-2.134359
1	0.684022	3.429418	-2.608947

1	-1.055132	3.499803	-2.921556
6	-0.390975	4.838569	-1.344928
1	-0.231038	5.698255	-2.003906
1	-1.379150	4.932670	-0.883111
1	0.360437	4.858815	-0.550263
6	-2.596803	1.806475	0.695512
6	-3.480572	2.287690	-0.443515
6	-3.340469	1.166006	1.779887
6	-4.543260	1.253175	-0.823435
1	-2.882593	2.551067	-1.318888
1	-3.973947	3.216338	-0.115308
6	-4.608191	0.733778	1.649442
1	-2.833908	1.037372	2.731162
6	-5.404310	0.853918	0.380330
1	-5.179840	1.647254	-1.623642
1	-4.045676	0.364187	-1.221606
1	-5.108905	0.288145	2.507436
1	-6.204751	1.593584	0.539623
1	-5.913884	-0.096536	0.174567
1	-1.856029	2.538032	1.024718
7	2.695802	-0.775884	1.150391
6	3.000769	-0.782855	2.488847
6	3.769626	-1.185808	0.516002
6	4.286472	-1.206164	2.661326
1	2.272011	-0.483098	3.226487
1	3.859610	-1.293179	-0.554761
1	4.891099	-1.347548	3.542668
1	5.683543	-1.789592	1.155369
7	4.762535	-1.459064	1.393092

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**W-<sup>3</sup>TS(C-D) Fe(his)**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2109.5539804  
Zero-point correction=                    0.679144 (Hartree/Particle)  
Thermal correction to Energy=            0.719294  
Thermal correction to Enthalpy=         0.720238  
Thermal correction to Gibbs Free Energy= 0.606672  
Sum of electronic and zero-point Energies= -2108.874836  
Sum of electronic and thermal Energies= -2108.834686  
Sum of electronic and thermal Enthalpies= -2108.833742  
Sum of electronic and thermal Free Energies= -2108.947308

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Cartesian Coordinates

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26	0.871640	-0.189552	0.243597
7	1.166850	-1.782200	-0.941947
6	1.681891	-1.805538	-2.204220
6	0.782859	-3.062185	-0.665276
6	1.610350	-3.137638	-2.750194
6	1.061502	-3.920011	-1.789604

1	1.945811	-3.417179	-3.740384
1	0.842286	-4.979051	-1.824628
7	-0.002341	-1.327678	1.633961
6	-0.566808	-0.926808	2.809374
6	-0.177681	-2.677444	1.568589
6	-1.128660	-2.054894	3.504014
6	-0.877355	-3.145406	2.736136
1	-1.640504	-2.002032	4.456091
1	-1.145793	-4.177247	2.921546
7	0.721473	1.378403	1.480180
6	1.276276	2.607510	1.293416
6	0.041224	1.445211	2.662571
6	0.906732	3.491790	2.370392
6	0.129116	2.772008	3.217005
1	1.213426	4.526659	2.451703
1	-0.336373	3.087858	4.141539
7	1.966017	0.898875	-1.051007
6	2.406274	2.175610	-0.849251
6	2.436905	0.523707	-2.276875
6	3.186336	2.616365	-1.978916
6	3.189312	1.596860	-2.873534
1	3.647912	3.591660	-2.065973
1	3.656390	1.554781	-3.848765
6	-0.915675	0.196828	-0.686253
6	2.269046	-0.726498	-2.846937
6	2.100804	2.972662	0.239572
6	0.192761	-3.492289	0.509374
6	-0.568237	0.373227	3.291077
1	2.506067	3.980057	0.249576
1	2.659978	-0.883927	-3.846896
1	-0.050163	-4.547166	0.586685
1	-1.055299	0.556873	4.243972
1	-1.798141	0.916792	0.179714
6	-1.693823	-1.018251	-1.068479
6	-1.658499	-1.602791	-2.345588
6	-2.513878	-1.624591	-0.104010
6	-2.401531	-2.743260	-2.631185
1	-1.038316	-1.156038	-3.111234
6	-3.267157	-2.755426	-0.394031
1	-2.572617	-1.192582	0.887564
6	-3.211526	-3.328012	-1.661329
1	-2.343890	-3.177710	-3.625866
1	-3.894627	-3.190186	0.379701
1	-3.793952	-4.216022	-1.892059
6	-0.696506	1.201680	-1.764123
8	-0.595783	2.447540	-1.250270
8	-0.622369	1.010289	-2.963705
6	-0.417634	3.504887	-2.187397
1	0.567520	3.408157	-2.656688
1	-1.171250	3.420989	-2.977248

6	-0.555268	4.803533	-1.419047
1	-0.421944	5.657498	-2.091347
1	-1.546479	4.872331	-0.959570
1	0.193733	4.860654	-0.623685
6	-2.720196	1.737744	0.672090
6	-3.612658	2.188790	-0.475788
6	-3.467038	1.074635	1.749261
6	-4.608542	1.097354	-0.877861
1	-3.012527	2.486642	-1.339723
1	-4.164730	3.086109	-0.154624
6	-4.708843	0.584124	1.595774
1	-2.976630	0.972252	2.713342
6	-5.479850	0.661137	0.306310
1	-5.243814	1.449314	-1.698847
1	-4.052782	0.232785	-1.253818
1	-5.207707	0.116942	2.443555
1	-6.319335	1.361646	0.439365
1	-5.936859	-0.313956	0.091347
1	-2.037966	2.516259	1.023977
7	2.729219	-0.663700	1.206699
6	3.023938	-0.595468	2.545828
6	3.814470	-1.086769	0.599450
6	4.315176	-0.986202	2.746784
1	2.283926	-0.270770	3.261302
1	3.912215	-1.246796	-0.464024
1	4.916832	-1.071310	3.637308
1	5.733060	-1.621423	1.280896
7	4.804423	-1.295732	1.495228

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**<sup>1</sup>CSSTs(C-D)<sub>Fe</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-1883.9429274  
Zero-point correction=                    0.598220 (Hartree/Particle)  
Thermal correction to Energy=            0.633954  
Thermal correction to Enthalpy=         0.634898  
Thermal correction to Gibbs Free Energy= 0.531627  
Sum of electronic and zero-point Energies= -1883.344707  
Sum of electronic and thermal Energies= -1883.308973  
Sum of electronic and thermal Enthalpies= -1883.308029  
Sum of electronic and thermal Free Energies= -1883.411301

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Cartesian Coordinates

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26	-0.521347	0.684655	0.925930
7	-0.213311	2.566958	0.270496
6	-1.068075	3.337023	-0.483212
6	0.937289	3.311022	0.392596
6	-0.428401	4.572542	-0.874278
6	0.817387	4.556435	-0.330429



1	-0.896474	5.347351	-1.468593
1	1.588488	5.314801	-0.384298
7	1.202424	0.806228	1.985844
6	1.703584	-0.115972	2.877069
6	2.136178	1.814405	1.940592
6	2.982537	0.316119	3.391751
6	3.250511	1.516749	2.809208
1	3.573410	-0.229258	4.117480
1	4.109377	2.160385	2.954112
7	-1.002165	-0.981997	1.959771
6	-2.192047	-1.676864	1.920425
6	-0.196011	-1.690074	2.825202
6	-2.108746	-2.872583	2.724218
6	-0.869265	-2.879482	3.289303
1	-2.914151	-3.584349	2.857672
1	-0.447361	-3.599030	3.980318
7	-2.476286	0.856749	0.377740
6	-3.493585	-0.039661	0.615657
6	-3.057772	1.894268	-0.313355
6	-4.738525	0.445593	0.066434
6	-4.466438	1.647921	-0.512297
1	-5.688428	-0.070108	0.137276
1	-5.145450	2.322407	-1.019021
6	0.180944	-0.129269	-0.792947
6	-2.392626	3.028358	-0.757991
6	-3.352356	-1.244020	1.290781
6	2.035006	2.962831	1.166352
6	1.067080	-1.292854	3.249270
1	-4.234438	-1.871348	1.386153
1	-2.964531	3.750394	-1.333290
1	2.865327	3.662202	1.198572
1	1.578082	-1.933968	3.962744
1	0.388353	-1.272116	-0.414835
6	1.478532	0.368017	-1.352351
6	1.586847	1.081473	-2.567341
6	2.678806	0.089908	-0.661480
6	2.828329	1.485744	-3.056403
1	0.687965	1.329193	-3.114924
6	3.918786	0.478865	-1.163195
1	2.634296	-0.438479	0.281038
6	4.003696	1.181301	-2.366765
1	2.873875	2.042901	-3.989051
1	4.819451	0.242200	-0.601836
1	4.969139	1.494068	-2.756518
6	-0.959527	-0.208955	-1.766148
8	-1.684071	-1.355150	-1.647721
8	-1.257320	0.647539	-2.580448
6	-2.834248	-1.461581	-2.515985
1	-3.536577	-0.661506	-2.268683
1	-2.511770	-1.316327	-3.552273

6	-3.446227	-2.833931	-2.299031
1	-4.332795	-2.949297	-2.932729
1	-2.738634	-3.630371	-2.554812
1	-3.747457	-2.961894	-1.254746
6	0.647458	-2.804699	-0.606900
6	0.768438	-3.168379	-2.066392
6	1.793669	-3.040513	0.229557
6	2.183378	-2.961805	-2.626160
1	0.024400	-2.632540	-2.658349
1	0.489854	-4.235219	-2.136501
6	2.989282	-3.430770	-0.283361
1	1.676405	-2.920056	1.300894
6	3.243882	-3.637720	-1.746110
1	2.237799	-3.350188	-3.649373
1	2.394733	-1.889770	-2.678169
1	3.804178	-3.657121	0.402814
1	3.273756	-4.724695	-1.936674
1	4.247182	-3.272064	-2.001767
1	-0.333110	-2.938541	-0.156126

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**<sup>10</sup>SS<sup>+</sup>TS(C-D)<sub>Fe</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-1883.9519413  
Zero-point correction=                    0.596982 (Hartree/Particle)  
Thermal correction to Energy=            0.632936  
Thermal correction to Enthalpy=         0.633880  
Thermal correction to Gibbs Free Energy= 0.530247  
Sum of electronic and zero-point Energies= -1883.354960  
Sum of electronic and thermal Energies= -1883.319005  
Sum of electronic and thermal Enthalpies= -1883.318061  
Sum of electronic and thermal Free Energies= -1883.421694

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Cartesian Coordinates

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26	-0.537506	0.675679	0.911056
7	0.032354	2.556537	0.466213
6	-0.621802	3.442504	-0.360441
6	1.232121	3.161212	0.768975
6	0.186708	4.613948	-0.590977
6	1.335273	4.442336	0.117145
1	-0.111112	5.456434	-1.202294
1	2.181070	5.112068	0.206681
7	1.083147	0.507052	2.095787
6	1.422024	-0.567570	2.888015
6	2.122495	1.401274	2.233851
6	2.700544	-0.351445	3.518857
6	3.132569	0.875006	3.116257
1	3.180371	-1.048498	4.194403
1	4.043023	1.393567	3.389008
7	-1.321219	-0.949351	1.798395

6	-2.598615	-1.452727	1.672345
6	-0.654116	-1.853704	2.597874
6	-2.721485	-2.708557	2.367566
6	-1.511192	-2.961823	2.937080
1	-3.628865	-3.296965	2.421003
1	-1.218118	-3.800741	3.555727
7	-2.398949	1.139303	0.239236
6	-3.552324	0.395079	0.365226
6	-2.757541	2.238465	-0.508506
6	-4.651329	1.042231	-0.307563
6	-4.153717	2.182093	-0.860987
1	-5.665215	0.663103	-0.337515
1	-4.673020	2.933948	-1.441581
6	0.170072	-0.094017	-0.769440
6	-1.914610	3.288075	-0.837464
6	-3.647173	-0.821909	1.020929
6	2.205018	2.631792	1.601934
6	0.628842	-1.686126	3.097391
1	-4.615404	-1.313634	1.033505
1	-2.317402	4.079912	-1.461346
1	3.097332	3.225998	1.772919
1	1.018950	-2.463730	3.747666
1	0.511724	-1.425254	-0.517263
6	1.450166	0.485661	-1.288079
6	1.522576	1.368804	-2.388627
6	2.666711	0.118539	-0.676743
6	2.750078	1.845600	-2.847319
1	0.609381	1.670830	-2.881666
6	3.892422	0.589745	-1.144260
1	2.651105	-0.560483	0.166298
6	3.943666	1.458957	-2.235004
1	2.769681	2.524586	-3.696593
1	4.808755	0.273584	-0.651467
1	4.897727	1.829300	-2.601813
6	-0.951081	-0.243493	-1.759645
8	-1.701908	-1.352082	-1.530737
8	-1.197599	0.507589	-2.688944
6	-2.782325	-1.579065	-2.460417
1	-3.517121	-0.775774	-2.350137
1	-2.389092	-1.530877	-3.480818
6	-3.378752	-2.940165	-2.149030
1	-4.214976	-3.143532	-2.827652
1	-2.634284	-3.733383	-2.274629
1	-3.749056	-2.977615	-1.119949
6	0.745227	-2.785930	-0.630098
6	0.852870	-3.152669	-2.106052
6	1.906498	-3.161156	0.175062
6	2.273437	-2.959924	-2.658278
1	0.133646	-2.583467	-2.701860
1	0.562402	-4.211255	-2.211513

6	3.071143	-3.600804	-0.353579
1	1.808094	-3.096223	1.255091
6	3.310366	-3.737280	-1.833139
1	2.313775	-3.274165	-3.708355
1	2.524989	-1.894283	-2.633962
1	3.876666	-3.904673	0.313986
1	3.288356	-4.807427	-2.100708
1	4.325355	-3.396984	-2.081425
1	-0.213432	-3.048615	-0.178321

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<sup>3</sup>TS(C-D)<sub>Fe</sub>  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-1883.9554463  
 Zero-point correction=                    0.596852 (Hartree/Particle)  
 Thermal correction to Energy=            0.633515  
 Thermal correction to Enthalpy=         0.634459  
 Thermal correction to Gibbs Free Energy= 0.524879  
 Sum of electronic and zero-point Energies= -1883.358595  
 Sum of electronic and thermal Energies= -1883.321931  
 Sum of electronic and thermal Enthalpies= -1883.320987  
 Sum of electronic and thermal Free Energies= -1883.430568

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 Cartesian Coordinates  
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26	-0.894792	0.933253	0.917332
7	-1.895266	1.947291	-0.504462
6	-3.110001	1.627169	-1.062812
6	-1.472708	3.079368	-1.156476
6	-3.459312	2.578598	-2.091201
6	-2.438483	3.474439	-2.156240
1	-4.367352	2.545428	-2.679814
1	-2.336305	4.334589	-2.806061
7	0.463381	2.420894	1.019522
6	1.497171	2.553426	1.918881
6	0.566603	3.495838	0.170313
6	2.270674	3.735582	1.624568
6	1.697146	4.316018	0.534011
1	3.132933	4.066789	2.189896
1	1.992096	5.222553	0.020282
7	-0.039849	0.067976	2.529130
6	-0.438677	-1.093369	3.148495
6	1.054766	0.513312	3.235967
6	0.435394	-1.396158	4.256305
6	1.358398	-0.394516	4.315577
1	0.333371	-2.256289	4.906479
1	2.168438	-0.265681	5.022703
7	-2.406950	-0.399430	1.008999
6	-2.480921	-1.505279	1.821108
6	-3.560248	-0.405715	0.259522
6	-3.701481	-2.233654	1.566630

6	-4.376526	-1.545721	0.603305
1	-4.000464	-3.137570	2.083039
1	-5.339727	-1.771753	0.162955
6	0.403401	-0.443146	-1.050313
6	-3.895636	0.540905	-0.701848
6	-1.553322	-1.848621	2.798448
6	-0.314914	3.788981	-0.864243
6	1.775637	1.668347	2.953444
1	-1.748257	-2.746831	3.377333
1	-4.839660	0.411884	-1.222986
1	-0.107745	4.672895	-1.460179
1	2.622713	1.897599	3.593538
1	0.911122	-1.556489	-0.254273
6	1.580193	0.138713	-1.675698
6	1.762384	0.237073	-3.080742
6	2.609874	0.639268	-0.840099
6	2.908782	0.814783	-3.611364
1	0.975345	-0.111785	-3.739228
6	3.770539	1.186981	-1.378017
1	2.475465	0.591154	0.233265
6	3.921994	1.281257	-2.763823
1	3.022701	0.896930	-4.689179
1	4.547740	1.560846	-0.717284
1	4.820683	1.724953	-3.184865
6	-0.646935	-0.989989	-1.913045
8	-1.053481	-2.248029	-1.606482
8	-1.193386	-0.312204	-2.775663
6	-2.176296	-2.744392	-2.367950
1	-3.026145	-2.073276	-2.217888
1	-1.920456	-2.728163	-3.432992
6	-2.475799	-4.148542	-1.875738
1	-3.321681	-4.564675	-2.434725
1	-1.614087	-4.809919	-2.016138
1	-2.737154	-4.134768	-0.813137
6	1.386023	-2.622786	0.133832
6	1.798049	-3.542504	-1.011841
6	2.485806	-2.245544	1.044603
6	3.173273	-3.175984	-1.590185
1	1.029289	-3.540317	-1.789061
1	1.833438	-4.568965	-0.613873
6	3.780685	-2.484091	0.761613
1	2.218467	-1.763092	1.980547
6	4.253955	-3.155901	-0.498955
1	3.449264	-3.884551	-2.380466
1	3.118299	-2.186819	-2.057515
1	4.539732	-2.216665	1.496210
1	4.567993	-4.183925	-0.252008
1	5.160034	-2.656333	-0.868134
1	0.493298	-2.972466	0.661589

W- <sup>1</sup>CSSTs(C-D) Fe

-----  
Number of imaginary frequencies: 1    Electronic energy:    HF=-1883.3847599  
Zero-point correction=                    0.607417 (Hartree/Particle)  
Thermal correction to Energy=            0.642255  
Thermal correction to Enthalpy=         0.643199  
Thermal correction to Gibbs Free Energy= 0.543408  
Sum of electronic and zero-point Energies= -1882.777343  
Sum of electronic and thermal Energies= -1882.742505  
Sum of electronic and thermal Enthalpies= -1882.741561  
Sum of electronic and thermal Free Energies= -1882.841352  
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Cartesian Coordinates

-----  
26    -0.367509   0.698549   1.072661  
7      -0.908239   2.422574   0.209559  
6      -2.161676   2.797309   -0.180950  
6      -0.073321   3.411437   -0.224597  
6      -2.118032   4.057781   -0.885322  
6      -0.818484   4.431248   -0.927212  
1      -2.981244   4.568216   -1.292315  
1      -0.384670   5.319490   -1.367984  
7      1.455336   1.479457   1.425528  
6      2.459905   0.947294   2.186910  
6      1.977927   2.606888   0.862708  
6      3.644235   1.768493   2.109430  
6      3.349761   2.790945   1.271130  
1      4.572350   1.566994   2.629001  
1      3.982502   3.611557   0.958719  
7      0.104825   -0.873634   2.237415  
6      -0.699686   -1.938342   2.544272  
6      1.291602   -1.106826   2.879293  
6      0.008535   -2.884871   3.367873  
6      1.243994   -2.361653   3.584993  
1      -0.408236   -3.808481   3.749130  
1      2.052177   -2.768754   4.179346  
7      -2.291060   0.124785   1.117001  
6      -2.781954   -1.071233   1.560859  
6      -3.367496   0.814679   0.639032  
6      -4.208607   -1.140008   1.354779  
6      -4.574854   0.039011   0.793808  
1      -4.835733   -1.977004   1.635218  
1      -5.564608   0.370537   0.506307  
6      0.061691   -0.144152   -0.833147  
6      -3.315120   2.063949   0.036001  
6      -2.035565   -2.058184   2.184136  
6      1.282869   3.484363   0.044268  
6      2.389564   -0.256154   2.867181  
1      -2.557237   -2.958862   2.495529  
1      -4.250820   2.486813   -0.318082

1	1.828871	4.331979	-0.358759
1	3.266946	-0.567247	3.427124
1	0.045325	-1.207247	-0.342033
6	1.397070	0.176891	-1.375919
6	1.605668	0.907151	-2.558832
6	2.531461	-0.281475	-0.681553
6	2.892881	1.139786	-3.029505
1	0.752530	1.301576	-3.094721
6	3.813963	-0.059860	-1.163110
1	2.399136	-0.798518	0.258609
6	4.003328	0.647361	-2.347276
1	3.027983	1.713415	-3.942334
1	4.666998	-0.422484	-0.596424
1	5.005462	0.831842	-2.723704
6	-1.115067	0.038347	-1.722549
8	-2.035576	-0.940601	-1.588034
8	-1.284109	0.965758	-2.487878
6	-3.211956	-0.815660	-2.391162
1	-3.785069	0.048078	-2.042474
1	-2.920312	-0.630017	-3.429714
6	-3.990145	-2.105637	-2.240912
1	-4.910174	-2.058362	-2.832248
1	-3.399931	-2.959624	-2.590426
1	-4.256716	-2.266442	-1.192701
6	0.082677	-2.648216	-0.849425
6	0.133645	-2.898822	-2.333301
6	1.203713	-3.103842	-0.067512
6	1.536107	-2.778722	-2.935310
1	-0.580116	-2.263624	-2.858981
1	-0.239409	-3.929724	-2.453873
6	2.350119	-3.504632	-0.655607
1	1.112054	-3.114792	1.012974
6	2.576580	-3.562171	-2.132503
1	1.516540	-3.134741	-3.970211
1	1.827222	-1.727371	-2.967804
1	3.155371	-3.869943	-0.020870
1	2.576856	-4.625408	-2.421177
1	3.583947	-3.192205	-2.357404
1	-0.903323	-2.720308	-0.391961

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**W- <sup>10</sup>SS<sup>TS</sup>(C-D)<sub>Fe</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-1883.3940076  
Zero-point correction=                    0.604802 (Hartree/Particle)  
Thermal correction to Energy=            0.639886  
Thermal correction to Enthalpy=         0.640831  
Thermal correction to Gibbs Free Energy= 0.540077  
Sum of electronic and zero-point Energies= -1882.789206  
Sum of electronic and thermal Energies= -1882.754121  
Sum of electronic and thermal Enthalpies= -1882.753177

Sum of electronic and thermal Free Energies= -1882.853931

.....  
Cartesian Coordinates  
.....

26	-0.436229	0.681835	0.982888
7	0.443135	2.442528	0.632619
6	-0.035576	3.443618	-0.169187
6	1.734286	2.798242	0.922683
6	0.973435	4.445340	-0.389880
6	2.071067	4.048159	0.296873
1	0.835518	5.336045	-0.988617
1	3.031950	4.538239	0.379927
7	1.142665	0.143606	2.076236
6	1.322100	-1.053126	2.717561
6	2.322612	0.820742	2.235897
6	2.642062	-1.134460	3.282034
6	3.261594	0.035683	2.988556
1	3.023521	-1.980304	3.839031
1	4.262635	0.354280	3.247861
7	-1.457779	-0.861108	1.715729
6	-2.789849	-1.142248	1.563128
6	-0.932042	-1.945750	2.370563
6	-3.100117	-2.440364	2.096819
6	-1.942371	-2.944916	2.590845
1	-4.085833	-2.887151	2.096171
1	-1.774202	-3.893631	3.083565
7	-2.177214	1.476827	0.352864
6	-3.432216	0.932243	0.442302
6	-2.337293	2.637552	-0.356197
6	-4.400752	1.776460	-0.206472
6	-3.716201	2.827701	-0.719377
1	-5.461579	1.568761	-0.259831
1	-4.093927	3.670786	-1.282596
6	0.141170	-0.072663	-0.726224
6	-1.327930	3.531960	-0.653143
6	-3.726964	-0.293254	1.004576
6	2.609257	2.058734	1.692742
6	0.364682	-2.043767	2.836361
1	-4.760917	-0.624026	0.985209
1	-1.580256	4.394342	-1.261582
1	3.603428	2.462323	1.854585
1	0.640971	-2.949631	3.367639
1	0.249979	-1.446584	-0.544963
6	1.495768	0.347159	-1.184296
6	1.707561	1.348214	-2.147079
6	2.624901	-0.278371	-0.635631
6	2.995515	1.696896	-2.537696
1	0.854226	1.849617	-2.583360
6	3.910582	0.062118	-1.037526
1	2.492636	-1.051629	0.110979



6	4.104772	1.056008	-1.991769
1	3.130254	2.479447	-3.279363
1	4.760431	-0.450191	-0.594739
1	5.108065	1.329573	-2.306382
6	-0.981823	0.009294	-1.706941
8	-1.919933	-0.924652	-1.458457
8	-1.080537	0.784346	-2.637842
6	-3.029000	-0.961573	-2.356415
1	-3.634434	-0.060748	-2.211036
1	-2.658951	-0.952951	-3.386436
6	-3.804577	-2.225850	-2.049522
1	-4.678094	-2.300379	-2.705152
1	-3.176183	-3.108574	-2.205321
1	-4.143552	-2.227599	-1.009631
6	0.251945	-2.791584	-0.748148
6	0.236386	-3.031152	-2.248746
6	1.405551	-3.385790	-0.071017
6	1.617223	-2.814665	-2.873673
1	-0.504586	-2.393694	-2.737455
1	-0.086162	-4.069793	-2.421775
6	2.506922	-3.800336	-0.723212
1	1.359993	-3.487699	1.008888
6	2.682045	-3.697099	-2.212430
1	1.578628	-3.017971	-3.949575
1	1.898176	-1.763321	-2.758589
1	3.318731	-4.256760	-0.159496
1	2.654583	-4.712387	-2.638059
1	3.682822	-3.306701	-2.438393
1	-0.706142	-2.974842	-0.256460

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**W- <sup>3</sup>TS(C-D) Fe**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-1883.392883  
Zero-point correction=                    0.605307 (Hartree/Particle)  
Thermal correction to Energy=            0.640683  
Thermal correction to Enthalpy=         0.641628  
Thermal correction to Gibbs Free Energy= 0.538318  
Sum of electronic and zero-point Energies= -1882.787576  
Sum of electronic and thermal Energies= -1882.752200  
Sum of electronic and thermal Enthalpies= -1882.751255  
Sum of electronic and thermal Free Energies= -1882.854565

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Cartesian Coordinates

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26	-0.446181	0.774280	1.076564
7	-1.027322	2.416376	0.076879
6	-2.279811	2.713635	-0.379074
6	-0.219869	3.421341	-0.370677
6	-2.261053	3.937941	-1.146544
6	-0.979353	4.368939	-1.155212

1	-3.128015	4.385906	-1.614191
1	-0.566628	5.252992	-1.623609
7	1.321912	1.669553	1.469486
6	2.331675	1.199255	2.262050
6	1.821597	2.773609	0.839019
6	3.493397	2.040602	2.144462
6	3.180357	3.011582	1.248067
1	4.423911	1.889965	2.676720
1	3.799712	3.824911	0.892798
7	0.046167	-0.709438	2.332044
6	-0.727788	-1.786863	2.666733
6	1.211957	-0.853313	3.033897
6	-0.015422	-2.655658	3.572480
6	1.184055	-2.069105	3.810939
1	-0.409339	-3.575878	3.984420
1	1.984117	-2.408752	4.456103
7	-2.362345	0.129524	1.086245
6	-2.806715	-1.072368	1.557448
6	-3.440665	0.730139	0.501255
6	-4.207385	-1.234872	1.268155
6	-4.605423	-0.107096	0.622562
1	-4.802099	-2.096070	1.545600
1	-5.591259	0.144681	0.252812
6	0.092811	-0.147936	-0.942161
6	-3.411700	1.945682	-0.169617
6	-2.039814	-1.987504	2.265988
6	1.119461	3.571803	-0.053040
6	2.281127	0.029283	3.005813
1	-2.529807	-2.897797	2.599060
1	-4.344316	2.303528	-0.595416
1	1.645289	4.416584	-0.487365
1	3.153604	-0.223982	3.600878
1	0.223998	-1.504864	-0.556189
6	1.391059	0.188570	-1.518183
6	1.565833	0.735909	-2.805816
6	2.536830	-0.055966	-0.735904
6	2.837759	1.019853	-3.280986
1	0.694180	0.958327	-3.408998
6	3.808124	0.198868	-1.229304
1	2.412911	-0.456968	0.261352
6	3.962206	0.740013	-2.503033
1	2.956690	1.455400	-4.268796
1	4.675676	-0.004598	-0.609189
1	4.955295	0.956111	-2.886899
6	-1.091391	-0.136645	-1.832645
8	-1.883564	-1.209781	-1.683296
8	-1.377396	0.796474	-2.558888
6	-3.096762	-1.209278	-2.443034
1	-3.720373	-0.377084	-2.104369
1	-2.860013	-1.048415	-3.499666

6	-3.765326	-2.546149	-2.205269
1	-4.708071	-2.596076	-2.759376
1	-3.123372	-3.367963	-2.538574
1	-3.978715	-2.675854	-1.140562
6	0.347315	-2.721896	-0.615819
6	0.428477	-3.243924	-2.041374
6	1.537556	-3.009673	0.204736
6	1.812018	-3.036182	-2.665179
1	-0.350406	-2.785291	-2.655186
1	0.202589	-4.319878	-2.003307
6	2.700019	-3.409859	-0.329993
1	1.453079	-2.876482	1.278434
6	2.921955	-3.636059	-1.797503
1	1.837498	-3.482171	-3.665419
1	1.997303	-1.966327	-2.793183
1	3.535395	-3.627702	0.333396
1	3.000271	-4.720813	-1.968864
1	3.893048	-3.216792	-2.089156
1	-0.595328	-2.965637	-0.118453

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**Conf1**

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Number of imaginary frequencies: 11	Electronic energy:	HF=-5382.32996648
Zero-point correction=	2.261473 (Hartree/Particle)	
Thermal correction to Energy=	2.394744	
Thermal correction to Enthalpy=	2.395688	
Thermal correction to Gibbs Free Energy=	2.052514	
Sum of electronic and zero-point Energies=	-5380.068494	
Sum of electronic and thermal Energies=	-5379.935223	
Sum of electronic and thermal Enthalpies=	-5379.934278	
Sum of electronic and thermal Free Energies=	-5380.277452	

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Cartesian Coordinates

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6	3.206294	6.629563	-3.731618
6	2.153051	7.670162	-3.333022
6	1.886598	8.765573	-4.385306
6	0.695647	9.639720	-3.963957
6	3.124156	9.636189	-4.653647
6	6.191664	-4.114068	-4.393527
6	7.283009	-3.198724	-3.855742
8	8.436604	-3.569574	-3.666328
6	5.862824	-5.327486	-3.483658
6	7.013160	-6.342651	-3.414358
6	5.413288	-4.885103	-2.083344
7	6.893837	-1.908639	-3.573156
6	7.877048	-0.900431	-3.187245
6	8.306413	-0.979335	-1.707015
8	9.352462	-0.454213	-1.345526
6	7.357604	0.507923	-3.496991

7	7.431158	-1.605534	-0.873523
6	7.702552	-1.819538	0.535800
6	6.815287	-0.983274	1.484562
6	7.052045	0.509664	1.399690
6	6.189902	1.339099	0.670343
6	8.151735	1.095902	2.043905
6	6.419585	2.714695	0.585144
6	8.385418	2.468918	1.961722
6	7.518058	3.284492	1.230380
6	0.631966	-2.844843	-4.585066
6	0.166074	-3.967144	-3.664248
8	0.925805	-4.583915	-2.903906
6	2.147509	-2.654686	-4.574808
7	-1.157020	-4.231776	-3.760740
6	-1.838415	-5.111186	-2.834886
6	0.103589	-7.228026	1.610397
6	0.934247	-6.585780	0.496424
8	0.053011	-6.363105	-0.602726
6	2.120891	-7.459074	0.074876
6	3.456181	-3.494206	6.571312
6	2.321854	-4.529425	6.589621
6	2.054122	-5.083129	5.182631
6	2.624205	-5.661406	7.582447
6	6.949953	3.401915	6.146951
6	5.542599	3.231694	5.585916
8	4.647157	3.721596	6.588995
6	5.230647	1.778263	5.225388
6	-3.118180	1.253599	5.829510
6	-3.647297	2.644972	5.434597
6	-5.146710	2.659068	5.215071
6	-6.018105	3.046924	6.242573
6	-5.694379	2.250944	3.989265
6	-7.402376	3.028137	6.058551
6	-7.078097	2.230085	3.804536
6	-7.937313	2.617762	4.835772
6	-5.656015	0.907523	-1.983282
6	-7.004627	0.213604	-1.885828
8	-7.984698	0.568749	-2.545674
6	-5.201803	1.743322	-0.757816
16	-4.332719	0.828599	0.584777
7	-7.056334	-0.876695	-1.060888
6	-8.311077	-1.595644	-0.880008
6	-8.659724	-2.507188	-2.067599
6	-10.048726	-3.166721	-1.971870
6	-10.394046	-3.885129	-3.285415
6	-10.165276	-4.135303	-0.783545
26	-1.904262	0.365543	-0.033524
6	-1.431592	3.732715	-0.291248
6	-0.999295	0.479980	3.250967
6	-3.250000	-2.701296	0.411984

6	-2.588927	0.209649	-3.391483
7	-1.354177	1.835823	1.251900
6	-1.185954	3.155574	0.951496
6	-0.648323	3.875113	2.102014
6	-0.466512	2.941521	3.086199
6	-0.939176	1.674024	2.542701
6	0.133929	3.128660	4.447721
6	-0.310545	5.339578	2.130944
6	1.068697	5.676246	1.523663
6	1.382476	7.175614	1.549924
7	-2.033377	-0.903796	1.522580
6	-1.563852	-0.708949	2.790458
6	-1.801036	-1.882230	3.612589
6	-2.487024	-2.775149	2.819702
6	-2.611184	-2.138125	1.510379
6	-1.330824	-2.063373	5.023427
6	-2.957904	-4.119539	3.124030
6	-3.284559	-4.619918	4.328195
7	-2.652757	-1.029584	-1.288203
6	-3.284433	-2.175362	-0.877355
6	-3.953523	-2.809438	-1.990027
6	-3.622672	-2.079229	-3.114736
6	-2.845781	-0.934649	-2.635416
6	-4.854180	-4.002341	-1.872237
6	-4.013829	-2.403036	-4.480371
6	-3.369526	-2.104857	-5.625550
7	-1.981276	1.708665	-1.553343
6	-2.245191	1.452454	-2.871065
6	-2.215289	2.683677	-3.646965
6	-1.945654	3.692276	-2.759322
6	-1.787853	3.057563	-1.455560
6	-2.490282	2.778470	-5.119055
6	-1.885677	5.171267	-3.020981
6	-3.196128	5.912733	-2.677522
6	-3.116510	7.419196	-2.943306
1	8.756265	-1.571883	0.688392
1	7.566459	-2.884053	0.766315
1	6.539458	-4.484116	-5.366440
1	5.268456	-3.548847	-4.574181
1	3.627701	-3.069926	7.568370
1	4.397266	-3.952132	6.237701
1	3.228146	-2.666778	5.888808
1	7.697198	3.102995	5.403866
1	7.126342	4.447012	6.422214
1	7.078329	2.785258	7.044213
1	3.299030	5.854806	-2.963411
1	2.934787	6.133152	-4.671754
1	4.197055	7.078419	-3.866831
1	0.722376	-7.421995	2.493975
1	-0.718450	-6.566247	1.901148

1	-0.322171	-8.178000	1.265002
1	-2.043083	1.282713	6.038563
1	-3.626263	0.889650	6.731733
1	-3.290334	0.531314	5.027182
1	-2.828062	-5.337847	-3.235397
1	-1.281084	-6.044251	-2.727771
1	-1.944883	-4.665362	-1.842160
1	0.147953	-1.921312	-4.255924
1	0.275119	-3.059908	-5.602101
1	-5.749764	1.573693	-2.849369
1	-4.892211	0.169421	-2.214561
1	-9.123738	-0.869051	-0.745769
1	-8.224687	-2.174607	0.045643
1	-4.059180	7.919692	-2.692853
1	-2.323287	7.887229	-2.345756
1	-2.900181	7.626505	-3.999615
1	2.366851	7.387352	1.115395
1	0.637415	7.746498	0.981282
1	1.380919	7.564327	2.576310
1	2.449795	8.149762	-2.388019
1	1.206861	7.151592	-3.124767
1	1.617823	8.261779	-5.327372
1	0.470006	10.399527	-4.722278
1	-0.208253	9.038279	-3.811190
1	0.909178	10.163935	-3.022839
1	2.905355	10.409811	-5.399852
1	3.449071	10.143872	-3.735326
1	3.969737	9.048076	-5.026542
1	5.005462	-5.823592	-3.960061
1	6.720380	-7.209225	-2.809086
1	7.279328	-6.705621	-4.414733
1	7.909663	-5.894720	-2.977246
1	5.095341	-5.748479	-1.487896
1	6.235137	-4.399286	-1.540894
1	4.564284	-4.192582	-2.132784
1	5.974677	-1.601608	-3.861646
1	8.796003	-1.090099	-3.749951
1	8.106289	1.242725	-3.191097
1	7.163724	0.626070	-4.569110
1	6.433543	0.719447	-2.945169
1	6.634594	-2.062485	-1.295671
1	7.019561	-1.332677	2.506047
1	5.759464	-1.205286	1.286655
1	5.318495	0.907175	0.185765
1	8.833938	0.468083	2.613703
1	5.734136	3.340787	0.019286
1	9.245499	2.901735	2.466666
1	7.696488	4.354825	1.166964
1	2.435925	-1.861347	-5.274588
1	2.480764	-2.370001	-3.573144

1	2.667041	-3.576661	-4.858656
1	-1.732940	-3.594373	-4.296963
1	1.318495	-5.621588	0.867667
1	0.500748	-5.827376	-1.289239
1	2.686186	-6.976461	-0.732012
1	2.807722	-7.633343	0.912973
1	1.765666	-8.429063	-0.293403
1	1.407587	-4.019625	6.928501
1	1.228194	-5.804485	5.187426
1	1.789716	-4.283524	4.480919
1	2.942619	-5.595412	4.788992
1	1.800884	-6.384800	7.625306
1	3.531049	-6.206988	7.288091
1	2.784227	-5.273246	8.596083
1	5.451782	3.847270	4.674709
1	3.743323	3.586071	6.263560
1	4.206391	1.679981	4.842690
1	5.910161	1.411792	4.447157
1	5.326290	1.138188	6.110555
1	-3.137683	2.970620	4.519999
1	-3.387203	3.367456	6.220477
1	-5.605849	3.370948	7.197234
1	-5.047203	1.948369	3.166214
1	-8.060641	3.337117	6.867973
1	-7.478251	1.910146	2.845879
1	-9.014670	2.603478	4.686869
1	-6.069703	2.250881	-0.317652
1	-4.536144	2.528795	-1.128098
1	-6.297471	-0.980227	-0.390859
1	-7.891083	-3.286576	-2.171446
1	-8.617825	-1.889317	-2.970786
1	-10.787860	-2.363461	-1.826893
1	-11.159384	-4.598815	-0.748033
1	-9.425507	-4.943281	-0.866021
1	-10.002114	-3.632602	0.175991
1	-1.287295	4.805167	-0.370262
1	-0.635036	0.493358	4.271195
1	-3.761839	-3.644655	0.566897
1	-2.836254	0.173053	-4.444544
1	-0.539614	2.799386	5.247964
1	1.063257	2.550990	4.552850
1	0.374478	4.180598	4.634607
1	-0.335956	5.703914	3.166766
1	-1.081557	5.912537	1.596900
1	1.104793	5.305281	0.491364
1	1.842534	5.123418	2.072942
1	-1.127474	-3.121101	5.226310
1	-0.409853	-1.501205	5.213492
1	-2.073696	-1.728540	5.761093
1	-3.049798	-4.786901	2.266859

1	-3.605204	-5.653051	4.431479
1	-3.270656	-4.022946	5.234475
1	-5.182107	-4.365421	-2.850925
1	-4.369133	-4.840649	-1.358029
1	-5.753678	-3.748861	-1.298207
1	-4.921489	-3.000880	-4.567823
1	-3.769111	-2.420267	-6.585249
1	-2.442778	-1.538701	-5.648020
1	-2.276124	3.781824	-5.501917
1	-1.882061	2.068679	-5.694842
1	-3.540785	2.557469	-5.351347
1	-1.647658	5.351291	-4.078399
1	-1.064221	5.626043	-2.447648
1	-3.444283	5.731023	-1.624483
1	-4.014494	5.472796	-3.261841
1	-9.683768	-4.699002	-3.484835
1	-11.399343	-4.324190	-3.249755
1	-10.356036	-3.195054	-4.136547
6	-0.122138	0.069825	-0.327058
6	0.980127	-0.172066	0.652103
6	1.804096	0.930841	0.972212
6	1.252868	-1.395195	1.313977
6	2.803887	0.859894	1.938902
1	1.612870	1.872999	0.471079
6	2.277535	-1.464167	2.269622
6	3.039689	-0.348702	2.599328
1	3.399809	1.739690	2.164995
1	2.450362	-2.427485	2.740785
1	3.821499	-0.426421	3.350655
6	0.460555	0.275860	-1.686223
8	0.522150	-0.611148	-2.520621
8	0.967130	1.509531	-1.903289
6	1.531885	1.729886	-3.211826
1	2.331750	1.001067	-3.384033
1	0.754590	1.558636	-3.962427
6	2.045093	3.156086	-3.248417
1	1.226751	3.860800	-3.073833
1	2.810558	3.315607	-2.481291
1	2.488100	3.371303	-4.227456
8	0.573531	-2.559613	1.120436
6	0.325449	-2.982528	-0.224501
1	-0.360458	-2.311830	-0.743811
1	1.264497	-3.051181	-0.784980
1	-0.121454	-3.972653	-0.144904

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**Conf2**

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Number of imaginary frequencies: 8    Electronic energy:    HF=-5382.3246545  
Zero-point correction=                    2.260429 (Hartree/Particle)  
Thermal correction to Energy=            2.396879



Thermal correction to Enthalpy=	2.397823
Thermal correction to Gibbs Free Energy=	2.038162
Sum of electronic and zero-point Energies=	-5380.064225
Sum of electronic and thermal Energies=	-5379.927775
Sum of electronic and thermal Enthalpies=	-5379.926831
Sum of electronic and thermal Free Energies=	-5380.286492

.....  
 Cartesian Coordinates  
 .....

6	2.179310	6.821458	-3.591402
6	0.984254	7.219859	-4.465936
6	0.267669	6.045898	-5.163450
6	-1.014440	6.533426	-5.854884
6	1.174335	5.320445	-6.170041
6	7.077798	-3.210682	-3.976103
6	7.985748	-2.092028	-3.484581
8	9.198731	-2.216970	-3.356149
6	7.160073	-4.512243	-3.135238
6	8.489762	-5.256289	-3.329253
6	6.875602	-4.248453	-1.649018
7	7.349900	-0.913742	-3.163743
6	8.108870	0.266435	-2.763262
6	8.483905	0.291470	-1.266202
8	9.344821	1.064992	-0.864630
6	7.356309	1.550606	-3.127538
7	7.775847	-0.553845	-0.469474
6	7.964624	-0.634000	0.965632
6	6.825587	0.026856	1.777119
6	6.722152	1.520847	1.560181
6	5.798173	2.058909	0.654781
6	7.583835	2.398948	2.233906
6	5.750097	3.435109	0.415749
6	7.531932	3.774294	2.005716
6	6.615713	4.297377	1.090536
6	1.390584	-2.970168	-4.381773
6	1.082346	-4.158174	-3.476639
8	1.911360	-4.626570	-2.683919
6	2.802901	-3.042547	-4.969594
7	-0.169591	-4.647534	-3.607869
6	-0.693243	-5.629675	-2.682875
6	1.432081	-7.318037	1.860893
6	1.840675	-6.222454	0.869629
8	1.500873	-6.679430	-0.435376
6	3.334758	-5.893218	0.964487
6	3.868753	-2.992413	6.875265
6	3.645538	-4.511800	6.884448
6	3.182467	-5.013199	5.508437
6	4.909586	-5.251422	7.347076
6	6.073547	4.417839	6.462757
6	4.767806	3.690422	6.161560

8	4.041015	3.646323	7.393959
6	4.995560	2.285124	5.601421
6	-3.422770	0.479569	5.828866
6	-4.620345	1.366747	5.439844
6	-5.908675	0.582383	5.293603
6	-6.740207	0.358828	6.400670
6	-6.278478	0.037324	4.055047
6	-7.911001	-0.392370	6.281858
6	-7.449295	-0.714656	3.935671
6	-8.269254	-0.933560	5.044976
6	-5.563436	-0.393520	-2.061453
6	-6.640400	-1.462636	-2.130193
8	-7.405805	-1.575669	-3.091651
6	-5.587163	0.544166	-0.824280
16	-4.513125	0.036045	0.584204
7	-6.701987	-2.326858	-1.071419
6	-7.762252	-3.325404	-1.011715
6	-7.487052	-4.560398	-1.884785
6	-8.663464	-5.551502	-1.970758
6	-8.375151	-6.639018	-3.017100
6	-9.001990	-6.188851	-0.613171
26	-1.937134	0.661019	-0.005562
6	-3.220433	3.783158	-0.401765
6	-1.128414	1.354186	3.202466
6	-2.078769	-2.648692	0.700409
6	-2.317169	0.037390	-3.307161
7	-2.133311	2.273007	1.174484
6	-2.751961	3.447006	0.864796
6	-2.760777	4.338852	2.020377
6	-2.089632	3.681660	3.016756
6	-1.724067	2.377915	2.474145
6	-1.790897	4.153223	4.408885
6	-3.370396	5.712837	2.050325
6	-2.447747	6.823458	1.502994
6	-3.111379	8.204410	1.509512
7	-1.561229	-0.453281	1.614303
6	-1.097100	0.011175	2.815554
6	-0.759694	-1.093050	3.689426
6	-1.126128	-2.246152	3.019493
6	-1.620567	-1.814401	1.716990
6	-0.110165	-0.969506	5.034164
6	-1.008728	-3.638177	3.427052
6	-0.894111	-4.128071	4.675335
7	-2.025807	-1.011565	-1.126063
6	-2.305300	-2.255341	-0.615691
6	-2.786858	-3.128067	-1.659440
6	-2.650217	-2.432238	-2.847021
6	-2.218658	-1.082214	-2.470201
6	-3.464062	-4.441186	-1.403160
6	-2.990112	-2.943335	-4.167749

6	-2.471778	-2.588563	-5.360744
7	-2.584729	1.730109	-1.557274
6	-2.552535	1.334687	-2.866703
6	-3.004876	2.419499	-3.730703
6	-3.354028	3.451868	-2.904246
6	-3.067174	3.004135	-1.544291
6	-3.101985	2.338707	-5.225053
6	-3.955082	4.779486	-3.269545
6	-5.491208	4.826648	-3.118449
6	-6.083009	6.192560	-3.480280
1	8.916624	-0.142639	1.182225
1	8.050214	-1.688701	1.256017
1	7.370856	-3.435995	-5.009845
1	6.033960	-2.872657	-4.007919
1	4.161598	-2.624671	7.866483
1	4.664760	-2.719279	6.169771
1	2.960556	-2.457904	6.572213
1	6.666683	4.537780	5.549586
1	5.869846	5.408327	6.882636
1	6.663200	3.851146	7.192866
1	2.594365	7.693945	-3.072946
1	1.878168	6.093414	-2.827479
1	2.989831	6.376499	-4.180347
1	1.626862	-7.000314	2.891177
1	0.365526	-7.543908	1.758052
1	1.996299	-8.237131	1.662090
1	-2.517025	1.081931	5.962782
1	-3.620467	-0.051943	6.768545
1	-3.223720	-0.264005	5.051869
1	-1.690034	-5.924453	-3.012063
1	-0.050335	-6.513755	-2.663321
1	-0.747596	-5.239006	-1.662582
1	1.292903	-2.068133	-3.764575
1	0.642874	-2.895948	-5.179202
1	-5.696271	0.193665	-2.977430
1	-4.590050	-0.875587	-2.123661
1	-8.696587	-2.858561	-1.348001
1	-7.887001	-3.610608	0.038676
1	-7.173575	6.198105	-3.367520
1	-5.677546	6.984410	-2.837189
1	-5.853735	6.463246	-4.519225
1	-2.435435	8.976171	1.122054
1	-4.016490	8.212126	0.888938
1	-3.406993	8.498931	2.524781
1	1.310878	7.943318	-5.229149
1	0.252216	7.748102	-3.839533
1	-0.024527	5.324044	-4.386189
1	-1.552008	5.701890	-6.326132
1	-1.696051	7.009089	-5.139868
1	-0.784243	7.268316	-6.638730

1	0.641228	4.490634	-6.649149
1	1.505986	6.005553	-6.962713
1	2.069997	4.904622	-5.694830
1	6.355762	-5.157263	-3.515670
1	8.487129	-6.195999	-2.763604
1	8.651793	-5.501792	-4.386160
1	9.333285	-4.646114	-2.996117
1	6.843736	-5.188271	-1.086702
1	7.659109	-3.622408	-1.203539
1	5.907194	-3.751564	-1.506577
1	6.375385	-0.801852	-3.408472
1	9.067099	0.236959	-3.290129
1	7.940076	2.414170	-2.800430
1	7.198808	1.616062	-4.209825
1	6.382880	1.595414	-2.623163
1	7.111729	-1.170328	-0.916062
1	7.009762	-0.188335	2.838200
1	5.874787	-0.456663	1.519532
1	5.105516	1.397578	0.138869
1	8.309092	1.998403	2.939352
1	5.030374	3.833183	-0.294700
1	8.210996	4.436147	2.537401
1	6.574930	5.367883	0.907333
1	3.051621	-2.119635	-5.505572
1	3.530836	-3.195394	-4.167472
1	2.900154	-3.879334	-5.671151
1	-0.838076	-4.113859	-4.152355
1	1.267055	-5.310016	1.112027
1	1.699405	-5.975464	-1.085922
1	3.606797	-5.122068	0.233174
1	3.601919	-5.524556	1.962812
1	3.931347	-6.787930	0.749024
1	2.845256	-4.729603	7.607965
1	3.010919	-6.096831	5.517995
1	2.249843	-4.529388	5.195044
1	3.941266	-4.804406	4.742075
1	4.744995	-6.335054	7.390811
1	5.742990	-5.069903	6.655151
1	5.226542	-4.918621	8.343314
1	4.201583	4.278570	5.419290
1	3.215101	3.165702	7.227345
1	4.040237	1.782042	5.402634
1	5.551700	2.319536	4.657544
1	5.557247	1.677538	6.320938
1	-4.391584	1.874522	4.495835
1	-4.752186	2.147836	6.201805
1	-6.468010	0.782780	7.366475
1	-5.659556	0.201337	3.172317
1	-8.544325	-0.550463	7.152437
1	-7.716513	-1.124537	2.964792

1	-9.182151	-1.516911	4.946940
1	-6.616822	0.646471	-0.456849
1	-5.278902	1.539040	-1.157666
1	-6.124323	-2.115202	-0.259640
1	-6.595374	-5.084054	-1.510407
1	-7.251107	-4.196207	-2.890652
1	-9.546936	-4.988206	-2.309564
1	-9.833847	-6.898523	-0.706779
1	-8.138830	-6.739949	-0.215711
1	-9.289934	-5.440418	0.133154
1	-3.662412	4.765969	-0.524788
1	-0.797707	1.589074	4.208349
1	-2.246716	-3.692445	0.942152
1	-2.450287	-0.143499	-4.365993
1	-2.190360	3.467938	5.167207
1	-0.709811	4.235563	4.587830
1	-2.226425	5.140087	4.596499
1	-3.654661	5.968657	3.080080
1	-4.306520	5.714766	1.475049
1	-2.136871	6.561832	0.483681
1	-1.528478	6.849988	2.103142
1	0.606107	-1.785284	5.191832
1	0.433897	-0.023815	5.129736
1	-0.835545	-1.015061	5.858210
1	-1.019415	-4.362312	2.612514
1	-0.804875	-5.197913	4.842422
1	-0.921258	-3.500187	5.559614
1	-3.679638	-4.985659	-2.326620
1	-2.876202	-5.104180	-0.758340
1	-4.421756	-4.263075	-0.899271
1	-3.735631	-3.739458	-4.172959
1	-2.823296	-3.050526	-6.279081
1	-1.709500	-1.821409	-5.462230
1	-3.363813	3.308670	-5.660632
1	-2.154083	2.017756	-5.676578
1	-3.868404	1.619649	-5.544889
1	-3.696637	5.030039	-4.307349
1	-3.513117	5.573774	-2.651502
1	-5.759211	4.564839	-2.087135
1	-5.933927	4.047405	-3.752197
1	-7.496323	-7.233121	-2.732053
1	-9.222032	-7.329351	-3.121427
1	-8.174184	-6.199135	-4.001125
6	-0.200667	1.061012	-0.440412
6	0.883590	0.169064	-0.882764
6	1.015627	-1.120074	-0.332898
6	1.900525	0.576469	-1.801290
6	2.106294	-1.942850	-0.607302
1	0.258996	-1.454436	0.358715
6	2.992134	-0.249036	-2.087557

6	3.097160	-1.504938	-1.480743
1	2.170123	-2.926498	-0.154338
1	3.749440	0.074515	-2.794023
1	3.940066	-2.149266	-1.717879
6	0.251242	2.495059	-0.344923
8	-0.172185	3.460582	-0.942930
8	1.270088	2.576044	0.568305
6	1.886614	3.864243	0.746242
1	2.935750	3.641517	0.960097
1	1.815575	4.421391	-0.192383
6	1.256211	4.646744	1.888490
1	0.207116	4.864917	1.675041
1	1.307482	4.075588	2.821336
1	1.792250	5.593816	2.031773
8	1.722236	1.789705	-2.390283
6	2.706824	2.294836	-3.268045
1	3.683987	2.390070	-2.773043
1	2.816656	1.661971	-4.159572
1	2.355259	3.283306	-3.568540

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**Conf3**

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Number of imaginary frequencies: 13    Electronic energy:    HF=-5382.30501543  
Zero-point correction=                    2.260410 (Hartree/Particle)  
Thermal correction to Energy=            2.392461  
Thermal correction to Enthalpy=         2.393405  
Thermal correction to Gibbs Free Energy= 2.053764  
Sum of electronic and zero-point Energies= -5380.044605  
Sum of electronic and thermal Energies= -5379.912554  
Sum of electronic and thermal Enthalpies= -5379.911610  
Sum of electronic and thermal Free Energies= -5380.251251

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Cartesian Coordinates

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6	3.374570	7.318053	-2.878258
6	2.390751	8.329666	-2.279199
6	2.523847	9.767644	-2.819898
6	1.376566	10.646952	-2.299510
6	3.883135	10.398908	-2.480500
6	6.090513	-3.334378	-4.858980
6	7.234917	-2.487488	-4.321369
8	8.409127	-2.839158	-4.366699
6	5.996925	-4.748983	-4.225976
6	7.127336	-5.676563	-4.696287
6	5.925320	-4.688396	-2.692166
7	6.860509	-1.293796	-3.749020
6	7.840674	-0.345968	-3.235684
6	8.182992	-0.533320	-1.741842
8	9.092884	0.117819	-1.237867
6	7.392094	1.099165	-3.481420

7	7.413549	-1.427809	-1.070198
6	7.586147	-1.722601	0.338585
6	6.398194	-1.277543	1.210261
6	6.126795	0.215398	1.247160
6	4.848082	0.709560	0.959843
6	7.124215	1.129414	1.622304
6	4.557508	2.072397	1.068546
6	6.845068	2.493968	1.713130
6	5.558042	2.970065	1.443466
6	0.570842	-1.898916	-4.953549
6	-0.227132	-3.180549	-4.814420
8	-0.088585	-4.128018	-5.588022
6	0.356540	-1.266801	-6.337787
7	-1.095819	-3.190528	-3.769721
6	-1.984531	-4.299001	-3.533249
6	-0.165246	-7.012578	0.630908
6	0.848523	-5.909181	0.312593
8	1.009618	-5.746807	-1.102699
6	2.236237	-6.224878	0.861392
6	3.206982	-4.028025	6.063195
6	2.716876	-5.255100	6.846872
6	1.710792	-6.071491	6.022307
6	3.896932	-6.126671	7.301330
6	6.883542	2.767806	6.556224
6	5.622466	1.931981	6.360792
8	5.115450	1.658643	7.672846
6	5.889913	0.637435	5.590202
6	-3.230808	0.953675	5.851279
6	-3.801002	2.326295	5.446617
6	-5.298693	2.289212	5.217215
6	-6.190758	2.609350	6.250537
6	-5.822136	1.899149	3.975286
6	-7.572046	2.541324	6.055977
6	-7.202999	1.829332	3.779921
6	-8.083016	2.149166	4.816851
6	-5.657793	1.666469	-1.971975
6	-7.025046	0.998116	-1.979721
8	-7.961352	1.429299	-2.659631
6	-5.057865	2.133719	-0.621764
16	-4.369379	0.853772	0.522264
7	-7.138494	-0.145412	-1.246644
6	-8.393159	-0.881982	-1.225661
6	-8.610943	-1.738134	-2.484245
6	-9.989808	-2.421054	-2.560328
6	-10.191730	-3.074950	-3.935981
6	-10.203288	-3.451481	-1.439350
26	-1.870391	0.226821	0.088558
6	-1.000794	3.513392	-0.206689
6	-1.203233	0.354357	3.431210
6	-3.355244	-2.814774	0.498530

6	-2.664088	0.164960	-3.249707
7	-1.292658	1.676892	1.380890
6	-0.949024	2.958518	1.066487
6	-0.461866	3.665569	2.246203
6	-0.482885	2.759463	3.268813
6	-1.021863	1.525740	2.710444
6	-0.019886	2.944343	4.683120
6	0.022981	5.088005	2.272782
6	1.494089	5.254984	1.834184
6	1.966475	6.711969	1.874061
7	-2.206652	-1.008697	1.669817
6	-1.786351	-0.820664	2.956914
6	-2.034142	-2.004801	3.756929
6	-2.655747	-2.910419	2.921585
6	-2.744366	-2.260561	1.618097
6	-1.640119	-2.198761	5.190083
6	-3.106856	-4.268395	3.190764
6	-3.425953	-4.813845	4.378030
7	-2.733521	-1.126231	-1.175883
6	-3.425281	-2.237006	-0.764687
6	-4.270929	-2.733132	-1.827853
6	-4.044874	-1.927393	-2.919663
6	-3.077387	-0.922607	-2.481197
6	-5.176540	-3.923606	-1.725859
6	-4.699386	-2.044506	-4.223885
6	-4.149785	-1.867242	-5.435364
7	-1.744118	1.538900	-1.444759
6	-2.047391	1.307910	-2.758477
6	-1.804108	2.497197	-3.562365
6	-1.389340	3.468477	-2.693295
6	-1.361150	2.847720	-1.372781
6	-2.036879	2.596004	-5.040916
6	-1.105505	4.915306	-2.986414
6	-2.323205	5.837144	-2.756011
6	-2.025694	7.309731	-3.055162
1	8.508593	-1.222477	0.642910
1	7.736721	-2.802825	0.466829
1	6.247094	-3.441725	-5.940245
1	5.132303	-2.817532	-4.729948
1	3.896416	-3.419453	6.661302
1	3.739489	-4.337234	5.154114
1	2.369276	-3.388925	5.760086
1	7.305246	3.060661	5.587888
1	6.655907	3.673083	7.128615
1	7.637974	2.194294	7.108812
1	3.175892	6.309117	-2.498800
1	3.288933	7.283080	-3.971966
1	4.414973	7.559709	-2.633670
1	-0.283668	-7.139044	1.713709
1	-1.152301	-6.768994	0.216552



1	0.161684	-7.965295	0.197575
1	-2.162856	1.018287	6.079557
1	-3.741787	0.581335	6.749565
1	-3.376349	0.225215	5.052355
1	-2.940291	-4.185543	-4.055390
1	-1.498731	-5.205835	-3.905799
1	-2.181747	-4.395154	-2.462283
1	1.624931	-2.165625	-4.844597
1	0.335474	-1.183231	-4.161088
1	-5.773211	2.541604	-2.623309
1	-4.944954	0.992932	-2.457622
1	-9.218563	-0.163775	-1.141253
1	-8.394914	-1.503727	-0.323792
1	-2.909912	7.936723	-2.890905
1	-1.223291	7.692588	-2.410712
1	-1.707383	7.448461	-4.096562
1	3.013969	6.803222	1.562007
1	1.364273	7.343285	1.207976
1	1.883266	7.129214	2.885801
1	2.504612	8.348575	-1.184868
1	1.366977	7.979664	-2.471210
1	2.438898	9.718302	-3.917160
1	1.434679	11.663084	-2.708604
1	0.399162	10.230072	-2.570732
1	1.410975	10.727421	-1.204870
1	3.949904	11.421406	-2.871989
1	4.027414	10.450097	-1.392831
1	4.718951	9.829409	-2.901234
1	5.047272	-5.168533	-4.586060
1	7.001269	-6.679263	-4.269844
1	7.125542	-5.774638	-5.788875
1	8.103954	-5.286278	-4.397969
1	5.762996	-5.687798	-2.273075
1	6.862475	-4.302496	-2.271022
1	5.099388	-4.052979	-2.348083
1	5.898936	-0.992402	-3.829745
1	8.775943	-0.540320	-3.768847
1	8.135660	1.781461	-3.063664
1	7.284019	1.295795	-4.553302
1	6.433918	1.304154	-2.986513
1	6.698451	-1.914843	-1.591865
1	6.591975	-1.642264	2.230315
1	5.494773	-1.799266	0.871209
1	4.055687	0.029152	0.662116
1	8.130112	0.776295	1.835263
1	3.542990	2.411324	0.878111
1	7.634281	3.185482	1.999089
1	5.338606	4.031469	1.529147
1	1.017734	-0.404255	-6.480866
1	0.562513	-2.001992	-7.121760

1	-0.676688	-0.920118	-6.463723
1	-1.215802	-2.352504	-3.217724
1	0.499579	-4.962364	0.755312
1	0.156774	-5.476648	-1.479053
1	2.945677	-5.444416	0.567035
1	2.216249	-6.282303	1.955808
1	2.596305	-7.181712	0.464452
1	2.198478	-4.893946	7.748096
1	1.343148	-6.938558	6.584868
1	0.842401	-5.465923	5.736117
1	2.174692	-6.446414	5.099677
1	3.554991	-6.985773	7.891634
1	4.449993	-6.516546	6.436191
1	4.602594	-5.555145	7.916763
1	4.886996	2.531556	5.797520
1	4.310090	1.127921	7.566776
1	4.969636	0.046231	5.486949
1	6.259373	0.847147	4.579939
1	6.630524	0.026378	6.121213
1	-3.297223	2.664090	4.533432
1	-3.569806	3.059917	6.231398
1	-5.797527	2.919676	7.217786
1	-5.158118	1.652294	3.146621
1	-8.247069	2.798615	6.869758
1	-7.583489	1.526371	2.807755
1	-9.158143	2.097774	4.659845
1	-5.819373	2.696121	-0.066433
1	-4.257163	2.842455	-0.858680
1	-6.373897	-0.373186	-0.610639
1	-7.820611	-2.500460	-2.546639
1	-8.491178	-1.075000	-3.348285
1	-10.754543	-1.636636	-2.448233
1	-11.187233	-3.929981	-1.524936
1	-9.443808	-4.243709	-1.489418
1	-10.143345	-2.996642	-0.444580
1	-0.721820	4.557664	-0.300109
1	-0.886162	0.366644	4.465662
1	-3.886113	-3.750841	0.635507
1	-2.972513	0.179896	-4.287462
1	-0.821961	2.770546	5.410906
1	0.796393	2.251981	4.929798
1	0.355323	3.959641	4.847183
1	-0.087968	5.495574	3.286599
1	-0.611892	5.715003	1.631147
1	1.611950	4.851423	0.820113
1	2.129735	4.637166	2.481936
1	-1.347116	-3.240857	5.369799
1	-0.797095	-1.557718	5.470491
1	-2.459982	-1.972279	5.885913
1	-3.189001	-4.911772	2.314531

1	-3.734488	-5.853728	4.444306
1	-3.423310	-4.250015	5.304899
1	-5.766381	-4.054771	-2.637785
1	-4.612013	-4.854649	-1.571374
1	-5.874539	-3.830442	-0.884910
1	-5.751588	-2.328782	-4.185611
1	-4.743455	-1.979878	-6.338324
1	-3.098685	-1.630698	-5.570449
1	-1.673657	3.549285	-5.438998
1	-1.526192	1.792892	-5.587670
1	-3.104068	2.523666	-5.290534
1	-0.776015	5.023493	-4.028965
1	-0.269081	5.275919	-2.370171
1	-2.663447	5.727276	-1.718752
1	-3.152575	5.489188	-3.385012
1	-9.449453	-3.866715	-4.105784
1	-11.186823	-3.530167	-4.021435
1	-10.084904	-2.341055	-4.743491
6	-0.157318	-0.363755	-0.035594
6	0.780568	-0.764064	-1.133930
6	1.019362	-2.131978	-1.340253
6	1.662132	0.165589	-1.740327
6	2.111274	-2.589092	-2.080357
1	0.364060	-2.849444	-0.859324
6	2.753292	-0.289375	-2.491576
6	2.984578	-1.659946	-2.637795
1	2.261742	-3.658247	-2.194712
1	3.436202	0.424244	-2.939695
1	3.846060	-1.998405	-3.206856
6	0.715346	-0.587248	1.178390
8	1.473567	0.250441	1.629748
8	0.641446	-1.857651	1.638889
6	1.434805	-2.180974	2.801930
1	1.352116	-1.360754	3.520236
1	0.944709	-3.066544	3.213499
6	2.889845	-2.456621	2.452968
1	2.963935	-3.188243	1.641212
1	3.388378	-1.534204	2.149378
1	3.411741	-2.858681	3.329145
8	1.416584	1.478836	-1.489539
6	2.239246	2.454860	-2.099936
1	3.278790	2.382475	-1.752334
1	2.212176	2.377205	-3.195366
1	1.821841	3.416782	-1.798660

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**Conf4**

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Number of imaginary frequencies:10	Electronic energy:	HF=-5382.32543821
Zero-point correction=	2.260978 (Hartree/Particle)	
Thermal correction to Energy=	2.395718	

Thermal correction to Enthalpy=	2.396662
Thermal correction to Gibbs Free Energy=	2.044978
Sum of electronic and zero-point Energies=	-5380.064460
Sum of electronic and thermal Energies=	-5379.929721
Sum of electronic and thermal Enthalpies=	-5379.928776
Sum of electronic and thermal Free Energies=	-5380.280461

.....  
 Cartesian Coordinates  
 .....

6	2.487692	7.040085	-3.236384
6	1.572806	8.022221	-2.495022
6	2.195083	9.402932	-2.204589
6	1.137329	10.363839	-1.640738
6	3.402192	9.315796	-1.257840
6	6.493586	-3.282479	-4.710060
6	7.534315	-2.259586	-4.277816
8	8.742360	-2.445843	-4.388236
6	6.642232	-4.667195	-4.025495
6	7.872300	-5.441126	-4.522623
6	6.632711	-4.548734	-2.494044
7	7.025280	-1.106949	-3.727009
6	7.883484	-0.009157	-3.301999
6	8.207653	-0.008272	-1.790894
8	8.992031	0.818778	-1.335359
6	7.301232	1.348270	-3.712752
7	7.578367	-0.958359	-1.050755
6	7.881460	-1.198921	0.347921
6	6.681309	-1.056488	1.296865
6	6.102068	0.338036	1.450805
6	4.713169	0.517486	1.467370
6	6.922703	1.461398	1.638386
6	4.148936	1.777314	1.679203
6	6.364934	2.722874	1.851297
6	4.976477	2.884240	1.879476
6	0.835292	-2.560324	-4.726256
6	0.472821	-3.798580	-3.919289
8	1.308070	-4.424366	-3.257835
6	2.099377	-2.772059	-5.567964
7	-0.831148	-4.157696	-3.980901
6	-1.363267	-5.177085	-3.106383
6	0.873874	-7.396129	1.146411
6	1.681420	-6.097560	1.044517
8	2.408512	-6.020759	-0.187426
6	2.717349	-5.985401	2.159208
6	3.953082	-3.703288	6.310714
6	3.762464	-4.843485	7.321218
6	2.665110	-5.813282	6.859311
6	5.083842	-5.584360	7.573805
6	6.745288	3.517989	6.328906
6	5.555847	2.625902	5.990621

8	4.674124	2.691327	7.117960
6	5.969397	1.183515	5.693569
6	-3.068869	0.408622	6.009955
6	-4.108200	1.485487	5.646912
6	-5.508090	0.923043	5.503726
6	-6.357494	0.824996	6.615330
6	-5.969384	0.458247	4.263217
6	-7.635217	0.274557	6.498451
6	-7.247279	-0.092764	4.145347
6	-8.084468	-0.187851	5.259351
6	-5.731498	0.359012	-1.768826
6	-6.966475	-0.526390	-1.774793
8	-7.923737	-0.333799	-2.528880
6	-5.454092	1.149021	-0.463400
16	-4.328590	0.307794	0.724215
7	-6.943769	-1.590982	-0.914864
6	-8.104327	-2.466111	-0.807876
6	-8.214798	-3.471001	-1.966046
6	-9.511422	-4.302974	-1.961393
6	-9.629082	-5.122784	-3.255519
6	-9.623427	-5.220336	-0.732662
26	-1.902282	0.486909	-0.167976
6	-2.348995	3.859974	-0.361252
6	-0.794919	0.790523	3.029004
6	-2.468838	-2.826413	0.336906
6	-2.793955	0.174897	-3.444212
7	-1.657957	2.027456	1.098511
6	-1.934755	3.338480	0.862146
6	-1.656704	4.142697	2.049580
6	-1.142668	3.281227	2.980018
6	-1.163743	1.955925	2.370529
6	-0.676590	3.581596	4.374158
6	-1.930583	5.615754	2.190034
6	-0.820831	6.545146	1.655066
6	-1.163459	8.029635	1.817768
7	-1.549930	-0.812019	1.350333
6	-1.012102	-0.510041	2.570895
6	-0.845100	-1.708808	3.367736
6	-1.378001	-2.744154	2.622738
6	-1.823598	-2.147916	1.366188
6	-0.252083	-1.776237	4.741585
6	-1.543907	-4.147724	2.967642
6	-0.878810	-4.864094	3.893608
7	-2.441232	-1.052985	-1.361803
6	-2.793478	-2.298325	-0.908929
6	-3.482584	-3.029706	-1.946750
6	-3.405194	-2.256786	-3.089929
6	-2.782409	-0.996396	-2.679413
6	-4.216982	-4.319612	-1.731372
6	-3.890507	-2.644046	-4.407916

6	-3.429346	-2.256037	-5.613152
7	-2.407594	1.776279	-1.632695
6	-2.668452	1.463151	-2.937777
6	-2.929544	2.670468	-3.711524
6	-2.855690	3.715186	-2.832073
6	-2.524634	3.132807	-1.534403
6	-3.243479	2.697440	-5.177597
6	-3.105581	5.173985	-3.091532
6	-4.538454	5.629804	-2.739914
6	-4.768926	7.122161	-2.998158
1	8.679708	-0.501228	0.609670
1	8.290104	-2.213681	0.454406
1	6.594503	-3.409703	-5.795815
1	5.480885	-2.901328	-4.526413
1	4.711516	-2.988195	6.651878
1	4.277002	-4.093864	5.337113
1	3.019100	-3.151081	6.150729
1	7.444612	3.563421	5.487031
1	6.406504	4.533592	6.558811
1	7.276028	3.127862	7.205473
1	1.956869	6.108623	-3.460588
1	2.834302	7.464666	-4.187575
1	3.375168	6.780525	-2.647869
1	0.311297	-7.430924	2.086554
1	0.154469	-7.474233	0.321445
1	1.539855	-8.265956	1.098524
1	-2.075153	0.853495	6.143396
1	-3.340110	-0.100819	6.942902
1	-2.999973	-0.344471	5.219084
1	-2.361863	-5.454169	-3.446088
1	-0.716951	-6.059171	-3.145327
1	-1.418120	-4.832190	-2.068369
1	1.009473	-1.758230	-3.999456
1	-0.002628	-2.245636	-5.359318
1	-5.886332	1.059230	-2.597572
1	-4.864408	-0.248196	-2.007887
1	-9.011165	-1.847574	-0.793124
1	-8.036510	-2.984919	0.154605
1	-5.793386	7.418333	-2.743572
1	-4.085507	7.739324	-2.400649
1	-4.601562	7.373947	-4.053498
1	-0.362342	8.671834	1.431765
1	-2.084201	8.285006	1.278334
1	-1.318147	8.288092	2.873083
1	1.245234	7.572909	-1.545229
1	0.659585	8.169591	-3.088304
1	2.547469	9.815797	-3.163460
1	1.557510	11.361359	-1.462601
1	0.289527	10.473076	-2.327829
1	0.742970	9.994513	-0.684572

1	3.823857	10.310117	-1.066205
1	3.107439	8.888699	-0.289871
1	4.203248	8.691221	-1.667539
1	5.747659	-5.234904	-4.317485
1	7.913321	-6.433228	-4.056424
1	7.834711	-5.582833	-5.609970
1	8.794690	-4.902996	-4.289050
1	6.638126	-5.540047	-2.027369
1	7.520409	-4.011020	-2.136439
1	5.736339	-4.026844	-2.136576
1	6.025812	-0.953224	-3.750032
1	8.845691	-0.166157	-3.798231
1	7.952948	2.143827	-3.344585
1	7.222032	1.421065	-4.802383
1	6.304906	1.500374	-3.278664
1	7.004316	-1.626251	-1.546277
1	7.013552	-1.422638	2.280551
1	5.886303	-1.743517	0.979466
1	4.046239	-0.326808	1.316597
1	8.003890	1.361090	1.600664
1	3.067586	1.871471	1.664032
1	7.017454	3.581927	1.989109
1	4.546541	3.868801	2.047332
1	2.422522	-1.833660	-6.031863
1	2.908411	-3.150886	-4.935891
1	1.928874	-3.504572	-6.365720
1	-1.495351	-3.534200	-4.421724
1	0.988431	-5.247466	1.126315
1	1.794421	-5.837108	-0.918093
1	3.270931	-5.044786	2.073082
1	2.232773	-6.016406	3.141159
1	3.435123	-6.812172	2.093897
1	3.438951	-4.398672	8.274625
1	2.504397	-6.614497	7.591305
1	1.709751	-5.294796	6.714206
1	2.936246	-6.283357	5.904616
1	4.960726	-6.378881	8.320231
1	5.452591	-6.049765	6.650051
1	5.862150	-4.901059	7.935035
1	5.051155	3.033644	5.099743
1	3.907812	2.131703	6.916889
1	5.090674	0.562993	5.475842
1	6.624842	1.135730	4.816960
1	6.491197	0.750904	6.555760
1	-3.808004	1.964071	4.707307
1	-4.104109	2.265598	6.420899
1	-6.014054	1.188711	7.582913
1	-5.336812	0.530105	3.378189
1	-8.280228	0.211718	7.372467
1	-7.584382	-0.442673	3.172805

1	-9.080627	-0.613910	5.162944
1	-6.399130	1.372675	0.048279
1	-5.014416	2.111172	-0.741155
1	-6.206065	-1.605192	-0.213802
1	-7.347010	-4.146364	-1.950904
1	-8.161347	-2.895435	-2.896321
1	-10.357102	-3.598246	-1.935093
1	-10.549182	-5.808895	-0.762371
1	-8.782628	-5.926508	-0.696130
1	-9.622862	-4.654844	0.205579
1	-2.510259	4.931561	-0.413208
1	-0.381798	0.903467	4.024955
1	-2.736055	-3.862917	0.511573
1	-3.105894	0.088320	-4.476944
1	-1.242108	3.015392	5.125417
1	0.382885	3.326609	4.513131
1	-0.788957	4.644502	4.611538
1	-2.099504	5.853965	3.248890
1	-2.871170	5.863185	1.678615
1	-0.640265	6.319983	0.596011
1	0.117292	6.321320	2.180334
1	0.794636	-2.113493	4.715954
1	-0.264618	-0.803335	5.240800
1	-0.802878	-2.483059	5.373645
1	-2.315439	-4.673936	2.405300
1	-1.132036	-5.905673	4.071907
1	-0.069316	-4.454554	4.488207
1	-4.559199	-4.760988	-2.672193
1	-3.608349	-5.073208	-1.217879
1	-5.104614	-4.146475	-1.110423
1	-4.697740	-3.377052	-4.403018
1	-3.876338	-2.635239	-6.527637
1	-2.614746	-1.546771	-5.729830
1	-3.308816	3.723884	-5.552919
1	-2.473866	2.179654	-5.764924
1	-4.200751	2.206422	-5.398539
1	-2.915480	5.398790	-4.149833
1	-2.389635	5.785350	-2.523936
1	-4.741117	5.397216	-1.686852
1	-5.252665	5.034645	-3.323458
1	-8.804997	-5.844459	-3.337992
1	-10.569061	-5.688498	-3.287547
1	-9.593516	-4.475319	-4.139579
6	-0.173119	0.489082	-0.690158
6	0.521748	1.332484	-1.708381
6	0.530375	0.919393	-3.047158
6	1.248512	2.497106	-1.370631
6	1.225956	1.624940	-4.032415
1	-0.042659	0.039628	-3.313045
6	1.950576	3.202989	-2.355304



6	1.940974	2.766258	-3.682584
1	1.200751	1.280152	-5.063040
1	2.516919	4.087981	-2.091017
1	2.494146	3.326377	-4.432616
6	0.808058	-0.499938	-0.140079
8	1.555447	-0.279821	0.796767
8	0.795343	-1.652008	-0.842454
6	1.678695	-2.705754	-0.387188
1	1.725912	-2.673309	0.703439
1	1.186768	-3.621278	-0.710151
6	3.061154	-2.605431	-1.012245
1	2.982492	-2.651593	-2.102228
1	3.564852	-1.680065	-0.714972
1	3.652583	-3.467738	-0.682646
8	1.220144	2.866277	-0.057730
6	1.791866	4.109951	0.299479
1	2.879201	4.115025	0.147541
1	1.341102	4.934629	-0.268386
1	1.569483	4.241873	1.359358

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**Conf5**

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Number of imaginary frequencies: 9    Electronic energy:    HF=-5382.3285664  
Zero-point correction=                    2.261258 (Hartree/Particle)  
Thermal correction to Energy=            2.396630  
Thermal correction to Enthalpy=         2.397574  
Thermal correction to Gibbs Free Energy= 2.042544  
Sum of electronic and zero-point Energies= -5380.067309  
Sum of electronic and thermal Energies= -5379.931936  
Sum of electronic and thermal Enthalpies= -5379.930992  
Sum of electronic and thermal Free Energies= -5380.286022

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Cartesian Coordinates

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6	2.880477	7.086332	-3.015320
6	1.660950	7.785715	-3.627332
6	1.345138	7.388984	-5.083609
6	0.010514	8.003451	-5.531971
6	2.469912	7.777281	-6.055885
6	6.391860	-3.397846	-4.607187
6	7.441393	-2.477610	-3.999127
8	8.616007	-2.800229	-3.856308
6	6.168688	-4.718703	-3.823678
6	7.369997	-5.670789	-3.918494
6	5.772300	-4.454265	-2.363497
7	6.986246	-1.243653	-3.591859
6	7.916019	-0.224391	-3.114329
6	8.345821	-0.408378	-1.643504
8	9.359512	0.140940	-1.229675
6	7.326769	1.177668	-3.305237

7	7.505866	-1.154269	-0.874689
6	7.785470	-1.476161	0.512377
6	6.858596	-0.768861	1.525955
6	7.032346	0.734094	1.582355
6	6.135253	1.592072	0.932651
6	8.107333	1.302007	2.282368
6	6.307288	2.977942	0.978697
6	8.283353	2.685108	2.331286
6	7.381774	3.529342	1.677951
6	0.775873	-2.390652	-4.712539
6	0.364041	-3.637995	-3.943261
8	1.163647	-4.309857	-3.275205
6	2.234914	-2.437015	-5.172072
7	-0.954004	-3.930474	-4.030992
6	-1.580392	-4.921305	-3.180781
6	0.461677	-7.324529	1.069859
6	1.243127	-6.479597	0.059482
8	0.375169	-6.247296	-1.049029
6	2.536293	-7.165259	-0.394117
6	3.624460	-3.883393	6.356424
6	2.555078	-4.973193	6.191205
6	2.361535	-5.339342	4.712622
6	2.897491	-6.213736	7.029222
6	6.774296	3.186324	6.558398
6	5.376135	2.964528	5.992333
8	4.459615	3.308549	7.036174
6	5.161016	1.526646	5.516598
6	-3.176006	0.582907	6.005169
6	-3.789240	1.971451	5.745410
6	-5.283832	1.912711	5.501394
6	-6.190389	2.138528	6.546702
6	-5.789756	1.596543	4.231284
6	-7.568308	2.050401	6.336810
6	-7.166914	1.506410	4.020437
6	-8.061329	1.732427	5.069693
6	-5.690186	0.804229	-1.819865
6	-7.012341	0.058766	-1.761122
8	-8.033058	0.464899	-2.321046
6	-5.272721	1.591501	-0.548507
16	-4.316377	0.648300	0.710723
7	-6.992979	-1.137413	-1.093058
6	-8.219088	-1.913769	-0.954407
6	-8.595893	-2.675092	-2.235220
6	-9.964283	-3.380064	-2.171905
6	-10.345536	-3.937496	-3.551965
6	-10.010353	-4.492599	-1.111751
26	-1.873962	0.414180	0.034531
6	-1.640260	3.810361	0.211684
6	-0.996550	0.174507	3.323173
6	-3.041083	-2.757186	0.086214

6	-2.562057	0.639453	-3.317585
7	-1.419986	1.742763	1.500298
6	-1.337780	3.097703	1.368595
6	-0.843239	3.699902	2.602699
6	-0.604386	2.664119	3.465042
6	-0.999148	1.447466	2.765506
6	-0.014669	2.717081	4.842958
6	-0.595493	5.167159	2.815289
6	0.756729	5.660684	2.256636
6	0.980083	7.160858	2.473073
7	-1.928050	-1.045386	1.420814
6	-1.486362	-0.979278	2.711744
6	-1.667817	-2.254027	3.383496
6	-2.292833	-3.080742	2.476856
6	-2.438529	-2.297720	1.251495
6	-1.208062	-2.576065	4.772479
6	-2.690658	-4.475951	2.608307
6	-3.009175	-5.133962	3.736458
7	-2.531636	-0.859516	-1.389266
6	-3.099049	-2.081815	-1.131102
6	-3.720039	-2.611082	-2.324314
6	-3.412032	-1.734934	-3.347278
6	-2.718251	-0.610944	-2.717848
6	-4.595410	-3.828089	-2.369352
6	-3.755699	-1.914208	-4.752082
6	-3.092847	-1.450136	-5.829142
7	-2.045779	1.930414	-1.302336
6	-2.326838	1.828780	-2.636920
6	-2.441106	3.150005	-3.237337
6	-2.229232	4.051966	-2.228112
6	-1.969268	3.266690	-1.026625
6	-2.771585	3.412034	-4.676963
6	-2.299233	5.552142	-2.287725
6	-3.646455	6.131206	-1.803933
6	-3.691966	7.661214	-1.862035
1	8.826099	-1.193565	0.691951
1	7.699523	-2.561936	0.648337
1	6.728341	-3.639517	-5.623501
1	5.430613	-2.876802	-4.701744
1	3.741503	-3.592943	7.407838
1	4.600729	-4.236918	5.997884
1	3.366362	-2.983228	5.785905
1	7.532398	3.000658	5.789826
1	6.881196	4.215639	6.916392
1	6.954174	2.509958	7.402215
1	3.002839	7.364050	-1.962111
1	2.770972	5.995220	-3.058311
1	3.809840	7.348270	-3.533652
1	1.072774	-7.531709	1.955761
1	-0.442303	-6.795898	1.388735

1	0.164939	-8.278118	0.616570
1	-2.107057	0.657446	6.234535
1	-3.669208	0.095425	6.855750
1	-3.292153	-0.061567	5.129421
1	-2.547098	-5.191316	-3.609655
1	-0.955387	-5.814657	-3.135042
1	-1.727091	-4.558293	-2.159595
1	0.629008	-1.539834	-4.038142
1	0.104344	-2.244625	-5.567882
1	-5.809151	1.512167	-2.648857
1	-4.896783	0.110826	-2.086087
1	-9.043914	-1.237430	-0.692733
1	-8.074988	-2.604690	-0.117076
1	-4.659093	8.045151	-1.516977
1	-2.912519	8.106711	-1.230408
1	-3.534618	8.026169	-2.885513
1	1.947335	7.484941	2.070647
1	0.198644	7.753226	1.980244
1	0.961309	7.415586	3.540457
1	1.799697	8.876580	-3.578052
1	0.780292	7.563205	-3.009228
1	1.236672	6.293493	-5.111715
1	-0.247179	7.696644	-6.552918
1	-0.810517	7.698556	-4.872090
1	0.059594	9.100667	-5.517244
1	2.217288	7.488503	-7.083381
1	2.634182	8.863540	-6.047642
1	3.419879	7.294432	-5.802103
1	5.313346	-5.205971	-4.312175
1	7.153419	-6.611318	-3.397341
1	7.599988	-5.911295	-4.963824
1	8.264353	-5.221844	-3.478104
1	5.519595	-5.391276	-1.854448
1	6.599564	-3.992500	-1.808680
1	4.894683	-3.799404	-2.296133
1	6.048852	-0.961383	-3.844759
1	8.844013	-0.319057	-3.685973
1	8.035980	1.920003	-2.931114
1	7.130492	1.378147	-4.364553
1	6.391221	1.293580	-2.744271
1	6.739185	-1.618421	-1.341818
1	7.072362	-1.202634	2.512606
1	5.814214	-1.015446	1.298745
1	5.281723	1.172256	0.407345
1	8.815840	0.652025	2.792067
1	5.595439	3.625706	0.473113
1	9.125244	3.103661	2.877256
1	7.515241	4.607384	1.716628
1	2.528508	-1.481553	-5.621385
1	2.886818	-2.640997	-4.317160

1	2.401272	-3.228884	-5.911965
1	-1.560565	-3.252535	-4.475935
1	1.499318	-5.519812	0.537676
1	0.807721	-5.651868	-1.694148
1	3.066262	-6.543190	-1.126129
1	3.212492	-7.342905	0.451794
1	2.309012	-8.127704	-0.868247
1	1.602281	-4.567901	6.563352
1	1.579835	-6.098128	4.587359
1	2.070977	-4.464844	4.118883
1	3.289859	-5.742348	4.285291
1	2.119048	-6.981413	6.941752
1	3.844055	-6.660676	6.696199
1	3.004348	-5.962432	8.091837
1	5.233669	3.643788	5.134583
1	3.563601	3.142761	6.703186
1	4.141866	1.389047	5.132287
1	5.855938	1.271985	4.707953
1	5.309544	0.825502	6.346468
1	-3.291124	2.421466	4.878367
1	-3.585504	2.623775	6.605715
1	-5.811151	2.390048	7.536269
1	-5.115290	1.421258	3.393463
1	-8.254545	2.233576	7.161106
1	-7.534101	1.260378	3.027387
1	-9.133680	1.664832	4.900735
1	-6.165205	2.006488	-0.063110
1	-4.670871	2.444930	-0.874756
1	-6.213009	-1.291786	-0.459610
1	-7.815018	-3.413769	-2.468114
1	-8.605809	-1.946757	-3.052987
1	-10.714963	-2.622049	-1.899232
1	-10.991114	-4.984748	-1.098737
1	-9.255728	-5.262689	-1.322402
1	-9.821109	-4.109444	-0.103065
1	-1.577604	4.891910	0.271936
1	-0.645597	0.084150	4.344414
1	-3.501881	-3.738056	0.122553
1	-2.812351	0.717380	-4.368004
1	-0.666732	2.253151	5.592536
1	0.946891	2.185786	4.882076
1	0.164005	3.750199	5.159293
1	-0.636606	5.396986	3.888495
1	-1.403255	5.754120	2.355959
1	0.807805	5.425808	1.185738
1	1.566087	5.090761	2.732345
1	-0.957218	-3.639663	4.856039
1	-0.317696	-1.997763	5.043284
1	-1.975898	-2.363248	5.529728
1	-2.727804	-5.039962	1.676060

1	-3.271314	-6.188189	3.709021
1	-3.045935	-4.649479	4.707001
1	-4.776903	-4.165124	-3.394592
1	-4.169190	-4.672616	-1.817095
1	-5.571686	-3.605638	-1.921001
1	-4.630454	-2.537940	-4.938553
1	-3.446315	-1.663036	-6.834154
1	-2.194068	-0.846104	-5.745481
1	-2.710852	4.479333	-4.913691
1	-2.087151	2.884641	-5.354438
1	-3.787481	3.078703	-4.927311
1	-2.123010	5.889968	-3.318630
1	-1.490212	5.992635	-1.686601
1	-3.834895	5.789532	-0.778625
1	-4.453234	5.709183	-2.416906
1	-9.625462	-4.699949	-3.878719
1	-11.338280	-4.405192	-3.534648
1	-10.357690	-3.145465	-4.309990
6	-0.075521	0.279611	-0.280039
6	1.024738	-0.044984	0.682058
6	1.784329	1.039244	1.179543
6	1.351017	-1.334760	1.171646
6	2.770924	0.879964	2.149074
1	1.549644	2.033655	0.818211
6	2.362815	-1.489543	2.131125
6	3.060901	-0.397482	2.634638
1	3.314643	1.747329	2.512975
1	2.575660	-2.500971	2.465047
1	3.833590	-0.543579	3.385271
6	0.549641	0.730115	-1.563802
8	0.732449	-0.015815	-2.511060
8	0.991951	2.010307	-1.549402
6	1.857663	2.409630	-2.636032
1	2.443214	3.233117	-2.216588
1	2.527435	1.577158	-2.872390
6	1.091439	2.855898	-3.871821
1	0.533114	2.019009	-4.297819
1	0.383814	3.651327	-3.621851
1	1.796093	3.230648	-4.625559
8	0.734096	-2.493402	0.807309
6	0.550512	-2.760724	-0.585484
1	-0.156468	-2.067360	-1.044589
1	1.508901	-2.715763	-1.115639
1	0.157988	-3.775446	-0.636527

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**Conf6**

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Number of imaginary frequencies: 9    Electronic energy:    HF=-5382.3285647  
Zero-point correction=                    2.261243 (Hartree/Particle)  
Thermal correction to Energy=            2.396630

Thermal correction to Enthalpy=	2.397574
Thermal correction to Gibbs Free Energy=	2.041750
Sum of electronic and zero-point Energies=	-5380.067322
Sum of electronic and thermal Energies=	-5379.931935
Sum of electronic and thermal Enthalpies=	-5379.930991
Sum of electronic and thermal Free Energies=	-5380.286815

.....  
 Cartesian Coordinates  
 .....

6	2.870335	7.093171	-3.007004
6	1.650165	7.790961	-3.619536
6	1.337324	7.396099	-5.076964
6	0.001832	8.008126	-5.526066
6	2.462503	7.788884	-6.046965
6	6.391364	-3.385297	-4.615024
6	7.440442	-2.464710	-4.006710
8	8.615618	-2.786076	-3.865713
6	6.171022	-4.707810	-3.833509
6	7.373447	-5.658154	-3.931597
6	5.776274	-4.446383	-2.372339
7	6.984179	-1.231975	-3.596978
6	7.913117	-0.212382	-3.118557
6	8.343764	-0.397772	-1.648154
8	9.356896	0.152328	-1.233988
6	7.322454	1.189350	-3.307482
7	7.505178	-1.145919	-0.880057
6	7.785612	-1.469266	0.506488
6	6.858086	-0.764549	1.521265
6	7.030469	0.738465	1.580350
6	6.132559	1.596843	0.932320
6	8.104994	1.306021	2.281364
6	6.303294	2.982780	0.981067
6	8.279711	2.689183	2.332993
6	7.377281	3.533832	1.681378
6	0.774374	-2.383575	-4.716237
6	0.364109	-3.632418	-3.948597
8	1.164800	-4.304893	-3.282455
6	2.232476	-2.429128	-5.178877
7	-0.953843	-3.925640	-4.035594
6	-1.578632	-4.918679	-3.186791
6	0.467949	-7.325694	1.059539
6	1.247927	-6.478387	0.049997
8	0.378897	-6.244805	-1.057394
6	2.541289	-7.162189	-0.405802
6	3.629876	-3.888696	6.349248
6	2.579753	-4.993183	6.159961
6	2.498886	-5.434220	4.691435
6	2.862747	-6.187777	7.082608
6	6.772769	3.183891	6.559412
6	5.377592	2.960332	5.986688

8	4.455528	3.312703	7.022828
6	5.163086	1.519562	5.519484
6	-3.175207	0.571327	6.007512
6	-3.786545	1.961455	5.751719
6	-5.281051	1.905341	5.506550
6	-6.188017	2.131022	6.551525
6	-5.786549	1.591803	4.235613
6	-7.565924	2.045335	6.340504
6	-7.163681	1.504097	4.023633
6	-8.058512	1.729974	5.072572
6	-5.693455	0.800843	-1.815969
6	-7.015150	0.054653	-1.756572
8	-8.037303	0.462013	-2.312931
6	-5.275407	1.587500	-0.544402
16	-4.317515	0.643890	0.713317
7	-6.993689	-1.143665	-1.092293
6	-8.219235	-1.920823	-0.953015
6	-8.598687	-2.678606	-2.235135
6	-9.966909	-3.383818	-2.170895
6	-10.350944	-3.937615	-3.551645
6	-10.010753	-4.499147	-1.113588
26	-1.875508	0.412842	0.035553
6	-1.643412	3.808452	0.222267
6	-0.996776	0.164141	3.323225
6	-3.041171	-2.759201	0.078458
6	-2.564588	0.647177	-3.315814
7	-1.421616	1.737352	1.504998
6	-1.339896	3.092669	1.376981
6	-0.844571	3.691589	2.612359
6	-0.604713	2.653483	3.471636
6	-0.999801	1.438662	2.769086
6	-0.013695	2.702882	4.849127
6	-0.597025	5.158320	2.828804
6	0.754741	5.653672	2.270665
6	0.977873	7.153312	2.490989
7	-1.928506	-1.050631	1.417674
6	-1.486736	-0.987970	2.708742
6	-1.668180	-2.264522	3.377120
6	-2.293270	-3.088767	2.468329
6	-2.438896	-2.302561	1.244997
6	-1.208221	-2.590119	4.765209
6	-2.691311	-4.484296	2.596177
6	-3.012263	-5.144287	3.722447
7	-2.532668	-0.857309	-1.391836
6	-3.099239	-2.080743	-1.137165
6	-3.719394	-2.607268	-2.332054
6	-3.411758	-1.728045	-3.352497
6	-2.719295	-0.605155	-2.719740
6	-4.594354	-3.824436	-2.381055
6	-3.754721	-1.903741	-4.757946



6	-3.091444	-1.436405	-5.833313
7	-2.048887	1.932674	-1.296931
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6	-1.972952	3.268175	-1.017391
6	-2.777229	3.423592	-4.666896
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1	6.726769	-3.624727	-5.632222
1	5.429268	-2.865414	-4.707310
1	3.668032	-3.546555	7.390837
1	4.631307	-4.251801	6.080960
1	3.410608	-3.019215	5.718104
1	7.535052	2.992238	5.796469
1	6.879022	4.215380	6.911283
1	6.946827	2.512816	7.408657
1	2.990673	7.369420	-1.953176
1	2.763210	6.001900	-3.051922
1	3.799854	7.357921	-3.523633
1	1.080088	-7.534114	1.944459
1	-0.436094	-6.798313	1.380286
1	0.171488	-8.278671	0.604791
1	-2.106442	0.643753	6.238455
1	-3.669997	0.081638	6.855908
1	-3.291105	-0.070139	5.129529
1	-2.544818	-5.189869	-3.616101
1	-0.952031	-5.810953	-3.142243
1	-1.726078	-4.557342	-2.165103
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1	0.101137	-2.235857	-5.569933
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1	-4.665234	8.046656	-1.491646
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1	1.231562	6.300399	-5.107203
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1	7.158805	-6.599870	-3.411788
1	7.602333	-5.896550	-4.977654
1	8.267806	-5.208799	-3.491636
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1	6.603691	-3.984496	-1.817856
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1	0.805211	5.421679	1.199108
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1	-9.631515	-4.699180	-3.881876
1	-11.343637	-4.405386	-3.533544
1	-10.364663	-3.143585	-4.307549
6	-0.077090	0.280276	-0.280339
6	1.023978	-0.044654	0.680770
6	1.782847	1.039620	1.179283
6	1.351585	-1.334750	1.168622
6	2.769988	0.880038	2.148185
1	1.547140	2.034262	0.819260
6	2.363720	-1.489699	2.127707

6	3.061170	-0.397739	2.632195
1	3.313199	1.747407	2.512838
1	2.577129	-2.501367	2.460703
1	3.834367	-0.544057	3.382266
6	0.547092	0.732932	-1.563813
8	0.730180	-0.011601	-2.512102
8	0.988222	2.013528	-1.547994
6	1.852838	2.415112	-2.634643
1	2.438119	3.238393	-2.214413
1	2.523027	1.583485	-2.872781
6	1.085313	2.862735	-3.869133
1	0.527187	2.026127	-4.295967
1	0.377375	3.657306	-3.617328
1	1.789084	3.239120	-4.622882
8	0.735930	-2.493628	0.802960
6	0.550899	-2.758821	-0.590050
1	-0.157550	-2.065587	-1.047066
1	1.508558	-2.711769	-1.121338
1	0.159555	-3.773943	-0.642252

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**Conf7**

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Number of imaginary frequencies: 9    Electronic energy:    HF=-5382.3290052  
Zero-point correction=                    2.261596 (Hartree/Particle)  
Thermal correction to Energy=            2.396679  
Thermal correction to Enthalpy=        2.397624  
Thermal correction to Gibbs Free Energy=    2.045693  
Sum of electronic and zero-point Energies=    -5380.067409  
Sum of electronic and thermal Energies=    -5379.932326  
Sum of electronic and thermal Enthalpies=   -5379.931382  
Sum of electronic and thermal Free Energies=   -5380.283313

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Cartesian Coordinates

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6	2.765869	7.597304	-1.172004
6	1.477757	7.370935	-1.972243
6	1.649330	7.421156	-3.503727
6	0.364805	6.953991	-4.204528
6	2.066487	8.812719	-4.004594
6	6.498585	-2.185918	-5.062607
6	7.534661	-1.390832	-4.280430
8	8.723791	-1.689683	-4.247412
6	6.372167	-3.669753	-4.626797
6	7.602154	-4.504440	-5.013208
6	6.053127	-3.797478	-3.129585
7	7.047827	-0.310754	-3.581159
6	7.948247	0.592410	-2.871361
6	8.375750	0.082063	-1.479211
8	9.344756	0.577664	-0.916911
6	7.328840	1.988633	-2.744393

7	7.590698	-0.891602	-0.942577
6	7.818196	-1.452592	0.374853
6	6.813959	-0.954863	1.441655
6	6.888008	0.536805	1.685686
6	5.990455	1.415853	1.065672
6	7.889881	1.077291	2.505176
6	6.104179	2.797332	1.241744
6	7.998663	2.455238	2.694778
6	7.107701	3.321904	2.057707
6	0.864305	-1.282801	-4.999655
6	0.446521	-2.657690	-4.496631
8	1.241512	-3.429014	-3.934916
6	2.227891	-1.310014	-5.698229
7	-0.848145	-2.963901	-4.702579
6	-1.450896	-4.137411	-4.108853
6	0.610079	-7.406115	-0.492044
6	1.260541	-6.619814	-1.632270
8	0.336772	-5.605655	-2.013231
6	1.617550	-7.508593	-2.828931
6	3.666686	-5.199261	5.472823
6	3.053596	-6.601539	5.600486
6	2.428860	-7.057807	4.273785
6	4.094754	-7.614809	6.098807
6	6.671987	1.695456	7.309623
6	5.352718	1.107555	6.820925
8	4.663576	0.645926	7.987579
6	5.553207	-0.023750	5.810960
6	-3.219793	-0.893609	6.068190
6	-4.158303	0.323041	5.963617
6	-5.593261	-0.067708	5.672792
6	-6.489498	-0.333750	6.718014
6	-6.043250	-0.203819	4.351079
6	-7.802723	-0.729579	6.456703
6	-7.356365	-0.600347	4.088767
6	-8.240496	-0.865074	5.137281
6	-5.684472	1.054014	-1.530065
6	-6.942394	0.237786	-1.776653
8	-7.862001	0.632967	-2.498910
6	-5.388652	1.456552	-0.062488
16	-4.340561	0.271330	0.878892
7	-6.985423	-0.992064	-1.181703
6	-8.163877	-1.834722	-1.332614
6	-8.225766	-2.552369	-2.691025
6	-9.532608	-3.329377	-2.939600
6	-9.590575	-3.834813	-4.389405
6	-9.725726	-4.495550	-1.956424
26	-1.869637	0.564926	0.126533
6	-2.166429	3.916562	0.700489
6	-0.893467	0.082450	3.347999
6	-2.520201	-2.756068	-0.173023

6	-2.679301	1.054196	-3.150229
7	-1.629793	1.765925	1.728375
6	-1.820864	3.111643	1.783813
6	-1.540533	3.613946	3.125751
6	-1.124595	2.535064	3.856845
6	-1.193063	1.382794	2.966029
6	-0.697722	2.489678	5.294700
6	-1.690601	5.043558	3.567903
6	-0.476846	5.943528	3.252021
6	-0.685866	7.397889	3.686540
7	-1.603548	-1.057801	1.308634
6	-1.113135	-1.064829	2.584581
6	-0.977891	-2.422293	3.074509
6	-1.479769	-3.242289	2.082786
6	-1.875204	-2.356190	0.992640
6	-0.366222	-2.818554	4.383674
6	-1.568571	-4.693998	2.023361
6	-1.575562	-5.564237	3.049978
7	-2.413016	-0.633353	-1.403418
6	-2.814772	-1.937189	-1.257577
6	-3.518570	-2.378656	-2.438015
6	-3.399567	-1.363458	-3.368455
6	-2.733461	-0.259588	-2.672956
6	-4.284088	-3.664714	-2.532917
6	-3.876741	-1.418946	-4.742777
6	-3.395995	-0.774069	-5.824975
7	-2.279200	2.180162	-1.013384
6	-2.518222	2.186040	-2.359506
6	-2.717502	3.547665	-2.839205
6	-2.625170	4.359642	-1.742102
6	-2.345495	3.482675	-0.608697
6	-3.011778	3.921114	-4.261766
6	-2.827290	5.846431	-1.660798
6	-4.251826	6.254643	-1.226531
6	-4.434444	7.772986	-1.135893
1	8.836821	-1.175421	0.658150
1	7.766421	-2.546854	0.312166
1	6.794114	-2.149398	-6.119015
1	5.512377	-1.709573	-4.989197
1	4.082284	-4.855893	6.428254
1	4.479811	-5.194661	4.734694
1	2.919850	-4.465844	5.146713
1	7.237515	2.120403	6.473179
1	6.488099	2.484074	8.046644
1	7.280235	0.917332	7.785514
1	2.582114	7.486269	-0.096889
1	3.537324	6.868589	-1.452688
1	3.183692	8.598386	-1.330872
1	1.271108	-8.208226	-0.143745
1	0.387682	-6.744968	0.351439

1	-0.330372	-7.854444	-0.834525
1	-2.197576	-0.581233	6.313664
1	-3.560660	-1.585538	6.848501
1	-3.188654	-1.438208	5.119521
1	-2.463662	-4.240657	-4.498495
1	-0.875733	-5.028404	-4.374911
1	-1.479714	-4.071518	-3.019239
1	0.917638	-0.633874	-4.115853
1	0.096665	-0.863582	-5.660019
1	-5.814293	1.955976	-2.139571
1	-4.832073	0.510111	-1.928418
1	-9.057744	-1.206914	-1.226143
1	-8.160002	-2.556648	-0.508614
1	-5.453844	8.035442	-0.829247
1	-3.743058	8.213721	-0.405988
1	-4.242543	8.255391	-2.103196
1	0.190394	8.016141	3.457183
1	-1.550092	7.842928	3.177386
1	-0.869481	7.467074	4.766421
1	0.723722	8.115119	-1.674164
1	1.066400	6.390352	-1.701844
1	2.450678	6.713252	-3.769400
1	0.483227	6.952025	-5.295393
1	0.088814	5.941035	-3.890262
1	-0.475333	7.619241	-3.963832
1	2.186448	8.818931	-5.095044
1	1.303549	9.561400	-3.751256
1	3.015232	9.142391	-3.566400
1	5.509810	-4.064892	-5.182099
1	7.454003	-5.554913	-4.734301
1	7.778986	-4.466228	-6.095196
1	8.501915	-4.131196	-4.517045
1	5.866910	-4.843231	-2.860243
1	6.893780	-3.445337	-2.518117
1	5.157188	-3.224858	-2.858045
1	6.092452	-0.017015	-3.734129
1	8.879669	0.650747	-3.442339
1	8.013026	2.635807	-2.190582
1	7.149127	2.424754	-3.733336
1	6.379956	1.955796	-2.195643
1	6.835069	-1.248257	-1.510340
1	7.022785	-1.501577	2.371014
1	5.797103	-1.233582	1.137256
1	5.189025	1.017533	0.447992
1	8.598193	0.410425	2.992649
1	5.405499	3.460006	0.737928
1	8.784103	2.852127	3.333103
1	7.194346	4.396300	2.197720
1	2.568744	-0.295022	-5.930182
1	2.965906	-1.792901	-5.050421

1	2.184894	-1.876953	-6.635546
1	-1.474163	-2.250964	-5.056393
1	2.186950	-6.159231	-1.250024
1	0.759259	-4.981405	-2.638472
1	2.057654	-6.909225	-3.635171
1	2.340177	-8.286256	-2.550335
1	0.716059	-7.994884	-3.220539
1	2.249849	-6.549885	6.350578
1	1.977169	-8.053074	4.368623
1	1.647112	-6.367419	3.935834
1	3.189116	-7.112024	3.483040
1	3.653760	-8.611121	6.226727
1	4.922570	-7.707374	5.382879
1	4.521647	-7.309599	7.062253
1	4.767995	1.910213	6.339844
1	3.832172	0.242392	7.692833
1	4.588921	-0.433473	5.483365
1	6.079419	0.331067	4.917383
1	6.133323	-0.836591	6.264004
1	-3.791232	0.984405	5.170053
1	-4.116508	0.892459	6.902637
1	-6.154562	-0.224979	7.748807
1	-5.374348	0.005705	3.515869
1	-8.483648	-0.926991	7.282136
1	-7.682855	-0.696048	3.056254
1	-9.263672	-1.169942	4.929069
1	-6.330742	1.599473	0.482638
1	-4.886711	2.428171	-0.078368
1	-6.260080	-1.208364	-0.500590
1	-7.369702	-3.236376	-2.783712
1	-8.112425	-1.784752	-3.464215
1	-10.368147	-2.626184	-2.798013
1	-10.656938	-5.037644	-2.164799
1	-8.898539	-5.213949	-2.037164
1	-9.768687	-4.154869	-0.916164
1	-2.271159	4.979887	0.888187
1	-0.530542	-0.059667	4.359976
1	-2.823943	-3.794444	-0.243955
1	-2.977530	1.220635	-4.177071
1	-1.328421	1.815133	5.888011
1	0.336641	2.134905	5.402398
1	-0.751889	3.480494	5.757586
1	-1.875524	5.075844	4.650172
1	-2.584189	5.482177	3.102390
1	-0.269773	5.902100	2.174857
1	0.410646	5.530880	3.750010
1	0.196960	-3.753752	4.276712
1	0.324324	-2.052178	4.751016
1	-1.118317	-2.984552	5.167597
1	-1.630397	-5.112082	1.018760



1	-1.630891	-6.633909	2.866981
1	-1.560639	-5.250469	4.088572
1	-4.667853	-3.842728	-3.541973
1	-3.679424	-4.535337	-2.252673
1	-5.146043	-3.640961	-1.854680
1	-4.699195	-2.114368	-4.913128
1	-3.844332	-0.921048	-6.803396
1	-2.568767	-0.071724	-5.772221
1	-3.009782	5.007498	-4.397892
1	-2.270284	3.500834	-4.953790
1	-3.995009	3.552273	-4.583902
1	-2.613337	6.302382	-2.636910
1	-2.103017	6.287911	-0.961449
1	-4.477901	5.792487	-0.257355
1	-4.973619	5.833026	-1.937933
1	-8.773724	-4.541251	-4.590420
1	-10.535479	-4.353808	-4.595683
1	-9.496716	-3.006786	-5.101925
6	-0.108740	0.660087	-0.259840
6	0.666581	1.760321	-0.910592
6	0.718061	1.839627	-2.307530
6	1.467499	2.659448	-0.162583
6	1.547932	2.755999	-2.961614
1	0.092079	1.166580	-2.882250
6	2.299407	3.577053	-0.815393
6	2.344011	3.618057	-2.213388
1	1.566576	2.788484	-4.047967
1	2.909891	4.264695	-0.240293
1	3.001111	4.331041	-2.705466
6	0.882726	-0.417821	0.075969
8	1.592924	-0.426647	1.063432
8	0.975751	-1.327159	-0.922127
6	2.075756	-2.267335	-0.821193
1	2.205037	-2.623166	-1.845299
1	2.966407	-1.716191	-0.499395
6	1.775636	-3.415460	0.129588
1	1.591197	-3.045145	1.139966
1	0.908235	-3.981463	-0.218193
1	2.638801	-4.094127	0.158810
8	1.358648	2.563615	1.188721
6	2.195097	3.355426	2.006633
1	3.256178	3.125933	1.842437
1	2.024641	4.428921	1.845979
1	1.924431	3.102773	3.032616

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**$\omega$ -Substrate**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-761.259606  
Zero-point correction=                    0.222793 (Hartree/Particle)  
Thermal correction to Energy=            0.238203  
Thermal correction to Enthalpy=         0.239147  
Thermal correction to Gibbs Free Energy= 0.178723  
Sum of electronic and zero-point Energies= -761.036813  
Sum of electronic and thermal Energies= -761.021403  
Sum of electronic and thermal Enthalpies= -761.020459  
Sum of electronic and thermal Free Energies= -761.080883  
.....

Cartesian Coordinates

-----  
6    -3.567523   -1.528803   0.055952  
6    -2.495284   -2.363628   0.340252  
6    -1.209510   -1.836284   0.410958  
6    -0.973775   -0.478931   0.185416  
6    -2.069945   0.354493   -0.118987  
6    -3.360074   -0.170150   -0.171237  
6    0.398391   0.060813   0.248314  
7    0.601906   1.269816   0.720688  
7    0.785248   2.307511   1.127951  
8    -1.773443   1.660333   -0.348978  
6    -2.819898   2.541178   -0.687540  
6    1.600702   -0.670683   -0.160975  
8    2.710847   0.076544   -0.006020  
8    1.608018   -1.806375   -0.584720  
1    -0.367356   -2.483005   0.624155  
1    -2.652845   -3.423142   0.513529  
1    -4.205681   0.468621   -0.398208  
1    -4.576328   -1.927373   0.005944  
1    -2.352901   3.514650   -0.840913  
1    -3.322753   2.228876   -1.611480  
1    -3.558550   2.617022   0.120515  
6    3.942301   -0.555701   -0.378552  
1    4.068727   -1.466418   0.214911  
1    3.887241   -0.849709   -1.431077  
6    5.053690   0.441726   -0.127451  
1    6.016752   -0.001337   -0.399577  
1    4.906680   1.345756   -0.725594  
1    5.089112   0.726572   0.928160  
-----

**ω-A<sub>Ir</sub>(Me)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-1978.9348032  
Zero-point correction=                    0.644697 (Hartree/Particle)  
Thermal correction to Energy=            0.686457  
Thermal correction to Enthalpy=         0.687402  
Thermal correction to Gibbs Free Energy= 0.569519  
Sum of electronic and zero-point Energies= -1978.290106  
-----

Sum of electronic and thermal Energies= -1978.248346  
Sum of electronic and thermal Enthalpies= -1978.247402  
Sum of electronic and thermal Free Energies= -1978.365284

.....  
Cartesian Coordinates  
.....

6	-4.094519	-2.878333	0.138152
6	-2.716566	-2.463837	-0.012640
7	-2.640105	-1.097746	-0.073456
6	-3.916649	-0.623765	0.049953
6	-4.842805	-1.734376	0.181247
6	-1.632421	-3.324006	-0.091310
6	-0.305895	-2.970076	-0.272506
7	0.162206	-1.690311	-0.387493
6	1.516646	-1.777118	-0.561950
6	1.921094	-3.170923	-0.578392
6	0.791112	-3.907800	-0.386626
6	2.369968	-0.692344	-0.683126
6	2.018696	0.647730	-0.632534
7	0.743820	1.121018	-0.492853
6	0.823668	2.486808	-0.493699
6	2.203159	2.898895	-0.639140
6	2.944476	1.759199	-0.720554
6	-0.247187	3.353148	-0.350081
6	-1.576707	3.004191	-0.174208
7	-2.050969	1.720942	-0.160802
6	-3.410465	1.798640	-0.020387
6	-3.821868	3.181206	0.038456
6	-2.684582	3.934859	-0.032771
77	-0.939590	0.013763	-0.227976
6	-4.269179	0.714587	0.076663
1	-0.027057	4.413887	-0.391829
1	-5.322932	0.941407	0.202013
1	-1.844847	-4.385288	-0.012102
1	3.420073	-0.913477	-0.836014
6	-0.645904	0.040394	1.796196
1	-1.343123	-0.658747	2.267568
1	0.384592	-0.259958	2.008663
1	-0.822515	1.053773	2.169239
6	4.437206	1.639964	-0.751893
1	4.748208	0.743865	-1.298862
1	4.869321	2.493176	-1.286771
6	5.002377	1.597503	0.685915
1	4.632100	0.702730	1.201699
1	4.676374	2.477681	1.243510
6	6.503930	1.572824	0.724900
8	7.236982	2.389862	1.216851
8	7.009374	0.467602	0.098342
1	7.975881	0.515075	0.179341
6	3.319349	-3.684276	-0.758169

1	3.833744	-3.142760	-1.559049
1	3.265946	-4.726129	-1.087886
6	4.186204	-3.636469	0.522835
1	3.592496	-3.884399	1.404685
1	4.991863	-4.374379	0.428491
6	4.853050	-2.303078	0.764764
8	4.743922	-1.629121	1.764205
8	5.619249	-1.943598	-0.279096
1	6.069124	-1.100253	-0.061761
6	0.634370	-5.393458	-0.300649
1	1.590212	-5.908595	-0.427459
1	0.227097	-5.692697	0.672418
1	-0.049894	-5.768420	-1.070947
6	2.666578	4.321344	-0.649681
1	2.427785	4.824539	0.294921
1	3.748492	4.388722	-0.794352
1	2.186686	4.891970	-1.453250
6	-4.560357	-4.298613	0.178648
1	-3.994631	-4.923603	-0.520489
1	-4.445554	-4.735861	1.178381
1	-5.618569	-4.363023	-0.091090
6	-5.235387	3.643410	0.198756
1	-5.871233	3.275200	-0.615019
1	-5.666128	3.282559	1.140373
1	-5.297225	4.734696	0.207808
6	-6.293601	-1.587791	0.295198
6	-7.094645	-2.355279	1.039484
1	-6.742099	-0.780096	-0.282804
1	-8.168445	-2.195723	1.054677
1	-6.705821	-3.148684	1.671325
6	-2.602454	5.397333	0.027834
6	-1.696531	6.102365	0.710690
1	-3.375018	5.939176	-0.517147
1	-1.712419	7.187934	0.705730
1	-0.929860	5.623510	1.313662

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 $\omega$  -**B**<sub>Ir(Me)</sub>  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2740.251031  
 Zero-point correction=                    0.870200 (Hartree/Particle)  
 Thermal correction to Energy=            0.928321  
 Thermal correction to Enthalpy=         0.929265  
 Thermal correction to Gibbs Free Energy= 0.775762  
 Sum of electronic and zero-point Energies= -2739.380831  
 Sum of electronic and thermal Energies= -2739.322710  
 Sum of electronic and thermal Enthalpies= -2739.321766  
 Sum of electronic and thermal Free Energies= -2739.475269

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 Cartesian Coordinates  
 .....

6	3.766197	-3.115576	-1.364544
6	3.510126	-1.726794	-1.067904
7	2.163685	-1.516591	-0.943444
6	1.547660	-2.714812	-1.171905
6	2.550656	-3.741923	-1.392256
6	4.491963	-0.765881	-0.865652
6	4.295041	0.547295	-0.473885
7	3.076667	1.131630	-0.267613
6	3.312233	2.426603	0.100712
6	4.736905	2.677987	0.148216
6	5.350909	1.512634	-0.220291
6	2.329605	3.361121	0.393335
6	0.960285	3.158648	0.360180
7	0.341724	1.993888	0.007079
6	-1.003431	2.209744	0.118725
6	-1.248892	3.561699	0.587169
6	-0.029704	4.152287	0.724883
77	1.253882	0.258230	-0.521622
7	-0.561802	-0.630593	-0.716556
6	-1.777230	-0.026551	-0.592853
6	-2.828429	-0.972504	-0.904279
6	-2.222240	-2.157853	-1.189474
6	-0.796814	-1.930725	-1.069265
6	-1.982404	1.278837	-0.175019
6	0.176111	-2.895416	-1.264057
8	-3.662040	-2.676966	1.927115
6	-2.961166	-1.564474	2.232185
8	-3.485890	-0.490949	2.450107
6	-1.517190	-1.835288	2.266455
7	-1.231578	-3.083695	1.957230
7	-1.090179	-4.170478	1.686165
6	-0.461833	-0.842411	2.551142
6	-0.791816	0.450051	2.966879
6	0.188494	1.406799	3.217721
6	1.526346	1.094743	3.045065
6	1.889214	-0.187051	2.634252
6	0.911041	-1.155241	2.405213
8	1.198266	-2.430731	2.049643
6	2.541722	-2.862540	2.064910
1	-0.165749	-3.890146	-1.525959
1	-3.011112	1.584706	-0.028606
1	2.667151	4.352882	0.676667
1	5.518361	-1.083637	-1.018273
1	-1.835556	0.709923	3.073821
1	-0.110215	2.405572	3.518686
1	2.935964	-0.427481	2.492536
1	2.298264	1.840902	3.202106
1	2.521302	-3.904792	1.743686
1	3.157377	-2.288528	1.366041
1	2.962415	-2.789224	3.076075

6	1.204730	0.729060	-2.509931
1	0.433002	1.486154	-2.681364
1	2.182058	1.118973	-2.812206
1	0.972261	-0.171792	-3.087053
6	-5.089693	-2.557308	1.943300
1	-5.434840	-3.348339	1.273479
1	-5.373894	-1.585945	1.533417
6	-5.638428	-2.735936	3.347405
1	-5.292191	-1.926453	3.995454
1	-6.732973	-2.715104	3.324912
1	-5.317591	-3.692916	3.769620
6	5.127525	-3.715349	-1.523356
1	5.067658	-4.780080	-1.763418
1	5.690340	-3.220953	-2.323768
1	5.716349	-3.619271	-0.602825
6	5.363286	3.967961	0.571719
1	6.393220	3.804789	0.902647
1	5.389924	4.695724	-0.248896
1	4.810866	4.426769	1.398749
6	2.308708	-5.176276	-1.561602
6	1.400721	-5.893726	-0.892610
1	2.955963	-5.690559	-2.271372
1	1.291350	-6.959486	-1.069190
1	0.753144	-5.450197	-0.140575
6	6.779499	1.215712	-0.316086
6	7.722632	2.061946	-0.739709
1	7.084037	0.214205	-0.012681
1	8.768262	1.770490	-0.761814
1	7.481913	3.058737	-1.097818
6	-2.844682	-3.471976	-1.537482
1	-3.935349	-3.398818	-1.573554
1	-2.502940	-3.833752	-2.514105
1	-2.587111	-4.235449	-0.793984
6	-4.281044	-0.625324	-0.984018
1	-4.889438	-1.526842	-0.850877
1	-4.559719	0.060951	-0.177198
6	-2.593692	4.165349	0.866433
1	-2.455986	5.022826	1.532174
1	-3.227725	3.458651	1.412525
6	-3.350448	4.655887	-0.390714
1	-2.661700	5.099903	-1.112142
1	-4.073718	5.421512	-0.085627
6	-4.611248	0.013400	-2.349771
1	-4.007047	0.917792	-2.490981
1	-4.385816	-0.683051	-3.160148
6	-4.141465	3.576857	-1.095906
8	-4.017447	3.271750	-2.263046
8	-5.019319	2.996698	-0.270495
1	-5.560154	2.341071	-0.775002
6	-6.045904	0.445295	-2.424511

8	-6.585094	1.216374	-1.648411
8	-6.727662	-0.107043	-3.430495
1	-7.628077	0.257314	-3.393092
6	0.303581	5.542134	1.167557
1	0.839192	6.090260	0.383275
1	-0.595721	6.114230	1.410558
1	0.944584	5.535860	2.057378

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 **$\omega$  -TS(B-C)<sub>Ir(Me)</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2740.2119109  
 Zero-point correction=                    0.866483 (Hartree/Particle)  
 Thermal correction to Energy=            0.924401  
 Thermal correction to Enthalpy=         0.925345  
 Thermal correction to Gibbs Free Energy=    0.774438  
 Sum of electronic and zero-point Energies=    -2739.345428  
 Sum of electronic and thermal Energies=    -2739.287510  
 Sum of electronic and thermal Enthalpies=   -2739.286566  
 Sum of electronic and thermal Free Energies=   -2739.437473

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 Cartesian Coordinates  
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6	3.382166	-3.411032	-1.017923
6	2.089474	-2.846771	-0.695447
7	2.144121	-1.482341	-0.777987
6	3.404039	-1.153806	-1.184685
6	4.198292	-2.360386	-1.335761
6	0.952713	-3.587443	-0.409736
6	-0.323133	-3.096072	-0.172924
7	-0.664850	-1.778880	-0.128929
6	-2.009436	-1.714649	0.093012
6	-2.544134	-3.057060	0.227809
6	-1.496441	-3.913890	0.054160
6	-2.749598	-0.544389	0.168185
6	-2.283282	0.749213	-0.014504
7	-0.991737	1.091998	-0.278297
6	-0.949608	2.442486	-0.432116
6	-2.271200	2.997379	-0.235325
6	-3.100075	1.947045	0.020881
6	0.178770	3.186943	-0.744697
6	1.454900	2.699287	-0.974090
7	1.809244	1.384026	-0.945570
6	3.106041	1.300306	-1.351998
6	3.616569	2.622308	-1.637171
6	2.605662	3.500661	-1.366601
77	0.595120	-0.191628	-0.466928
6	3.846265	0.131650	-1.456177
1	0.042241	4.256419	-0.851775
1	4.865953	0.232737	-1.813372
1	1.062588	-4.667411	-0.414459

1	-3.803442	-0.651253	0.396814
6	0.908308	0.114029	1.692175
6	0.973193	1.511897	2.209278
6	-0.207602	2.123830	2.649777
6	2.130136	2.318278	2.111863
6	-0.254384	3.476660	2.970651
1	-1.110363	1.531418	2.700283
6	2.091525	3.662856	2.475122
6	0.897085	4.244338	2.890725
1	-1.195136	3.916939	3.285043
1	2.985100	4.271478	2.408059
1	0.880060	5.298998	3.150468
6	0.055710	-0.840533	2.498220
8	-1.084782	-0.589237	2.820633
8	0.630227	-2.024514	2.716074
8	3.256650	1.710008	1.677613
6	4.455407	2.446538	1.600269
1	5.194248	1.756404	1.189861
1	4.350655	3.304222	0.926357
1	4.778982	2.787213	2.592134
7	3.406436	-1.286277	1.817860
7	2.561861	-0.630558	2.096201
6	0.057457	-0.346700	-2.482963
1	-1.024389	-0.498536	-2.575136
1	0.328110	0.567741	-3.024448
1	0.568511	-1.197302	-2.950229
6	-4.589398	1.978082	0.174354
1	-4.935957	1.153197	0.805174
1	-4.893713	2.902035	0.679448
6	-5.273134	1.903135	-1.209520
1	-5.028274	0.947608	-1.689752
1	-4.915958	2.712563	-1.849113
6	-6.768447	2.019762	-1.130319
8	-7.463632	2.874433	-1.613782
8	-7.318687	1.004839	-0.397342
1	-8.280075	1.140596	-0.406482
6	-3.975289	-3.416375	0.497980
1	-4.392060	-2.780189	1.285845
1	-4.007997	-4.437995	0.888597
6	-4.895843	-3.353886	-0.744043
1	-4.369140	-3.690842	-1.638836
1	-5.753943	-4.016634	-0.578484
6	-5.466421	-1.983556	-1.024107
8	-5.382178	-1.385076	-2.072560
8	-6.119111	-1.496654	0.044971
1	-6.510086	-0.630604	-0.195674
6	-1.485397	-5.410332	0.075070
1	-2.480817	-5.818641	0.269266
1	-1.145624	-5.817519	-0.884471
1	-0.812057	-5.796835	0.849988



6	-2.597377	4.454330	-0.318603
1	-2.401911	4.852423	-1.321272
1	-3.649593	4.643716	-0.087499
1	-1.989029	5.032169	0.387651
6	3.715852	-4.867177	-0.958501
1	3.221651	-5.353484	-0.110504
1	3.403690	-5.394508	-1.868653
1	4.795023	-5.009119	-0.847808
6	5.014250	2.917858	-2.080281
1	5.748225	2.594597	-1.331162
1	5.254649	2.398248	-3.014994
1	5.163207	3.988586	-2.242995
6	5.609932	-2.374179	-1.715842
6	6.203620	-3.303591	-2.469942
1	6.215355	-1.548524	-1.342301
1	7.265762	-3.253098	-2.689369
1	5.648931	-4.127266	-2.909980
6	2.679969	4.961632	-1.432881
6	2.129657	5.809746	-0.558427
1	3.265512	5.372771	-2.254816
1	2.240112	6.883431	-0.677785
1	1.570850	5.459656	0.305277
6	-0.217430	-3.042609	3.269199
1	-0.522173	-2.742254	4.276543
1	-1.113492	-3.125284	2.649045
6	0.585157	-4.325758	3.272248
1	1.475397	-4.232969	3.901565
1	-0.028399	-5.146670	3.656852
1	0.904038	-4.569355	2.254428

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$\omega$  -C<sub>Ir</sub>(Me)

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2740.2371944  
Zero-point correction=                    0.865609 (Hartree/Particle)  
Thermal correction to Energy=            0.925299  
Thermal correction to Enthalpy=         0.926243  
Thermal correction to Gibbs Free Energy= 0.769338  
Sum of electronic and zero-point Energies= -2739.371585  
Sum of electronic and thermal Energies= -2739.311895  
Sum of electronic and thermal Enthalpies= -2739.310951  
Sum of electronic and thermal Free Energies= -2739.467856

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Cartesian Coordinates

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6	3.209476	-3.200208	-1.409501
6	1.942514	-2.662208	-0.964600
7	1.974892	-1.300821	-1.028864
6	3.187371	-0.938755	-1.530857
6	3.978018	-2.130474	-1.783952
6	0.848794	-3.424513	-0.578238

6	-0.415654	-2.954196	-0.253887
7	-0.775404	-1.644935	-0.190232
6	-2.111409	-1.596340	0.082200
6	-2.621890	-2.948729	0.229388
6	-1.568710	-3.789331	0.018047
6	-2.863131	-0.437097	0.192768
6	-2.405949	0.868348	0.066274
7	-1.118183	1.231369	-0.165472
6	-1.060541	2.590274	-0.176664
6	-2.385423	3.127635	0.048769
6	-3.220629	2.059081	0.191998
6	0.080492	3.350109	-0.398430
6	1.343662	2.879817	-0.727752
7	1.669718	1.569491	-0.899545
6	2.923063	1.521939	-1.426529
6	3.448281	2.861741	-1.556875
6	2.485052	3.708597	-1.084217
77	0.469207	-0.042235	-0.487914
6	3.611042	0.361522	-1.755112
1	-0.039133	4.427086	-0.369192
1	4.591925	0.488679	-2.201342
1	0.979101	-4.501652	-0.588961
1	-3.911764	-0.559286	0.436065
6	0.809008	0.156146	1.484391
6	1.570058	1.233698	2.108235
6	0.895062	2.255579	2.789977
6	2.961594	1.359809	1.890842
6	1.557850	3.419856	3.163181
1	-0.169923	2.142848	2.962591
6	3.625464	2.521153	2.277033
6	2.915164	3.550214	2.893521
1	1.015172	4.218401	3.658892
1	4.687719	2.637627	2.098377
1	3.441655	4.457787	3.173720
6	-0.153476	-0.507637	2.413436
8	-1.178461	-0.012717	2.832197
8	0.251962	-1.748405	2.683598
8	3.563071	0.282083	1.352137
6	4.957271	0.309289	1.160290
1	5.212774	-0.656982	0.723604
1	5.248852	1.106345	0.464960
1	5.485406	0.436835	2.113624
7	3.250765	-3.122977	1.939421
7	3.232767	-2.324349	2.697762
6	-0.173070	0.031442	-2.512848
1	-1.176442	-0.397835	-2.622672
1	-0.197472	1.066924	-2.873448
1	0.518703	-0.536505	-3.148083
6	-4.711981	2.068822	0.323318
1	-5.054379	1.233842	0.943437

1	-5.036738	2.983865	0.831037
6	-5.374794	1.993278	-1.070700
1	-5.113446	1.043423	-1.553814
1	-5.017511	2.809540	-1.701502
6	-6.872546	2.092347	-1.013347
8	-7.570495	2.935550	-1.512351
8	-7.421604	1.075314	-0.282128
1	-8.384296	1.199571	-0.307576
6	-4.039882	-3.327773	0.539564
1	-4.443172	-2.699594	1.341021
1	-4.047990	-4.351205	0.926664
6	-4.996340	-3.272458	-0.675524
1	-4.493328	-3.608236	-1.584272
1	-5.845556	-3.939345	-0.483644
6	-5.579994	-1.904328	-0.940423
8	-5.517232	-1.300514	-1.987115
8	-6.214460	-1.424804	0.143045
1	-6.611892	-0.558551	-0.086959
6	-1.542662	-5.285648	0.010210
1	-2.508556	-5.707554	0.300593
1	-1.302689	-5.670126	-0.988206
1	-0.788623	-5.681066	0.700995
6	-2.715432	4.586564	0.070116
1	-2.522158	5.052134	-0.903454
1	-3.768069	4.755374	0.313846
1	-2.111853	5.121156	0.812951
6	3.571302	-4.650023	-1.391429
1	3.172448	-5.143086	-0.498881
1	3.179125	-5.179381	-2.268781
1	4.658191	-4.774258	-1.387998
6	4.814358	3.196864	-2.065917
1	5.598009	2.771637	-1.425972
1	4.971560	2.803813	-3.077125
1	4.972295	4.278082	-2.097141
6	5.348165	-2.115939	-2.293943
6	5.889440	-3.032607	-3.101376
1	5.968879	-1.276241	-1.980997
1	6.924751	-2.957810	-3.419515
1	5.314688	-3.868689	-3.488853
6	2.582229	5.163011	-0.950583
6	2.112093	5.874669	0.077982
1	3.107517	5.685458	-1.749576
1	2.225405	6.954170	0.110557
1	1.624986	5.398176	0.924536
6	-0.666882	-2.573525	3.414184
1	-0.821304	-2.148676	4.410886
1	-1.625194	-2.571490	2.886630
6	-0.061026	-3.959304	3.467332
1	0.884583	-3.953370	4.017328
1	-0.749147	-4.650689	3.963785

1 0.131442 -4.319807 2.452615

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$\omega$  -TS(C-P)<sub>IR(Me)</sub>

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2630.8045366  
Zero-point correction=                    0.854123 (Hartree/Particle)  
Thermal correction to Energy=            0.909102  
Thermal correction to Enthalpy=         0.910046  
Thermal correction to Gibbs Free Energy= 0.764742  
Sum of electronic and zero-point Energies= -2629.950414  
Sum of electronic and thermal Energies= -2629.895435  
Sum of electronic and thermal Enthalpies= -2629.894491  
Sum of electronic and thermal Free Energies= -2630.039794

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Cartesian Coordinates

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6 3.511580 -3.248880 -1.120076  
6 2.191928 -2.729308 -0.837079  
7 2.214732 -1.362857 -0.877440  
6 3.484332 -0.985307 -1.199949  
6 4.317338 -2.165986 -1.354233  
6 1.071102 -3.502525 -0.573246  
6 -0.208400 -3.045032 -0.291714  
7 -0.585905 -1.737771 -0.232761  
6 -1.910003 -1.709296 0.089765  
6 -2.394978 -3.065688 0.270567  
6 -1.340806 -3.893573 0.019329  
6 -2.676376 -0.559023 0.203195  
6 -2.257751 0.745139 -0.019201  
7 -0.984127 1.123341 -0.320411  
6 -0.981418 2.475886 -0.466619  
6 -2.316905 2.991616 -0.253998  
6 -3.108257 1.918945 0.029757  
6 0.135815 3.259178 -0.721871  
6 1.437304 2.814708 -0.881764  
7 1.817490 1.505943 -0.914827  
6 3.148029 1.473798 -1.208014  
6 3.653881 2.822880 -1.335853  
6 2.600274 3.660964 -1.110128  
77 0.617939 -0.116310 -0.561924  
6 3.915563 0.325930 -1.349144  
1 -0.022408 4.328411 -0.795637  
1 4.956831 0.471840 -1.615029  
1 1.206693 -4.578861 -0.590685  
1 -3.713214 -0.692809 0.488225  
6 0.111788 -0.213573 -2.586773  
1 -0.959976 -0.411634 -2.701669  
1 0.345613 0.732244 -3.088728  
1 0.666783 -1.018525 -3.082419  
6 -4.593265 1.902626 0.219458

1	-4.891781	1.089093	0.887594
1	-4.917606	2.831528	0.700659
6	-5.309169	1.752792	-1.140718
1	-5.042153	0.790317	-1.593809
1	-5.001872	2.549861	-1.819298
6	-6.805639	1.809218	-1.032466
8	-7.549381	2.586752	-1.570681
8	-7.294218	0.836572	-0.205251
1	-8.257052	0.926034	-0.208132
6	-3.791161	-3.462143	0.647867
1	-4.172468	-2.819220	1.447050
1	-3.763270	-4.473281	1.063292
6	-4.794766	-3.458246	-0.528554
1	-4.323714	-3.812887	-1.446368
1	-5.625724	-4.130049	-0.284612
6	-5.413438	-2.110248	-0.812650
8	-5.417524	-1.549910	-1.885523
8	-5.999021	-1.596930	0.281460
1	-6.431071	-0.754674	0.038493
6	-1.284779	-5.388011	0.049554
1	-2.250660	-5.822340	0.316781
1	-1.001189	-5.793537	-0.927614
1	-0.547149	-5.745863	0.777165
6	-2.691620	4.435880	-0.348443
1	-2.517628	4.826984	-1.356516
1	-3.746529	4.592183	-0.110337
1	-2.098213	5.043886	0.343563
6	3.881572	-4.696945	-1.104880
1	3.345386	-5.236178	-0.318136
1	3.646185	-5.185529	-2.057409
1	4.953754	-4.817105	-0.928560
6	5.081953	3.172802	-1.603794
1	5.732520	2.810682	-0.799963
1	5.434115	2.724777	-2.539247
1	5.218715	4.253905	-1.675490
6	5.745348	-2.131262	-1.665492
6	6.405054	-3.028163	-2.403554
1	6.306393	-1.292605	-1.254266
1	7.473315	-2.937618	-2.570428
1	5.899814	-3.860790	-2.882635
6	2.636904	5.124586	-1.079253
6	1.988240	5.899016	-0.205341
1	3.274340	5.601368	-1.822972
1	2.072147	6.980177	-0.248743
1	1.379730	5.475573	0.588482
6	1.091944	0.059616	1.590698
6	1.138666	1.415391	2.174917
6	0.507716	-1.024233	2.414314
6	-0.004109	2.143306	2.500838
6	2.381868	2.038671	2.313235

8	-0.587443	-0.921392	2.921923
8	1.263531	-2.131401	2.434947
6	0.112706	3.463287	2.930877
1	-0.973944	1.671186	2.400272
6	2.515899	3.351392	2.720919
8	3.496382	1.297484	1.969055
6	1.361025	4.069705	3.028653
1	-0.783906	4.018637	3.185597
1	3.503072	3.792113	2.795594
6	3.266315	-0.042673	2.060744
1	1.445291	5.100833	3.355892
1	3.100186	-0.430218	3.067279
1	3.992040	-0.608232	1.474834
1	2.293524	-0.319871	1.321506
6	0.645591	-3.314032	2.970291
1	-0.403054	-3.326630	2.662822
1	1.170543	-4.134847	2.477110
6	0.786328	-3.375401	4.478961
1	0.240358	-2.552023	4.944215
1	0.374689	-4.317661	4.852316
1	1.837945	-3.319515	4.773975

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 $\omega$  -<sup>5</sup>A<sub>Fe(his)</sub>  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2183.9142918  
 Zero-point correction=                    0.676437 (Hartree/Particle)  
 Thermal correction to Energy=            0.721804  
 Thermal correction to Enthalpy=         0.722749  
 Thermal correction to Gibbs Free Energy=    0.591105  
 Sum of electronic and zero-point Energies=    -2183.237855  
 Sum of electronic and thermal Energies=    -2183.192487  
 Sum of electronic and thermal Enthalpies=   -2183.191543  
 Sum of electronic and thermal Free Energies=   -2183.323187

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 Cartesian Coordinates  
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6	-1.642063	-3.449653	-0.670214
6	-0.344663	-2.795661	-0.638072
7	-0.514756	-1.448141	-0.497489
6	-1.851171	-1.210238	-0.427454
6	-2.578750	-2.464174	-0.545000
6	0.881422	-3.449152	-0.730950
6	2.158715	-2.876856	-0.721219
7	2.411227	-1.549973	-0.570358
6	3.755910	-1.370545	-0.659273
6	4.404529	-2.661044	-0.876133
6	3.403863	-3.598698	-0.892284
6	4.394628	-0.138170	-0.513002
6	3.807080	1.120176	-0.361653
7	2.464453	1.365985	-0.313440

6	2.297232	2.703052	-0.148912
6	3.595477	3.355497	-0.099504
6	4.537561	2.364181	-0.236121
6	1.062400	3.353116	-0.015250
6	-0.203743	2.778432	-0.028060
7	-0.450300	1.443310	-0.126617
6	-1.796437	1.276953	-0.141277
6	-2.456054	2.574057	-0.022229
6	-1.465546	3.507715	0.045669
6	-1.584825	4.995896	0.145315
6	-3.939619	2.780502	-0.044903
6	-4.500693	2.715817	-1.468557
6	-6.002023	2.852791	-1.505417
8	-6.725539	2.981101	-0.546129
6	-2.441813	0.046382	-0.261966
6	6.025264	2.505880	-0.303232
6	3.796353	4.797513	0.034166
6	4.804711	5.391818	0.679420
6	3.518638	-5.074456	-1.113433
6	5.834639	-2.914680	-1.065363
6	6.682894	-2.154226	-1.763870
6	-4.069724	-2.597937	-0.478238
6	-4.579178	-2.545818	0.965165
6	-6.082166	-2.631188	1.054061
8	-6.842811	-2.735784	0.121472
6	-1.851455	-4.924889	-0.811450
8	-6.475315	2.813227	-2.766268
8	-6.509733	-2.576342	2.331387
1	1.098033	4.431684	0.107418
1	-3.528062	0.066819	-0.239673
1	0.841032	-4.529180	-0.845646
1	5.479007	-0.162925	-0.517945
1	6.464861	1.779755	-0.994879
1	6.301393	3.508679	-0.644069
1	6.494437	2.350379	0.676545
1	4.563460	-5.395641	-1.143604
1	3.014967	-5.639482	-0.320047
1	3.058470	-5.368663	-2.064457
1	-1.395656	-5.305699	-1.732959
1	-1.401375	-5.472981	0.025063
1	-2.914900	-5.178633	-0.838631
1	-2.627915	5.309470	0.245009
1	-1.036458	5.383602	1.012027
1	-1.174108	5.487111	-0.745011
1	3.047419	5.430853	-0.440911
1	4.887731	6.473941	0.712832
1	5.563657	4.824428	1.210233
1	6.219559	-3.827305	-0.609746
1	7.731035	-2.423016	-1.854028
1	6.355924	-1.260531	-2.287918

1	-4.442842	2.026439	0.570787
1	-4.201551	3.745829	0.399553
1	-4.064521	3.502346	-2.095621
1	-4.230893	1.770117	-1.954238
1	-7.440059	2.896528	-2.696804
1	-4.393653	-3.536638	-0.938143
1	-4.554348	-1.804487	-1.057869
1	-4.151228	-3.363225	1.557896
1	-4.257411	-1.622747	1.462349
1	-7.478466	-2.629051	2.294677
7	1.136802	-0.312387	2.031487
6	1.978143	-1.111383	2.648597
6	0.446489	0.365091	3.006726
7	1.858383	-0.978877	3.989048
1	2.672725	-1.779394	2.160247
6	0.881883	-0.037221	4.235845
1	-0.307972	1.091818	2.744685
1	2.393273	-1.477906	4.681497
1	0.599347	0.248861	5.236243
26	0.985930	-0.073903	-0.131483

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$\omega$ -<sup>10</sup>SSC<sub>Fe(cys)</sub>

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3157.1760494  
Zero-point correction=                    0.863942 (Hartree/Particle)  
Thermal correction to Energy=            0.926258  
Thermal correction to Enthalpy=        0.927202  
Thermal correction to Gibbs Free Energy= 0.760961  
Sum of electronic and zero-point Energies= -3156.312108  
Sum of electronic and thermal Energies= -3156.249791  
Sum of electronic and thermal Enthalpies= -3156.248847  
Sum of electronic and thermal Free Energies= -3156.415088

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Cartesian Coordinates

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6	-0.796161	-3.793127	3.373636
6	0.445812	-3.249245	3.078041
6	0.522210	-2.017233	2.430221
6	-0.624585	-1.313453	2.054671
6	-1.873084	-1.850010	2.427848
6	-1.959983	-3.088372	3.062606
6	-0.538237	-0.084740	1.239866
8	-2.951731	-1.072619	2.145955
6	-4.227542	-1.578598	2.428872
26	-0.572466	-0.132703	-0.717501
7	-2.037698	1.228749	-0.918893
6	-1.919934	2.571800	-1.051876
6	-3.224516	3.183730	-1.240692
6	-4.131439	2.159223	-1.224400
6	-3.365749	0.946220	-1.033705



6	-0.722824	3.274667	-1.054289
6	0.525359	2.707112	-0.892429
7	0.770453	1.373887	-0.770783
6	2.109330	1.247964	-0.593325
6	2.744127	2.554652	-0.565081
6	1.756004	3.465960	-0.771593
6	-3.935992	-0.314719	-0.995705
6	-3.263027	-1.514315	-0.830417
7	-1.916423	-1.642981	-0.727987
6	-1.658115	-2.973223	-0.647182
6	-2.882810	-3.733411	-0.673465
6	-3.900448	-2.824708	-0.784306
6	2.794317	0.051567	-0.459472
6	2.232253	-1.215866	-0.488023
7	0.910588	-1.491180	-0.599441
6	0.793113	-2.844635	-0.539160
6	2.097404	-3.462912	-0.396427
6	2.998958	-2.445947	-0.361640
6	-0.395896	-3.544435	-0.561631
6	0.082448	1.054473	1.931272
8	-0.666595	2.176590	1.887551
8	1.173556	1.038014	2.479374
1	-0.341398	-4.625869	-0.490138
1	-5.005701	-0.372163	-1.154349
1	-0.768582	4.350514	-1.190101
1	3.869646	0.110940	-0.322716
1	1.486931	-1.592648	2.175090
1	1.358160	-3.782082	3.332265
1	-2.925093	-3.509999	3.321454
1	-0.874144	-4.760602	3.863715
1	-4.931773	-0.820213	2.081246
1	-4.422196	-2.515236	1.891755
1	-4.370975	-1.737610	3.508123
16	-0.480854	-0.399797	-3.065211
6	-0.296568	1.249732	-3.810145
1	-1.153514	1.892253	-3.578581
1	0.611052	1.752652	-3.458653
1	-0.231757	1.141032	-4.898681
6	1.840843	4.959717	-0.801541
1	1.432479	5.365961	-1.734856
1	1.271412	5.407948	0.023271
1	2.876595	5.302645	-0.714903
6	2.326625	-4.935968	-0.277070
1	1.800943	-5.341112	0.596573
1	1.957863	-5.472494	-1.159721
1	3.390021	-5.169518	-0.165880
6	-5.622593	2.232463	-1.302560
1	-5.990559	2.034101	-2.317555
1	-6.088139	1.500116	-0.634315
1	-5.973891	3.227289	-1.009934

6	-2.962209	-5.220016	-0.529420
1	-2.363363	-5.730401	-1.293140
1	-2.580063	-5.532454	0.450655
1	-3.992016	-5.580058	-0.612774
6	-5.324516	-3.151261	-0.845758
6	-6.356868	-2.451460	-0.360763
1	-5.553631	-4.101146	-1.330769
1	-7.375120	-2.811301	-0.478796
1	-6.227561	-1.515034	0.172402
6	-3.456509	4.618713	-1.370199
6	-4.422297	5.203619	-2.087690
1	-2.770569	5.264483	-0.820731
1	-4.532780	6.284311	-2.102942
1	-5.113027	4.629245	-2.698213
6	4.492278	-2.519135	-0.273052
6	5.148461	-2.279380	-1.636356
1	4.807652	-3.495956	0.107098
1	4.875270	-1.783373	0.443964
1	4.783840	-3.010309	-2.368997
1	4.868643	-1.300549	-2.041999
6	4.176748	2.789986	-0.202752
6	4.358885	2.688276	1.316249
1	4.510717	3.775419	-0.545148
1	4.834752	2.065175	-0.694030
1	3.790357	3.473191	1.828723
1	3.937074	1.748690	1.694936
6	6.650411	-2.373471	-1.591815
8	7.320634	-2.718295	-0.645924
8	7.212339	-2.030009	-2.771476
1	8.169760	-2.120644	-2.641855
6	5.797926	2.780498	1.744162
8	6.761813	2.841336	1.014950
8	5.927210	2.786489	3.088764
1	6.881806	2.823276	3.259019
6	-0.052130	3.346202	2.414513
6	-1.053686	4.477507	2.293568
1	0.861008	3.555685	1.845033
1	0.239918	3.173413	3.456091
1	-0.614687	5.412744	2.659519
1	-1.348600	4.608126	1.248509
1	-1.953676	4.262027	2.877402
7	-3.506428	1.864148	2.799307
7	-4.264475	1.879929	2.000406

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**M06-A<sub>Ir</sub>(Me)**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-1978.1796225  
Zero-point correction=                    0.634596 (Hartree/Particle)  
Thermal correction to Energy=            0.676988  
Thermal correction to Enthalpy=        0.677933

Thermal correction to Gibbs Free Energy=	0.558493
Sum of electronic and zero-point Energies=	-1977.545026
Sum of electronic and thermal Energies=	-1977.502634
Sum of electronic and thermal Enthalpies=	-1977.501690
Sum of electronic and thermal Free Energies=	-1977.621129

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 Cartesian Coordinates  
 .....

6	-4.041205	-3.012147	-0.004472
6	-2.680364	-2.545994	-0.103121
7	-2.653067	-1.175136	-0.117481
6	-3.948625	-0.749950	-0.007858
6	-4.836118	-1.893976	0.060381
6	-1.558857	-3.362859	-0.171614
6	-0.239380	-2.956969	-0.291608
7	0.178524	-1.653216	-0.358613
6	1.542786	-1.679482	-0.465819
6	2.006119	-3.050236	-0.480812
6	0.901576	-3.843673	-0.368745
6	2.359555	-0.562036	-0.554491
6	1.955182	0.764135	-0.526172
7	0.661656	1.187986	-0.383377
6	0.690498	2.557647	-0.366260
6	2.049802	3.020699	-0.525694
6	2.833720	1.906418	-0.632958
6	-0.415642	3.378891	-0.206679
6	-1.735801	2.979414	-0.053239
7	-2.162727	1.679134	-0.096108
6	-3.527962	1.698959	0.020356
6	-3.991652	3.058221	0.118788
6	-2.879324	3.860786	0.100845
77	-0.990280	0.008772	-0.196241
6	-4.344806	0.577066	0.060787
1	-0.233840	4.451829	-0.226139
1	-5.412480	0.763367	0.172548
1	-1.733937	-4.437639	-0.128476
1	3.429141	-0.743046	-0.647572
6	-0.867078	0.003289	1.848172
1	-1.882390	0.082493	2.257630
1	-0.399399	-0.935578	2.171803
1	-0.263258	0.863559	2.164938
6	4.316696	1.845930	-0.792034
1	4.609373	0.984923	-1.412160
1	4.672499	2.743097	-1.319716
6	5.048116	1.759289	0.561540
1	4.821339	0.804014	1.051082
1	4.712308	2.581905	1.205344
6	6.522468	1.926450	0.348681
8	7.101923	2.975739	0.233819
8	7.178184	0.739605	0.226041

1	8.110859	0.963232	0.052900
6	3.447247	-3.433483	-0.546743
1	3.955048	-2.811848	-1.296723
1	3.549301	-4.468602	-0.898208
6	4.161690	-3.283690	0.816273
1	3.561513	-2.623901	1.461501
1	4.252869	-4.243907	1.334517
6	5.530249	-2.661042	0.751890
8	6.535933	-3.094274	1.256614
8	5.493626	-1.488403	0.084615
1	6.366468	-1.050420	0.155146
6	0.822206	-5.329261	-0.321115
1	1.816167	-5.786819	-0.393879
1	0.368491	-5.682191	0.616146
1	0.213375	-5.732627	-1.143005
6	2.461578	4.451198	-0.547798
1	2.183534	4.966495	0.383079
1	3.546955	4.557815	-0.665120
1	1.983909	5.001876	-1.370634
6	-4.457604	-4.440037	-0.032728
1	-3.802479	-5.040236	-0.677464
1	-4.439381	-4.900778	0.966495
1	-5.482493	-4.536292	-0.413623
6	-5.417477	3.458940	0.264453
1	-6.032076	3.086621	-0.567535
1	-5.857351	3.061657	1.190691
1	-5.527710	4.548763	0.297786
6	-6.283975	-1.802160	0.138430
6	-7.098279	-2.680380	0.734550
1	-6.735380	-0.928996	-0.340821
1	-8.177338	-2.543248	0.725909
1	-6.721047	-3.547850	1.273826
6	-2.866896	5.312113	0.217301
6	-1.955002	6.055285	0.853428
1	-3.715135	5.827767	-0.241659
1	-2.040087	7.139106	0.890042
1	-1.114539	5.613188	1.386757

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**M06-B<sub>Ir</sub>(Me)**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2739.2358889  
Zero-point correction=                    0.856192 (Hartree/Particle)  
Thermal correction to Energy=            0.914296  
Thermal correction to Enthalpy=         0.915240  
Thermal correction to Gibbs Free Energy= 0.761242  
Sum of electronic and zero-point Energies= -2738.379697  
Sum of electronic and thermal Energies= -2738.321593  
Sum of electronic and thermal Enthalpies= -2738.320649  
Sum of electronic and thermal Free Energies= -2738.474647

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### Cartesian Coordinates

6	3.522576	-2.910543	-1.965283
6	3.405985	-1.637799	-1.301710
7	2.085594	-1.290204	-1.191552
6	1.352901	-2.289087	-1.771113
6	2.245184	-3.340313	-2.225858
6	4.474334	-0.897883	-0.807148
6	4.413952	0.304517	-0.117924
7	3.264312	0.990833	0.159760
6	3.630335	2.142016	0.806228
6	5.062543	2.178563	0.975215
6	5.556927	1.038569	0.389651
6	2.750027	3.135121	1.222638
6	1.375054	3.158115	1.043102
7	0.647403	2.178100	0.425693
6	-0.656767	2.583454	0.436603
6	-0.765376	3.871584	1.091396
6	0.495898	4.227738	1.470899
77	1.368268	0.448491	-0.385720
7	-0.527177	-0.106168	-0.895506
6	-1.665339	0.622305	-0.696845
6	-2.801366	-0.090563	-1.236163
6	-2.319491	-1.239822	-1.796400
6	-0.890878	-1.243490	-1.565786
6	-1.723705	1.865045	-0.082642
6	-0.023585	-2.252489	-1.960096
8	-4.109497	-4.034186	1.993289
6	-3.310509	-3.062738	2.479431
8	-3.596162	-2.357117	3.422266
6	-2.061330	-2.968274	1.718549
7	-1.948040	-3.802366	0.710248
7	-1.855224	-4.527561	-0.159864
6	-0.980573	-2.012436	2.004463
6	-1.276512	-0.753642	2.539929
6	-0.272485	0.158966	2.827438
6	1.052786	-0.164932	2.550837
6	1.374996	-1.411504	2.012868
6	0.365454	-2.343927	1.757936
8	0.597882	-3.588459	1.274346
6	1.929546	-4.046164	1.204754
1	-0.461858	-3.095202	-2.493100
1	-2.707031	2.326003	-0.004260
1	3.188647	3.998279	1.722974
1	5.467511	-1.308021	-0.988267
1	-2.315299	-0.506638	2.741099
1	-0.523333	1.135755	3.238033
1	2.416262	-1.657097	1.815698
1	1.851909	0.544195	2.762979
1	1.876802	-5.076990	0.842895

1	2.529035	-3.454893	0.498164
1	2.405189	-4.026964	2.196893
6	1.581818	1.352941	-2.212249
1	0.991465	2.279017	-2.226682
1	2.643730	1.578921	-2.378993
1	1.219974	0.666835	-2.989797
6	-5.351669	-4.228899	2.683564
1	-6.002847	-4.706172	1.943201
1	-5.768790	-3.249876	2.947589
6	-5.165145	-5.094409	3.906265
1	-4.528260	-4.588794	4.640554
1	-6.134005	-5.300888	4.377211
1	-4.702568	-6.051511	3.637102
6	4.805894	-3.617881	-2.228060
1	4.642148	-4.562797	-2.758585
1	5.489289	-3.008546	-2.836449
1	5.337486	-3.858372	-1.295480
6	5.809306	3.244826	1.695366
1	6.754616	2.853992	2.093500
1	6.060279	4.093515	1.041327
1	5.230873	3.646679	2.537497
6	1.867338	-4.621191	-2.805771
6	0.817679	-5.366405	-2.441993
1	2.535038	-5.010876	-3.579312
1	0.612966	-6.321469	-2.921171
1	0.142369	-5.067289	-1.639926
6	6.931589	0.577389	0.297993
6	8.019125	1.352071	0.215004
1	7.074644	-0.506833	0.297846
1	9.016322	0.919820	0.170290
1	7.954922	2.437571	0.159680
6	-3.065029	-2.289913	-2.542575
1	-4.147555	-2.113479	-2.512792
1	-2.768193	-2.316129	-3.601316
1	-2.879107	-3.293576	-2.135539
6	-4.211052	0.397657	-1.207032
1	-4.905197	-0.455678	-1.229443
1	-4.415732	0.939519	-0.271156
6	-2.046183	4.628563	1.219231
1	-1.965730	5.373898	2.021507
1	-2.847216	3.943179	1.527168
6	-2.450140	5.333214	-0.095552
1	-1.873906	4.895097	-0.925639
1	-2.210289	6.401561	-0.075467
6	-4.532160	1.326496	-2.394544
1	-3.892070	2.215790	-2.351857
1	-4.347050	0.793733	-3.335910
6	-3.897805	5.195968	-0.494850
8	-4.598935	6.090674	-0.898367
8	-4.304537	3.916504	-0.411329

1	-5.202483	3.813355	-0.806653
6	-5.965108	1.756412	-2.323891
8	-6.396730	2.725576	-1.729881
8	-6.782746	0.898982	-2.948329
1	-7.689436	1.227810	-2.807584
6	0.946750	5.465476	2.164177
1	1.653072	6.041014	1.548603
1	0.102489	6.126361	2.394323
1	1.457264	5.241911	3.111954

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**M06-TS(B-C)<sub>Ir(Me)</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2739.2103201  
 Zero-point correction=                    0.853326 (Hartree/Particle)  
 Thermal correction to Energy=            0.911463  
 Thermal correction to Enthalpy=         0.912407  
 Thermal correction to Gibbs Free Energy= 0.762790  
 Sum of electronic and zero-point Energies= -2738.356994  
 Sum of electronic and thermal Energies= -2738.298857  
 Sum of electronic and thermal Enthalpies= -2738.297913  
 Sum of electronic and thermal Free Energies= -2738.447531

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 Cartesian Coordinates  
 -----

6	3.398373	-3.370139	-1.083153
6	2.113699	-2.821337	-0.729218
7	2.156035	-1.452147	-0.798347
6	3.406231	-1.110773	-1.233384
6	4.203196	-2.307373	-1.414750
6	0.984234	-3.572564	-0.429387
6	-0.294448	-3.096724	-0.170508
7	-0.650617	-1.780741	-0.121308
6	-1.996445	-1.732198	0.109303
6	-2.512761	-3.077245	0.253526
6	-1.454363	-3.924916	0.071410
6	-2.751082	-0.568722	0.179955
6	-2.301864	0.732255	-0.006234
7	-1.009794	1.092200	-0.254199
6	-0.987221	2.444191	-0.421528
6	-2.317891	2.978892	-0.246499
6	-3.135461	1.914620	0.008688
6	0.133795	3.200181	-0.741103
6	1.419924	2.730658	-0.968778
7	1.790567	1.417910	-0.943657
6	3.084421	1.348580	-1.371329
6	3.576230	2.673190	-1.656929
6	2.556610	3.544178	-1.368380
77	0.596360	-0.177502	-0.460158
6	3.831041	0.183953	-1.496980
1	-0.018320	4.271130	-0.861160

1	4.846441	0.298233	-1.875395
1	1.103280	-4.656150	-0.445637
1	-3.809576	-0.687383	0.405778
6	0.931513	0.108914	1.732927
6	0.918085	1.489107	2.273032
6	-0.277266	2.017473	2.782606
6	2.018778	2.373057	2.156221
6	-0.393860	3.355373	3.143896
1	-1.138361	1.362218	2.863231
6	1.912910	3.701106	2.563682
6	0.703497	4.196510	3.041810
1	-1.348077	3.728069	3.511680
1	2.770416	4.364342	2.482223
1	0.632561	5.242995	3.335559
6	0.142855	-0.917547	2.495960
8	-1.013850	-0.755762	2.821338
8	0.797507	-2.069140	2.680476
8	3.166288	1.852702	1.665304
6	4.321755	2.652247	1.617288
1	5.109539	2.011534	1.207413
1	4.182357	3.520124	0.953758
1	4.615166	2.996666	2.620449
7	3.474865	-1.157333	1.680721
7	2.633531	-0.539552	2.067276
6	0.032011	-0.318750	-2.475997
1	0.286559	0.612102	-3.002709
1	0.557196	-1.160662	-2.949905
1	-1.050728	-0.487389	-2.550924
6	-4.622104	1.920058	0.132721
1	-4.970699	1.085191	0.757877
1	-4.957366	2.838369	0.638046
6	-5.274664	1.835406	-1.258633
1	-5.000842	0.879200	-1.733299
1	-4.914251	2.648833	-1.898948
6	-6.766984	1.921505	-1.221418
8	-7.470712	2.728727	-1.768530
8	-7.308905	0.933547	-0.445482
1	-8.274794	1.052819	-0.489167
6	-3.929894	-3.455448	0.539466
1	-4.348906	-2.832483	1.342148
1	-3.942590	-4.483427	0.925799
6	-4.866140	-3.397457	-0.683421
1	-4.351403	-3.736778	-1.589407
1	-5.721159	-4.065876	-0.504392
6	-5.443915	-2.035629	-0.955394
8	-5.363675	-1.426216	-1.997594
8	-6.100006	-1.563973	0.118838
1	-6.500737	-0.700326	-0.128111
6	-1.427807	-5.413536	0.109370
1	-1.069633	-5.838183	-0.839314



1	-0.760278	-5.790461	0.899622
1	-2.423484	-5.833359	0.295250
6	-2.670872	4.420973	-0.350141
1	-2.502508	4.812659	-1.363824
1	-3.725168	4.597265	-0.103405
1	-2.064074	5.032496	0.334124
6	3.747058	-4.815443	-1.032149
1	3.235526	-5.323437	-0.203246
1	3.473445	-5.346474	-1.956436
1	4.827357	-4.947834	-0.890637
6	4.958482	2.988362	-2.110288
1	5.713021	2.671189	-1.374141
1	5.203402	2.480205	-3.053766
1	5.094977	4.064557	-2.268238
6	5.596392	-2.307046	-1.826162
6	6.213602	-3.270193	-2.519746
1	6.182260	-1.431473	-1.532869
1	7.270391	-3.197216	-2.767170
1	5.685292	-4.147553	-2.889584
6	2.627148	4.997030	-1.412123
6	2.033519	5.841279	-0.559430
1	3.261419	5.420133	-2.196228
1	2.152670	6.917937	-0.661619
1	1.430392	5.488934	0.278004
6	0.032853	-3.148533	3.234480
1	-0.338677	-2.852128	4.224458
1	-0.839308	-3.328577	2.589880
6	0.950905	-4.341470	3.292832
1	1.811612	-4.147446	3.943994
1	0.415543	-5.217328	3.678798
1	1.330662	-4.575385	2.288701

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**M06-C<sub>Ir(Me)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2739.2286384  
 Zero-point correction=                    0.851597 (Hartree/Particle)  
 Thermal correction to Energy=            0.911934  
 Thermal correction to Enthalpy=         0.912878  
 Thermal correction to Gibbs Free Energy= 0.755238  
 Sum of electronic and zero-point Energies= -2738.377041  
 Sum of electronic and thermal Energies= -2738.316705  
 Sum of electronic and thermal Enthalpies= -2738.315760  
 Sum of electronic and thermal Free Energies= -2738.473401

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 Cartesian Coordinates  
 -----

6	3.173283	-3.341240	-1.250970
6	1.917736	-2.747350	-0.867326
7	1.998661	-1.389206	-0.985508
6	3.236997	-1.085868	-1.465927

6	3.992565	-2.309155	-1.649050
6	0.782997	-3.455090	-0.481100
6	-0.476548	-2.932197	-0.224545
7	-0.788534	-1.605589	-0.225700
6	-2.133378	-1.498831	-0.022361
6	-2.702132	-2.822664	0.137745
6	-1.673765	-3.713262	0.017723
6	-2.849360	-0.310580	0.037901
6	-2.337063	0.976011	-0.073285
7	-1.032369	1.286917	-0.294032
6	-0.924323	2.644460	-0.323794
6	-2.227885	3.232218	-0.106538
6	-3.103551	2.194491	0.056264
6	0.250326	3.355190	-0.543788
6	1.507195	2.832466	-0.830655
7	1.792048	1.505540	-0.949017
6	3.057072	1.393664	-1.447898
6	3.628307	2.706439	-1.615795
6	2.683753	3.606378	-1.190913
77	0.521962	-0.053996	-0.528403
6	3.708246	0.196165	-1.719980
1	0.168319	4.440791	-0.553106
1	4.707152	0.276160	-2.148612
1	0.876971	-4.540104	-0.440119
1	-3.920683	-0.392594	0.210170
6	0.847297	0.206215	1.467389
6	1.736878	1.180514	2.070251
6	1.203230	2.283754	2.759196
6	3.138408	1.130288	1.862288
6	2.006520	3.353247	3.131763
1	0.128642	2.306036	2.933987
6	3.943883	2.197446	2.252327
6	3.370966	3.309355	2.865164
1	1.569297	4.216817	3.629199
1	5.017255	2.169903	2.081473
1	4.010056	4.143881	3.149743
6	-0.242373	-0.251836	2.364613
8	-1.211923	0.398293	2.696990
8	-0.026262	-1.522163	2.724508
8	3.609089	-0.018771	1.344195
6	4.999074	-0.201498	1.253573
1	5.145651	-1.217822	0.872741
1	5.456767	0.512777	0.550233
1	5.478061	-0.103894	2.239485
7	2.834535	-3.083278	2.112810
7	2.845371	-2.303573	2.896713
6	-0.040974	-0.004539	-2.582927
1	-1.027244	-0.468562	-2.728781
1	-0.083757	1.034683	-2.938808
1	0.702244	-0.548591	-3.184524

6	-4.574552	2.267342	0.296368
1	-4.899439	1.460403	0.970482
1	-4.823745	3.211670	0.802236
6	-5.387038	2.189594	-1.010647
1	-5.264850	1.201515	-1.471719
1	-5.024222	2.956850	-1.706044
6	-6.828849	2.483002	-0.725880
8	-7.321669	3.578319	-0.639312
8	-7.563290	1.358842	-0.497786
1	-8.463722	1.664674	-0.284623
6	-4.161092	-3.074588	0.329199
1	-4.559955	-2.357646	1.060618
1	-4.320458	-4.068945	0.766978
6	-4.959154	-2.963734	-0.990808
1	-4.352510	-2.414694	-1.727191
1	-5.172170	-3.948415	-1.419633
6	-6.260064	-2.213647	-0.887294
8	-7.334506	-2.591668	-1.283344
8	-6.071720	-1.001266	-0.326780
1	-6.904817	-0.488965	-0.372697
6	-1.722501	-5.200935	0.058745
1	-2.730111	-5.562739	0.296855
1	-1.437843	-5.641330	-0.907714
1	-1.037530	-5.617518	0.811760
6	-2.506943	4.694342	-0.088602
1	-2.253127	5.165312	-1.049010
1	-3.566708	4.901140	0.104278
1	-1.922722	5.213024	0.684884
6	3.490106	-4.791373	-1.161160
1	2.980734	-5.261182	-0.309626
1	3.191671	-5.342710	-2.065646
1	4.569302	-4.944242	-1.031484
6	5.011621	2.977612	-2.093388
1	5.768489	2.600934	-1.388348
1	5.210419	2.498621	-3.062425
1	5.192564	4.052206	-2.211692
6	5.367991	-2.358556	-2.114352
6	5.947018	-3.369750	-2.772151
1	5.977590	-1.475423	-1.899990
1	6.993725	-3.324270	-3.064609
1	5.396232	-4.260704	-3.068885
6	2.839041	5.050452	-1.105435
6	2.331380	5.836027	-0.149196
1	3.456619	5.512945	-1.880479
1	2.500144	6.910787	-0.153099
1	1.758172	5.429054	0.683743
6	-1.078553	-2.163631	3.456617
1	-1.242755	-1.629872	4.402269
1	-2.004118	-2.091035	2.866320
6	-0.649374	-3.592580	3.659615

1	0.258662	-3.647910	4.272554
1	-1.439325	-4.166970	4.157604
1	-0.434191	-4.057326	2.687836

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**M06-TS(C-P)<sub>Ir(Me)</sub>**  
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Number of imaginary frequencies: 1    Electronic energy:    HF=-2629.7348728  
 Zero-point correction=                    0.841658 (Hartree/Particle)  
 Thermal correction to Energy=            0.897629  
 Thermal correction to Enthalpy=         0.898574  
 Thermal correction to Gibbs Free Energy= 0.750567  
 Sum of electronic and zero-point Energies= -2628.893215  
 Sum of electronic and thermal Energies= -2628.837243  
 Sum of electronic and thermal Enthalpies= -2628.836299  
 Sum of electronic and thermal Free Energies= -2628.984306

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 Cartesian Coordinates  
 .....

6	3.484903	-3.412438	-0.958435
6	2.197099	-2.830761	-0.670752
7	2.263774	-1.467182	-0.793878
6	3.533657	-1.159972	-1.195111
6	4.319811	-2.374995	-1.298641
6	1.048421	-3.549820	-0.362190
6	-0.225442	-3.040952	-0.149410
7	-0.558722	-1.717407	-0.192075
6	-1.902642	-1.631686	0.029547
6	-2.445935	-2.956996	0.243137
6	-1.405793	-3.833754	0.130424
6	-2.641926	-0.456895	0.039705
6	-2.166465	0.828639	-0.181414
7	-0.865791	1.150766	-0.439261
6	-0.809155	2.501667	-0.616309
6	-2.127443	3.071533	-0.452010
6	-2.969819	2.032291	-0.168950
6	0.346998	3.232930	-0.862095
6	1.634051	2.734978	-1.002538
7	1.960635	1.407365	-1.000401
6	3.277665	1.311530	-1.357996
6	3.829258	2.630686	-1.548798
6	2.820325	3.522773	-1.288539
77	0.702757	-0.155229	-0.581787
6	3.994686	0.122805	-1.467582
1	0.231699	4.310048	-0.969862
1	5.028649	0.212763	-1.799513
1	1.150916	-4.634058	-0.312007
1	-3.709645	-0.553514	0.228720
6	0.241999	-0.334285	-2.604184
1	-0.806055	-0.643846	-2.724395
1	0.388841	0.633646	-3.104956

1	0.895442	-1.086666	-3.070224
6	-4.441545	2.089533	0.073271
1	-4.747731	1.331791	0.810482
1	-4.711376	3.066291	0.501725
6	-5.254622	1.887957	-1.220122
1	-5.113974	0.866240	-1.594504
1	-4.907306	2.600381	-1.978722
6	-6.701141	2.178308	-0.956353
8	-7.216050	3.266816	-0.974465
8	-7.410138	1.067600	-0.613247
1	-8.315838	1.373777	-0.424401
6	-3.897117	-3.229570	0.460264
1	-4.307071	-2.483570	1.154256
1	-4.032918	-4.201861	0.951965
6	-4.701969	-3.207804	-0.860243
1	-4.113268	-2.679422	-1.625715
1	-4.889028	-4.218491	-1.237859
6	-6.021860	-2.488978	-0.785516
8	-7.091327	-2.919119	-1.139781
8	-5.859371	-1.238590	-0.304997
1	-6.708395	-0.755374	-0.367381
6	-1.421061	-5.317814	0.247039
1	-2.431338	-5.693875	0.449242
1	-1.071079	-5.803184	-0.675371
1	-0.769960	-5.672378	1.060435
6	-2.440315	4.522497	-0.564667
1	-2.216150	4.910033	-1.568768
1	-3.499957	4.725929	-0.366808
1	-1.848316	5.119791	0.145270
6	3.808815	-4.860540	-0.852129
1	3.237533	-5.344960	-0.049506
1	3.588701	-5.407351	-1.781418
1	4.876012	-5.004718	-0.638963
6	5.245575	2.915502	-1.907262
1	5.945127	2.526608	-1.152957
1	5.521822	2.454108	-2.866275
1	5.429061	3.992670	-1.991970
6	5.726144	-2.410355	-1.660478
6	6.360572	-3.415440	-2.275038
1	6.310350	-1.523034	-1.400477
1	7.425656	-3.360764	-2.489196
1	5.840819	-4.310378	-2.612942
6	2.923275	4.974417	-1.274632
6	2.292084	5.793373	-0.425525
1	3.607296	5.414206	-2.005754
1	2.430529	6.871362	-0.476168
1	1.643898	5.415303	0.366156
6	1.123098	0.120020	1.726106
6	1.074489	1.479621	2.244382
6	0.394774	-0.915940	2.480373

6	-0.114646	2.214246	2.378279
6	2.249294	2.118630	2.677559
8	-0.739386	-0.778951	2.889645
8	1.109658	-2.052165	2.584683
6	-0.089961	3.538504	2.789374
1	-1.052575	1.729263	2.119820
6	2.296898	3.440467	3.090062
8	3.358181	1.309248	2.877891
6	1.112885	4.165304	3.120143
1	-1.026255	4.092467	2.844521
1	3.246108	3.867850	3.404389
6	3.501538	0.346512	1.977103
1	1.124710	5.207523	3.433443
1	4.047355	-0.524365	2.344656
1	3.665760	0.658850	0.938066
1	2.216007	-0.219924	1.489398
6	0.430409	-3.172364	3.168429
1	-0.598623	-3.200681	2.784958
1	0.971386	-4.046302	2.785500
6	0.463371	-3.110160	4.676685
1	-0.100835	-2.242992	5.036916
1	0.014744	-4.014806	5.105563
1	1.495718	-3.034526	5.039902

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**M06-<sup>5</sup>A<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-2395.189857  
Zero-point correction=                    0.630786 (Hartree/Particle)  
Thermal correction to Energy=            0.676574  
Thermal correction to Enthalpy=         0.677519  
Thermal correction to Gibbs Free Energy= 0.545985  
Sum of electronic and zero-point Energies= -2394.559071  
Sum of electronic and thermal Energies= -2394.513282  
Sum of electronic and thermal Enthalpies= -2394.512338  
Sum of electronic and thermal Free Energies= -2394.643872

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Cartesian Coordinates

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26	1.013773	-0.111179	0.414920
7	2.387114	-1.505460	-0.470429
6	2.126590	-2.821678	-0.693103
6	3.355637	-3.553290	-0.885770
6	4.374064	-2.631033	-0.807153
6	3.734762	-1.351271	-0.524188
6	0.851015	-3.393222	-0.736831
6	-0.367892	-2.733806	-0.598502
7	-0.509273	-1.400607	-0.369318
6	-1.841439	-1.151508	-0.315802
6	-2.592925	-2.379699	-0.517217
6	-1.668850	-3.372009	-0.687304

6	-2.410582	0.107765	-0.117113
6	-1.735733	1.321018	0.029641
7	-0.386355	1.463461	0.052819
6	-0.132830	2.793665	0.173916
6	-1.376186	3.540625	0.234825
6	-2.380869	2.617863	0.152333
6	1.135690	3.367185	0.220177
6	2.360982	2.704296	0.108220
6	3.666923	3.347390	0.166020
6	4.593680	2.337310	0.034809
6	3.835761	1.112397	-0.101381
7	2.499649	1.367948	-0.052215
6	4.402935	-0.147905	-0.294823
1	0.807017	-4.469736	-0.913075
1	5.489508	-0.202478	-0.268366
1	1.171551	4.448849	0.357156
1	-3.501752	0.152642	-0.101648
16	1.104348	-0.469877	2.755182
6	1.665140	-2.218511	2.758222
1	2.646803	-2.326838	2.276337
1	1.750603	-2.568609	3.795136
1	0.953189	-2.869835	2.232890
6	-1.488386	5.022153	0.341783
1	-0.970585	5.407737	1.232311
1	-1.042739	5.529517	-0.527186
1	-2.536155	5.344916	0.407066
6	-1.903327	-4.826298	-0.908783
1	-1.435788	-5.180635	-1.839567
1	-1.483681	-5.434699	-0.093587
1	-2.974998	-5.058529	-0.971164
6	3.451348	-5.011493	-1.173454
1	2.922139	-5.608657	-0.416643
1	3.005057	-5.265733	-2.146848
1	4.493257	-5.354849	-1.197756
6	6.075819	2.453947	-0.032023
1	6.544239	2.406965	0.963452
1	6.519421	1.648410	-0.632875
1	6.373332	3.412614	-0.480422
6	5.787167	-2.909886	-0.999211
6	6.711705	-2.105876	-1.540053
1	6.111964	-3.908554	-0.688111
1	7.748086	-2.425708	-1.633904
1	6.465641	-1.118341	-1.927922
6	3.878629	4.775714	0.288165
6	4.963894	5.398455	0.769125
1	3.051285	5.404514	-0.054940
1	5.020490	6.485275	0.797237
1	5.813179	4.855778	1.180585
6	-4.078236	-2.510373	-0.460176
6	-4.566591	-2.683478	0.973819

1	-4.420632	-3.367840	-1.058147
1	-4.571670	-1.632776	-0.903342
1	-4.103077	-3.568143	1.438149
1	-4.245756	-1.840248	1.604470
6	-3.851172	2.868088	0.097341
6	-4.341354	2.989648	-1.341188
1	-4.112619	3.787659	0.640942
1	-4.409725	2.065628	0.601024
1	-3.807667	3.798431	-1.865393
1	-4.105661	2.080959	-1.915903
6	-6.054665	-2.822031	1.080294
8	-6.845693	-2.821477	0.166160
8	-6.450107	-2.960150	2.364966
1	-7.419759	-3.032991	2.330338
6	-5.812288	3.254512	-1.450483
8	-6.587044	3.410939	-0.536622
8	-6.211115	3.311319	-2.741290
1	-7.168929	3.479555	-2.707631

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**M06-<sup>5</sup>B<sub>Fe(cys)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-3156.2464063  
 Zero-point correction=                    0.853567 (Hartree/Particle)  
 Thermal correction to Energy=            0.915332  
 Thermal correction to Enthalpy=         0.916276  
 Thermal correction to Gibbs Free Energy= 0.751414  
 Sum of electronic and zero-point Energies= -3155.392840  
 Sum of electronic and thermal Energies= -3155.331075  
 Sum of electronic and thermal Enthalpies= -3155.330130  
 Sum of electronic and thermal Free Energies= -3155.494992

.....  
 Cartesian Coordinates  
 .....

6	7.133498	-3.182998	-1.096923
6	5.992814	-3.685389	-1.706997
6	4.937292	-2.833361	-2.015772
6	4.986056	-1.469668	-1.709743
6	6.143603	-0.980015	-1.063569
6	7.209926	-1.829606	-0.778964
6	3.847760	-0.597740	-2.025986
7	4.023011	0.696377	-2.179247
7	4.136447	1.814808	-2.341355
8	6.140386	0.339905	-0.741995
6	7.209301	0.845825	0.014048
26	-0.460892	0.516151	1.193390
7	0.925267	2.064552	0.655913
6	0.632854	3.368099	0.430227
6	1.850339	4.167790	0.429360
6	2.884360	3.286381	0.644504
6	2.277241	1.981916	0.797953



6	-0.654952	3.873143	0.225578
6	-1.833466	3.135201	0.136528
7	-1.909773	1.783321	0.252367
6	-3.206766	1.446271	0.041045
6	-4.008519	2.636875	-0.197541
6	-3.146613	3.695323	-0.142148
6	2.991789	0.813640	1.067988
6	2.487916	-0.486428	1.146396
7	1.193518	-0.819977	0.900945
6	1.135871	-2.179279	0.855992
6	2.443384	-2.747335	1.078557
6	3.290152	-1.691223	1.321744
6	-3.697372	0.141726	-0.003693
6	-2.962679	-1.037952	0.126891
7	-1.638258	-1.108446	0.407800
6	-1.306534	-2.430046	0.409791
6	-2.473571	-3.243448	0.123549
6	-3.510768	-2.369322	-0.060494
6	-0.022130	-2.925753	0.624108
6	2.452952	-1.054011	-2.187392
8	1.634148	-0.024262	-2.413391
8	2.104496	-2.216208	-2.141482
1	0.098009	-4.009774	0.589886
1	4.073012	0.914872	1.167894
1	-0.746343	4.953257	0.103596
1	-4.761693	0.028428	-0.202563
1	4.037207	-3.220884	-2.482949
1	5.917417	-4.743301	-1.953131
1	8.096297	-1.443441	-0.281825
1	7.970278	-3.837892	-0.857520
1	6.972636	1.894852	0.217129
1	7.308536	0.307449	0.968422
1	8.159759	0.791662	-0.540029
6	-0.318126	-1.109836	3.947150
1	0.744848	-1.276710	3.724706
1	-0.475786	-1.279791	5.020056
1	-0.904884	-1.853525	3.390874
16	-0.832133	0.601946	3.524796
6	-3.435096	5.145123	-0.323440
1	-4.501051	5.326249	-0.513163
1	-3.154821	5.729414	0.565281
1	-2.875478	5.569122	-1.170554
6	-2.479288	-4.730587	0.040643
1	-1.782291	-5.098579	-0.726585
1	-2.173255	-5.189945	0.992113
1	-3.475444	-5.122623	-0.203351
6	2.764290	-4.198676	1.020369
1	2.225416	-4.775301	1.786939
1	2.480760	-4.613025	0.041199
1	3.836086	-4.386307	1.160776

6	4.347912	3.554255	0.632762
1	4.768181	3.656632	1.645913
1	4.884811	2.735876	0.131396
1	4.569853	4.482394	0.089282
6	1.901189	5.597341	0.188864
6	2.817770	6.456497	0.654021
1	1.099509	6.002550	-0.436154
1	2.779018	7.514416	0.400123
1	3.615767	6.143681	1.325986
6	4.690716	-1.792333	1.689732
6	5.368608	-0.962600	2.494862
1	5.223057	-2.663649	1.293738
1	6.416742	-1.148075	2.730745
1	4.898165	-0.103941	2.972254
6	-4.927075	-2.677090	-0.416807
6	-5.900350	-2.499572	0.768529
1	-5.007119	-3.712895	-0.781905
1	-5.270612	-2.028426	-1.238087
1	-5.559077	-3.105288	1.616360
1	-5.927885	-1.445521	1.069583
6	-5.485268	2.621636	-0.427576
6	-5.902442	2.006242	-1.781171
1	-5.888690	3.641667	-0.356968
1	-5.962510	2.053467	0.382961
1	-6.116283	2.772050	-2.534899
1	-5.063465	1.408187	-2.171557
6	-7.270971	-2.926638	0.351979
8	-8.093755	-2.256571	-0.244314
8	-7.518298	-4.215030	0.642903
1	-8.401377	-4.405220	0.278506
6	-7.080928	1.066827	-1.740188
8	-7.970278	1.022075	-2.558275
8	-6.994338	0.220652	-0.701074
1	-7.679020	-0.483852	-0.756023
6	0.228744	-0.332610	-2.473100
6	-0.502368	0.963538	-2.691710
1	-0.064818	-0.802684	-1.526277
1	0.066422	-1.057758	-3.282868
1	-1.585523	0.784369	-2.681059
1	-0.278248	1.663218	-1.877420
1	-0.225512	1.423818	-3.649382

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**M06-<sup>3</sup>TS(B-C)<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3156.170865  
Zero-point correction=                    0.852971 (Hartree/Particle)  
Thermal correction to Energy=            0.913071  
Thermal correction to Enthalpy=        0.914016  
Thermal correction to Gibbs Free Energy= 0.759291  
Sum of electronic and zero-point Energies= -3155.317894

Sum of electronic and thermal Energies=	-3155.257794
Sum of electronic and thermal Enthalpies=	-3155.256849
Sum of electronic and thermal Free Energies=	-3155.411574

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 Cartesian Coordinates  
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6	-0.112058	-4.125408	2.990659
6	0.946851	-3.244116	2.839440
6	0.707853	-1.929191	2.450190
6	-0.577447	-1.435313	2.181484
6	-1.641881	-2.364293	2.337823
6	-1.407863	-3.676441	2.748646
6	-0.806768	-0.049904	1.692804
7	-2.264630	0.481878	2.551926
7	-3.142763	1.119213	2.195441
8	-2.895075	-1.918778	2.066785
6	-3.991331	-2.736986	2.340205
26	-0.713888	0.086497	-0.590184
7	-2.245795	1.352472	-0.625792
6	-2.198278	2.709958	-0.624717
6	-3.535491	3.275382	-0.613872
6	-4.398034	2.211233	-0.595440
6	-3.574394	1.028212	-0.623415
6	-1.039932	3.471266	-0.677569
6	0.243764	2.961298	-0.644934
7	0.561608	1.640456	-0.536436
6	1.922558	1.583057	-0.546132
6	2.492056	2.909980	-0.625063
6	1.439355	3.775003	-0.694085
6	-4.089423	-0.251566	-0.708988
6	-3.337686	-1.411736	-0.829880
7	-1.983016	-1.466073	-0.738590
6	-1.645920	-2.784639	-0.806279
6	-2.817863	-3.603243	-0.929385
6	-3.889878	-2.744236	-0.980270
6	2.677646	0.426866	-0.494317
6	2.160708	-0.856911	-0.489028
7	0.842994	-1.174541	-0.569400
6	0.793566	-2.538188	-0.629758
6	2.121873	-3.106109	-0.536829
6	2.978740	-2.051377	-0.435568
6	-0.355322	-3.292472	-0.750986
6	0.166291	0.975133	2.155138
8	-0.417049	2.187769	2.308812
8	1.361258	0.835919	2.357724
1	-0.243870	-4.376094	-0.781121
1	-5.171797	-0.358888	-0.700403
1	-1.147978	4.552975	-0.754038
1	3.759049	0.531288	-0.466056
1	1.543087	-1.245773	2.340956

1	1.972009	-3.569309	3.020040
1	-2.243271	-4.362783	2.868742
1	0.053729	-5.157274	3.301423
1	-4.879260	-2.153019	2.072738
1	-3.983678	-3.657675	1.731585
1	-4.039727	-3.013013	3.406977
6	-2.114973	0.524915	-3.609025
1	-2.426653	1.526128	-3.281919
1	-2.041488	0.524080	-4.704737
1	-2.890885	-0.195812	-3.313687
16	-0.491547	0.061732	-2.927393
6	1.451675	5.262355	-0.766214
1	2.475099	5.653534	-0.829937
1	0.901555	5.635118	-1.642265
1	0.982876	5.715926	0.121317
6	2.417509	-4.563983	-0.503924
1	1.938280	-5.044205	0.363249
1	2.046332	-5.077380	-1.402844
1	3.496191	-4.758447	-0.440310
6	-2.816595	-5.091223	-0.975884
1	-2.278012	-5.477255	-1.853789
1	-2.323083	-5.512956	-0.086342
1	-3.835548	-5.496592	-1.017768
6	-5.880111	2.215275	-0.472418
1	-6.388101	2.086855	-1.441356
1	-6.223694	1.405192	0.185054
1	-6.228521	3.165038	-0.045763
6	-3.828153	4.695380	-0.563413
6	-4.914843	5.303958	-1.055967
1	-3.079445	5.318118	-0.063665
1	-5.060508	6.376870	-0.943443
1	-5.680894	4.761005	-1.608223
6	-5.284152	-3.126195	-1.125248
6	-6.253891	-2.452951	-1.757369
1	-5.549032	-4.093748	-0.683627
1	-7.270443	-2.839979	-1.800564
1	-6.062908	-1.513936	-2.274559
6	4.460098	-2.071351	-0.258529
6	5.236335	-1.755167	-1.555039
1	4.776518	-3.062209	0.102573
1	4.766334	-1.346142	0.510857
1	4.922574	-2.445782	-2.347055
1	5.027195	-0.726229	-1.871169
6	3.958886	3.187680	-0.612589
6	4.633605	2.853314	0.736954
1	4.144208	4.242622	-0.859150
1	4.441865	2.604250	-1.408602
1	4.777528	3.745958	1.355808
1	3.974591	2.179398	1.309320
6	6.702137	-1.899758	-1.298774

8	7.442282	-1.067517	-0.808952
8	7.157834	-3.126879	-1.605511
1	8.095508	-3.135011	-1.341946
6	5.963778	2.152292	0.635267
8	6.940787	2.392393	1.305547
8	5.925135	1.165139	-0.276673
1	6.749473	0.630385	-0.262610
6	0.441568	3.249960	2.692360
6	-0.421484	4.482296	2.809242
1	1.233395	3.377584	1.937968
1	0.937820	3.000274	3.641957
1	0.183741	5.358647	3.076076
1	-0.926181	4.676296	1.852604
1	-1.196814	4.344766	3.573044

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**M06-10SSC<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 0    Electronic energy:    HF=-3156.2127576  
Zero-point correction=                    0.851668 (Hartree/Particle)  
Thermal correction to Energy=            0.913756  
Thermal correction to Enthalpy=         0.914700  
Thermal correction to Gibbs Free Energy=    0.752316  
Sum of electronic and zero-point Energies=    -3155.361090  
Sum of electronic and thermal Energies=    -3155.299001  
Sum of electronic and thermal Enthalpies=   -3155.298057  
Sum of electronic and thermal Free Energies= -3155.460441

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Cartesian Coordinates

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6	-0.980687	-3.694972	3.510973
6	0.280123	-3.181286	3.241804
6	0.399621	-1.970380	2.564009
6	-0.722422	-1.253914	2.132716
6	-1.993320	-1.758475	2.479302
6	-2.119800	-2.978149	3.142858
6	-0.567501	-0.056862	1.298277
8	-3.052434	-0.970784	2.150170
6	-4.334745	-1.453507	2.435947
26	-0.553859	-0.139290	-0.662840
7	-2.024517	1.198964	-0.948327
6	-1.908435	2.545372	-1.088489
6	-3.197401	3.148361	-1.369860
6	-4.099081	2.111782	-1.407926
6	-3.343661	0.913141	-1.146102
6	-0.715555	3.252029	-1.035193
6	0.531643	2.686245	-0.851689
7	0.783082	1.350651	-0.724683
6	2.131947	1.239342	-0.577269
6	2.756959	2.544931	-0.578686
6	1.755117	3.451536	-0.760751

6	-3.910841	-0.349468	-1.086906
6	-3.236591	-1.528229	-0.826001
7	-1.889440	-1.638210	-0.675225
6	-1.630186	-2.969024	-0.544175
6	-2.848328	-3.735791	-0.568840
6	-3.870640	-2.836208	-0.736823
6	2.830492	0.050783	-0.441007
6	2.267267	-1.214021	-0.414197
7	0.936832	-1.480597	-0.486006
6	0.818355	-2.833830	-0.405361
6	2.117707	-3.455691	-0.278738
6	3.027564	-2.440910	-0.280250
6	-0.371316	-3.536582	-0.423505
6	0.125670	1.063999	1.945684
8	-0.622024	2.188555	1.964553
8	1.253551	1.032277	2.409410
1	-0.315443	-4.620659	-0.329531
1	-4.972866	-0.426837	-1.302490
1	-0.757467	4.332215	-1.174176
1	3.913972	0.116989	-0.340721
1	1.381831	-1.563060	2.329527
1	1.176364	-3.723280	3.543446
1	-3.103300	-3.376097	3.383123
1	-1.093476	-4.648618	4.027156
1	-5.036693	-0.692179	2.079685
1	-4.542067	-2.399518	1.909856
1	-4.482686	-1.601339	3.519116
16	-0.414437	-0.474667	-2.992384
6	0.003183	1.124551	-3.760259
1	-0.778827	1.874619	-3.573796
1	0.957172	1.521616	-3.384988
1	0.091601	0.981579	-4.845455
6	1.843141	4.938144	-0.795731
1	1.391517	5.356619	-1.707121
1	1.320958	5.401213	0.057271
1	2.887006	5.277258	-0.761840
6	2.352727	-4.921132	-0.164307
1	1.831015	-5.346402	0.706539
1	1.990230	-5.464651	-1.049398
1	3.420803	-5.150234	-0.053211
6	-5.574953	2.179901	-1.583850
1	-5.878384	2.103034	-2.639430
1	-6.083798	1.371862	-1.040580
1	-5.964697	3.134985	-1.204265
6	-2.923259	-5.206184	-0.354315
1	-2.284379	-5.756711	-1.059803
1	-2.584766	-5.470484	0.659716
1	-3.946671	-5.584978	-0.466825
6	-5.282588	-3.171895	-0.798552
6	-6.341451	-2.430590	-0.443067

1	-5.490800	-4.184535	-1.159577
1	-7.352546	-2.820582	-0.546555
1	-6.246827	-1.428716	-0.026505
6	-3.424480	4.571241	-1.524377
6	-4.424415	5.162482	-2.193209
1	-2.695843	5.223696	-1.033067
1	-4.514388	6.246839	-2.224656
1	-5.165428	4.594925	-2.753716
6	4.515481	-2.539134	-0.239561
6	5.111522	-2.544545	-1.642952
1	4.830186	-3.453955	0.282983
1	4.955141	-1.711542	0.336301
1	4.686972	-3.368263	-2.238764
1	4.837247	-1.633036	-2.195012
6	4.184491	2.810340	-0.241970
6	4.352437	2.901733	1.272435
1	4.535125	3.745109	-0.703997
1	4.847858	2.025985	-0.632596
1	3.771423	3.744981	1.678534
1	3.921576	2.016344	1.767686
6	6.603374	-2.684433	-1.652001
8	7.316518	-2.859359	-0.692049
8	7.102520	-2.602284	-2.905335
1	8.065296	-2.702213	-2.806048
6	5.777781	3.061242	1.701867
8	6.750314	3.068078	0.983197
8	5.882311	3.208142	3.041068
1	6.836102	3.285274	3.217140
6	0.020979	3.354357	2.461274
6	-0.983727	4.477252	2.391104
1	0.910599	3.561722	1.844438
1	0.375016	3.175485	3.486938
1	-0.530335	5.426315	2.706279
1	-1.352819	4.583743	1.361521
1	-1.847620	4.268446	3.033762
7	-3.622012	2.197714	2.158772
7	-4.461202	1.713610	1.625897

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**M06-<sup>1</sup>OSS<sup>r</sup>TS(C-D)<sub>Fe(cys)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-3046.724714  
Zero-point correction=                    0.840839 (Hartree/Particle)  
Thermal correction to Energy=            0.898025  
Thermal correction to Enthalpy=         0.898969  
Thermal correction to Gibbs Free Energy= 0.751089  
Sum of electronic and zero-point Energies= -3045.883875  
Sum of electronic and thermal Energies= -3045.826689  
Sum of electronic and thermal Enthalpies= -3045.825745  
Sum of electronic and thermal Free Energies= -3045.973625

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Cartesian Coordinates

6	3.027106	0.794259	3.367216
6	2.184047	1.847392	3.018137
6	0.934289	1.592949	2.464132
6	0.473223	0.285663	2.258226
6	1.309227	-0.756263	2.707092
6	2.576083	-0.512974	3.225431
6	-0.797057	-0.030346	1.574940
8	0.921681	-2.073624	2.618208
6	-0.442082	-2.284325	2.679106
26	-0.798198	-0.075074	-0.498802
7	-2.442778	1.066174	-0.586887
6	-2.494637	2.422377	-0.614197
6	-3.867476	2.886741	-0.653578
6	-4.652215	1.759168	-0.642714
6	-3.743570	0.641875	-0.610524
6	-1.391960	3.265340	-0.632720
6	-0.072825	2.858101	-0.618567
7	0.356394	1.568120	-0.543681
6	1.713859	1.624032	-0.597571
6	2.174127	2.995335	-0.700689
6	1.051236	3.768744	-0.703632
6	-4.152639	-0.680548	-0.628294
6	-3.312560	-1.781904	-0.620764
7	-1.953290	-1.721833	-0.532984
6	-1.518221	-3.012931	-0.494659
6	-2.625410	-3.927572	-0.528197
6	-3.760473	-3.161986	-0.637718
6	2.554536	0.527362	-0.541158
6	2.139313	-0.789087	-0.436510
7	0.849104	-1.211190	-0.453997
6	0.902439	-2.572779	-0.403072
6	2.272898	-3.030508	-0.302121
6	3.047428	-1.911140	-0.310324
6	-0.189779	-3.416223	-0.428125
6	-1.983360	0.612979	2.153684
8	-3.011588	-0.269514	2.300546
8	-2.101006	1.779343	2.483523
1	0.003914	-4.488496	-0.389013
1	-5.222963	-0.873399	-0.644514
1	-1.580438	4.336326	-0.691550
1	3.625183	0.708225	-0.571675
1	0.282493	2.411224	2.164398
1	2.506533	2.879569	3.162623
1	3.186344	-1.367119	3.517250
1	4.027903	0.987395	3.750877
1	-0.896070	-2.032101	3.647737
1	-0.925892	-1.276137	1.817812
1	-0.703369	-3.263005	2.273772



6	-2.271192	0.038266	-3.534591
1	-2.722253	0.999631	-3.252034
1	-2.192913	0.001182	-4.629322
1	-2.942907	-0.768527	-3.208247
16	-0.603154	-0.159961	-2.829126
6	0.925181	5.249929	-0.792792
1	1.906243	5.740589	-0.819512
1	0.379603	5.558525	-1.696725
1	0.376405	5.661975	0.066806
6	2.683722	-4.453049	-0.156324
1	2.315603	-5.073148	-0.986749
1	3.776278	-4.557756	-0.130509
1	2.286577	-4.889704	0.772620
6	-2.508380	-5.411769	-0.497370
1	-1.938097	-5.756082	0.378368
1	-3.492957	-5.894555	-0.463171
1	-1.989182	-5.799042	-1.386727
6	-6.137287	1.664810	-0.598668
1	-6.585651	1.562022	-1.599455
1	-6.471034	0.800641	-0.007239
1	-6.567145	2.568254	-0.144786
6	-4.267289	4.280717	-0.648972
6	-5.390855	4.793475	-1.168169
1	-3.573063	4.971142	-0.161420
1	-5.613320	5.856169	-1.089123
1	-6.110510	4.183052	-1.711911
6	-5.120032	-3.665201	-0.740965
6	-6.136882	-3.140512	-1.436823
1	-5.309909	-4.600890	-0.204358
1	-7.117892	-3.612464	-1.438477
1	-6.020645	-2.247924	-2.049469
6	4.526519	-1.800703	-0.160763
6	5.239493	-1.561469	-1.508261
1	4.928201	-2.723053	0.283662
1	4.783158	-0.982900	0.531007
1	5.001657	-2.389580	-2.189658
1	4.896064	-0.625264	-1.964978
6	3.597839	3.438700	-0.822252
6	4.504091	3.094263	0.378429
1	3.604428	4.527623	-0.967573
1	4.047305	3.021269	-1.734552
1	5.133545	3.963359	0.626285
1	3.915792	2.864933	1.275476
6	6.717833	-1.489121	-1.311275
8	7.403043	-0.483405	-1.276193
8	7.269564	-2.698708	-1.124360
1	8.212470	-2.536638	-0.943023
6	5.466230	1.948395	0.194864
8	5.807576	1.193893	1.081185
8	5.947837	1.865900	-1.052724

1	6.555032	1.085861	-1.089313
6	-4.239843	0.287670	2.742985
6	-5.243294	-0.837753	2.801579
1	-4.551313	1.079753	2.044373
1	-4.098424	0.765311	3.723918
1	-6.226634	-0.465929	3.118218
1	-5.346128	-1.310356	1.815150
1	-4.919660	-1.610907	3.510218

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**M06-<sup>5</sup>A<sub>Fe(his)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2183.1626512  
 Zero-point correction=                    0.666249 (Hartree/Particle)  
 Thermal correction to Energy=            0.712885  
 Thermal correction to Enthalpy=         0.713829  
 Thermal correction to Gibbs Free Energy= 0.579596  
 Sum of electronic and zero-point Energies= -2182.496402  
 Sum of electronic and thermal Energies= -2182.449766  
 Sum of electronic and thermal Enthalpies= -2182.448822  
 Sum of electronic and thermal Free Energies= -2182.583056

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 Cartesian Coordinates  
 .....

6	-1.632420	-3.438629	-0.733803
6	-0.344657	-2.781984	-0.694660
7	-0.514960	-1.434124	-0.554585
6	-1.856318	-1.204508	-0.480930
6	-2.576306	-2.453919	-0.609262
6	0.885100	-3.435385	-0.774364
6	2.157570	-2.860883	-0.753552
7	2.405321	-1.528486	-0.605376
6	3.753659	-1.355424	-0.672945
6	4.405101	-2.644094	-0.878532
6	3.400984	-3.582925	-0.901012
6	4.392725	-0.128544	-0.500626
6	3.801476	1.127710	-0.339384
7	2.456268	1.367916	-0.305287
6	2.290408	2.703902	-0.108623
6	3.583789	3.355627	-0.033475
6	4.529325	2.362829	-0.182004
6	1.056873	3.347599	0.038538
6	-0.209362	2.770416	0.005766
7	-0.451759	1.437392	-0.138611
6	-1.802426	1.274136	-0.141594
6	-2.458010	2.560571	0.030065
6	-1.464084	3.494212	0.116054
6	-1.592236	4.970695	0.259169
6	-3.932540	2.786998	0.022957
6	-4.469519	2.962004	-1.393063
6	-5.955154	3.173147	-1.427910

8	-6.690480	3.205690	-0.470580
6	-2.448439	0.047265	-0.288193
6	6.009457	2.506331	-0.238597
6	3.777913	4.785764	0.128219
6	4.832379	5.387323	0.691681
6	3.516424	-5.051984	-1.112980
6	5.825480	-2.906775	-1.050770
6	6.721374	-2.117102	-1.654198
6	-4.058369	-2.613664	-0.540572
6	-4.541979	-2.777150	0.895927
6	-6.031266	-2.936688	0.993975
8	-6.806371	-2.956375	0.068723
6	-1.845441	-4.906130	-0.873238
8	-6.399760	3.329718	-2.690209
8	-6.428300	-3.063067	2.276186
1	1.089314	4.425924	0.195980
1	-3.539151	0.065443	-0.257351
1	0.846713	-4.520017	-0.885816
1	5.480429	-0.155701	-0.479899
1	6.466646	1.744925	-0.884066
1	6.288992	3.492525	-0.632609
1	6.478206	2.412173	0.752754
1	4.561501	-5.383350	-1.102805
1	2.979571	-5.619407	-0.339344
1	3.092157	-5.354990	-2.081413
1	-1.370845	-5.303401	-1.781806
1	-1.422393	-5.462447	-0.023925
1	-2.912603	-5.155346	-0.926598
1	-2.639616	5.274910	0.379241
1	-1.038952	5.348035	1.131204
1	-1.196755	5.499349	-0.620503
1	2.974854	5.421955	-0.254206
1	4.895823	6.471819	0.749678
1	5.652975	4.827346	1.137072
1	6.174653	-3.871101	-0.669334
1	7.765048	-2.412917	-1.736330
1	6.443418	-1.171124	-2.116929
1	-4.463764	1.955042	0.507504
1	-4.192497	3.676147	0.614716
1	-3.985305	3.814671	-1.893901
1	-4.226779	2.090686	-2.020585
1	-7.362899	3.453780	-2.621135
1	-4.383079	-3.485068	-1.126548
1	-4.571254	-1.755336	-0.997433
1	-4.068672	-3.650057	1.372160
1	-4.241848	-1.918857	1.516405
1	-7.396982	-3.156305	2.247137
7	1.084424	-0.338208	1.976080
6	1.910015	-1.150566	2.596538
6	0.375572	0.323622	2.947770

7	1.762610	-1.042395	3.938003
1	2.616041	-1.816324	2.111059
6	0.782553	-0.101276	4.179494
1	-0.375363	1.059225	2.681746
1	2.282591	-1.555657	4.635600
1	0.478876	0.168021	5.181328
26	0.980347	-0.068159	-0.174491

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**M06-<sup>5</sup>B<sub>Fe(his)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2944.2216418  
 Zero-point correction=                    0.890116 (Hartree/Particle)  
 Thermal correction to Energy=            0.951134  
 Thermal correction to Enthalpy=         0.952078  
 Thermal correction to Gibbs Free Energy= 0.792011  
 Sum of electronic and zero-point Energies= -2943.331526  
 Sum of electronic and thermal Energies= -2943.270508  
 Sum of electronic and thermal Enthalpies= -2943.269564  
 Sum of electronic and thermal Free Energies= -2943.429631

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 Cartesian Coordinates  
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6	2.571846	3.553322	1.226697
6	2.202549	2.156098	1.226185
7	0.898668	2.017232	0.850599
6	0.417483	3.260099	0.585170
6	1.467152	4.249881	0.801200
6	3.073888	1.105280	1.510747
6	2.849014	-0.262703	1.340278
7	1.688204	-0.815091	0.893427
6	1.882004	-2.163046	0.813181
6	3.226866	-2.494253	1.219574
6	3.829891	-1.305542	1.575024
6	0.908145	-3.090697	0.425514
6	-0.412511	-2.829728	0.069759
7	-0.964384	-1.585996	0.005783
6	-2.259832	-1.741266	-0.380721
6	-2.564227	-3.153663	-0.543243
6	-1.409920	-3.833329	-0.270526
7	-1.708321	1.233267	-0.148388
6	-2.891814	0.676456	-0.527870
6	-3.857053	1.718886	-0.801721
6	-3.229891	2.911502	-0.548431
6	-1.880158	2.586334	-0.139451
6	-3.147840	-0.694268	-0.626823
6	-0.898163	3.521477	0.196817
8	5.929123	-1.567654	-1.140988
6	5.247164	-0.403592	-1.175561
8	5.694247	0.642565	-0.747535
6	3.926039	-0.575594	-1.793753

7	3.657832	-1.833723	-2.088892
7	3.510574	-2.938905	-2.301148
6	2.967588	0.506894	-2.076041
6	3.367800	1.845348	-2.005059
6	2.480156	2.885182	-2.262090
6	1.166050	2.604367	-2.604053
6	0.739059	1.282392	-2.691288
6	1.624119	0.239311	-2.427821
8	1.266237	-1.068242	-2.487320
6	0.010769	-1.398103	-3.034650
1	-1.185198	4.570628	0.136371
1	-4.152821	-0.974857	-0.939696
1	1.213424	-4.137592	0.420406
1	4.072550	1.391902	1.839208
1	4.394268	2.066273	-1.731235
1	2.821525	3.916452	-2.178860
1	-0.296098	1.066825	-2.944872
1	0.456808	3.407858	-2.799031
1	-0.046611	-2.490888	-3.023507
1	-0.813533	-0.998137	-2.427224
1	-0.075487	-1.032175	-4.069279
6	7.267670	-1.510870	-0.634816
1	7.464898	-2.523934	-0.266070
1	7.302971	-0.820279	0.215347
6	8.233739	-1.103744	-1.721192
1	8.025253	-0.080875	-2.055647
1	9.264593	-1.137819	-1.347568
1	8.157308	-1.777265	-2.583210
6	3.941497	4.065771	1.501083
1	3.987077	5.159795	1.446984
1	4.303236	3.765012	2.494885
1	4.661357	3.669496	0.768540
6	3.831781	-3.853545	1.186973
1	4.914571	-3.788766	1.011630
1	3.689801	-4.400921	2.131285
1	3.401040	-4.467109	0.385357
6	1.408541	5.680170	0.546005
6	0.714384	6.293135	-0.420451
1	2.033502	6.301094	1.194732
1	0.747554	7.374231	-0.537785
1	0.115147	5.740846	-1.143332
6	5.181266	-1.074468	2.054768
6	5.925097	-1.931205	2.765636
1	5.620247	-0.107145	1.791928
1	6.939747	-1.676794	3.067002
1	5.546408	-2.897340	3.095712
6	-3.786834	4.288859	-0.652187
1	-4.825516	4.281665	-1.006332
1	-3.777583	4.804133	0.319059
1	-3.206282	4.913887	-1.346276

6	-5.266067	1.496637	-1.241625
1	-5.630072	2.366861	-1.808127
1	-5.329428	0.633981	-1.922307
6	-3.924197	-3.673000	-0.876569
1	-3.862095	-4.711607	-1.228289
1	-4.341765	-3.096375	-1.713266
6	-4.889992	-3.597241	0.327123
1	-4.472526	-2.898424	1.070329
1	-4.994422	-4.565243	0.828700
6	-6.214787	1.250908	-0.051520
1	-5.904461	0.346802	0.485858
1	-6.172460	2.109275	0.631174
6	-6.276514	-3.081064	0.034902
8	-7.300412	-3.551839	0.466568
8	-6.233277	-1.967913	-0.717574
1	-7.127613	-1.555931	-0.773296
6	-7.614616	1.064088	-0.549551
8	-8.131471	0.011186	-0.870054
8	-8.264503	2.228340	-0.681234
1	-9.138252	2.016403	-1.057437
6	-1.167818	-5.302391	-0.287184
1	-0.859713	-5.674985	0.700402
1	-2.067463	-5.857469	-0.579808
1	-0.368921	-5.574960	-0.991806
7	-0.819651	0.048381	2.629261
6	-0.594140	0.933298	3.573233
6	-1.617691	-0.923065	3.180781
7	-1.216927	0.573219	4.720630
1	0.004394	1.830357	3.456794
6	-1.876634	-0.615850	4.485538
1	-1.943011	-1.774113	2.591781
1	-1.197412	1.083544	5.592211
1	-2.452031	-1.115240	5.252405
26	-0.076292	0.201457	0.585785

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**M06-<sup>1</sup>CSS<sup>T</sup>S(B-C)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2944.1499078  
Zero-point correction=                    0.889657 (Hartree/Particle)  
Thermal correction to Energy=            0.950554  
Thermal correction to Enthalpy=        0.951498  
Thermal correction to Gibbs Free Energy= 0.794483  
Sum of electronic and zero-point Energies= -2943.260251  
Sum of electronic and thermal Energies= -2943.199354  
Sum of electronic and thermal Enthalpies= -2943.198410  
Sum of electronic and thermal Free Energies= -2943.355425

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Cartesian Coordinates

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6	3.321439	-3.610822	-0.583853
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6	2.079681	-2.952539	-0.263260
7	2.159391	-1.604050	-0.502884
6	3.416968	-1.393266	-0.995676
6	4.159634	-2.635846	-1.067120
6	0.926942	-3.626235	0.119035
6	-0.323658	-3.048966	0.259136
7	-0.584510	-1.714064	0.140435
6	-1.936438	-1.592298	0.271702
6	-2.552717	-2.883907	0.498583
6	-1.540870	-3.797803	0.500498
6	-2.643006	-0.402086	0.229022
6	-2.093651	0.853759	0.030049
7	-0.773343	1.106410	-0.196407
6	-0.684142	2.453492	-0.400281
6	-1.978673	3.083439	-0.264419
6	-2.862654	2.079814	0.009419
6	0.470756	3.134078	-0.748119
6	1.708717	2.548596	-0.965387
7	1.964143	1.213637	-0.874593
6	3.240133	1.045761	-1.326554
6	3.827048	2.308386	-1.702926
6	2.884307	3.265542	-1.434757
6	3.916385	-0.162609	-1.392837
1	0.391285	4.206719	-0.912242
1	4.927165	-0.140242	-1.798708
1	0.996214	-4.706955	0.243557
1	-3.720654	-0.454039	0.370949
6	1.035416	0.172120	1.691849
6	1.096860	1.589897	2.177651
6	-0.078004	2.200170	2.634748
6	2.251057	2.404287	2.097699
6	-0.127717	3.545308	2.984536
1	-0.981187	1.602840	2.693393
6	2.209206	3.744974	2.478696
6	1.018620	4.320568	2.909251
1	-1.071031	3.975434	3.316847
1	3.108453	4.352955	2.418534
1	1.001425	5.373303	3.188550
6	0.209576	-0.749121	2.560910
8	-0.924191	-0.497347	2.903907
8	0.827253	-1.899382	2.865204
8	3.391203	1.815288	1.665543
6	4.573918	2.568013	1.578060
1	5.335975	1.879309	1.198044
1	4.464881	3.406792	0.872573
1	4.886040	2.949331	2.562437
7	3.529944	-1.130032	1.866552
7	2.652016	-0.484027	2.079432
6	-4.336405	2.192676	0.218921
1	-4.688917	1.446209	0.946766

1	-4.578505	3.178981	0.642312
6	-5.128968	2.026226	-1.092439
1	-5.023470	1.000399	-1.466842
1	-4.732630	2.725399	-1.839829
6	-6.567111	2.380334	-0.864500
8	-7.021469	3.495763	-0.840326
8	-7.350800	1.295081	-0.614772
1	-8.244144	1.644028	-0.442035
6	-4.024946	-3.091865	0.631418
1	-4.443032	-2.326139	1.298663
1	-4.231977	-4.056333	1.114580
6	-4.751597	-3.039139	-0.731634
1	-4.106378	-2.515326	-1.453933
1	-4.937074	-4.040996	-1.133220
6	-6.057025	-2.290900	-0.736019
8	-7.099852	-2.679713	-1.202149
8	-5.911447	-1.065076	-0.193179
1	-6.737705	-0.556069	-0.320173
6	-1.611769	-5.272738	0.692438
1	-2.642998	-5.606836	0.861167
1	-1.230550	-5.820688	-0.181481
1	-1.015246	-5.601689	1.557045
6	-2.230202	4.545316	-0.389022
1	-1.629426	5.116375	0.335003
1	-1.967673	4.923840	-1.387479
1	-3.285221	4.792084	-0.215376
6	3.606245	-5.056555	-0.373225
1	3.080819	-5.447031	0.508083
1	3.303690	-5.677306	-1.230718
1	4.681367	-5.220608	-0.222706
6	5.218054	2.494842	-2.199912
1	5.423956	3.545717	-2.436032
1	5.965063	2.179235	-1.455229
1	5.410891	1.906843	-3.108636
6	5.533372	-2.751933	-1.523576
6	6.092202	-3.827433	-2.091490
1	6.161759	-1.868425	-1.380886
1	7.140711	-3.830161	-2.381688
1	5.524307	-4.730755	-2.309180
6	3.057774	4.705061	-1.556108
6	2.547640	5.637491	-0.741238
1	3.706379	5.038659	-2.371683
1	2.746426	6.694694	-0.905741
1	1.936818	5.378900	0.124582
6	0.038810	-2.880789	3.555026
1	-0.976243	-2.876109	3.137840
1	0.518523	-3.833729	3.301670
6	0.036872	-2.628933	5.043336
1	-0.460950	-1.680081	5.271538
1	-0.499025	-3.432234	5.563942



1	1.061552	-2.591897	5.432926
7	0.234503	-0.515910	-2.259874
6	0.587884	-1.545707	-2.997941
6	-0.492673	0.316670	-3.077069
7	0.115654	-1.413163	-4.260597
1	1.176398	-2.390658	-2.660638
6	-0.577432	-0.224068	-4.327125
1	-0.903385	1.246526	-2.704130
1	0.259154	-2.068220	-5.015280
1	-1.052512	0.118308	-5.235587
26	0.722515	-0.232556	-0.267799

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**M06-<sup>1</sup>OSSC<sub>Fe(his)</sub>**  
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Number of imaginary frequencies: 0    Electronic energy:    HF=-2834.7278582  
 Zero-point correction=                    0.881753 (Hartree/Particle)  
 Thermal correction to Energy=            0.940918  
 Thermal correction to Enthalpy=         0.941862  
 Thermal correction to Gibbs Free Energy= 0.787428  
 Sum of electronic and zero-point Energies= -2833.846105  
 Sum of electronic and thermal Energies= -2833.786940  
 Sum of electronic and thermal Enthalpies= -2833.785996  
 Sum of electronic and thermal Free Energies= -2833.940430

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 Cartesian Coordinates  
 .....

6	3.368743	-3.393324	-0.645198
6	2.088146	-2.792874	-0.374547
7	2.129121	-1.438390	-0.571228
6	3.398446	-1.161894	-0.987973
6	4.193511	-2.371121	-1.048991
6	0.952457	-3.517017	-0.044556
6	-0.305871	-2.976584	0.148925
7	-0.605855	-1.646800	0.081384
6	-1.950149	-1.563174	0.298744
6	-2.519272	-2.875035	0.525302
6	-1.488274	-3.762051	0.436177
6	-2.684813	-0.392234	0.328216
6	-2.172181	0.878876	0.131663
7	-0.872817	1.167807	-0.169075
6	-0.808563	2.527848	-0.286270
6	-2.103799	3.121505	-0.062072
6	-2.957399	2.087921	0.207394
6	0.333201	3.256941	-0.573760
6	1.586488	2.715595	-0.795310
7	1.865250	1.380774	-0.799392
6	3.154989	1.273582	-1.229215
6	3.724391	2.572573	-1.492784
6	2.758231	3.487410	-1.170240
6	3.864882	0.090091	-1.347415

1	0.235351	4.337649	-0.653074
1	4.886503	0.160242	-1.719403
1	1.051096	-4.599337	0.037121
1	-3.749603	-0.471327	0.536067
6	0.941515	0.137990	1.512241
6	1.423899	1.388514	2.116589
6	0.513390	2.313089	2.630252
6	2.797201	1.693072	2.157706
6	0.941071	3.552746	3.101649
1	-0.544092	2.050435	2.630097
6	3.227885	2.933498	2.620990
6	2.294341	3.862775	3.080458
1	0.214939	4.268934	3.482912
1	4.286199	3.182658	2.635333
1	2.642571	4.830922	3.438616
6	0.351175	-0.811232	2.485488
8	-0.706103	-0.621129	3.048867
8	1.123315	-1.888039	2.676601
8	3.623043	0.698750	1.748249
6	4.997327	0.966608	1.683198
1	5.466828	0.062995	1.281414
1	5.208952	1.814386	1.010937
1	5.418030	1.182601	2.677749
6	-4.419140	2.163530	0.500750
1	-4.716982	1.385961	1.219968
1	-4.654384	3.129281	0.972389
6	-5.277372	2.026295	-0.772043
1	-5.174425	1.014592	-1.184263
1	-4.935102	2.756458	-1.516236
6	-6.707645	2.343539	-0.456558
8	-7.193615	3.445076	-0.422069
8	-7.437437	1.240185	-0.134288
1	-8.327302	1.564819	0.094650
6	-3.973730	-3.123630	0.749431
1	-4.364259	-2.382777	1.459965
1	-4.123370	-4.102197	1.224820
6	-4.790880	-3.063422	-0.561686
1	-4.204918	-2.518406	-1.317787
1	-4.987747	-4.062538	-0.964437
6	-6.105846	-2.338742	-0.460574
8	-7.177181	-2.747287	-0.835628
8	-5.936422	-1.109490	0.067815
1	-6.781586	-0.618031	0.025390
6	-1.506332	-5.242135	0.597925
1	-2.515794	-5.609405	0.819826
1	-1.162279	-5.760286	-0.308863
1	-0.850402	-5.568402	1.419664
6	-2.389291	4.582263	-0.102869
1	-2.156138	5.017778	-1.084931
1	-3.445548	4.794464	0.104369

1	-1.788686	5.131037	0.637911
6	3.701449	-4.832113	-0.459851
1	3.132251	-5.277278	0.366684
1	3.491779	-5.434057	-1.357472
1	4.768879	-4.955151	-0.234053
6	5.113066	2.822621	-1.969140
1	5.868150	2.437290	-1.267081
1	5.305535	2.336928	-2.936737
1	5.306292	3.894778	-2.091506
6	5.596218	-2.415949	-1.422796
6	6.238655	-3.452871	-1.973736
1	6.172916	-1.507200	-1.227189
1	7.301604	-3.400743	-2.199260
1	5.729061	-4.377229	-2.241192
6	2.885838	4.937560	-1.175065
6	2.366818	5.766102	-0.261705
1	3.493463	5.366136	-1.977480
1	2.517904	6.841810	-0.327868
1	1.806392	5.396156	0.598148
6	0.558393	-2.915187	3.498787
1	0.359066	-2.509674	4.499831
1	-0.409130	-3.213465	3.066109
6	1.544179	-4.053737	3.524697
1	2.503416	-3.730745	3.946476
1	1.159232	-4.882772	4.131031
1	1.728941	-4.419013	2.505208
7	0.172333	-0.345657	-2.375995
6	0.692046	-1.231765	-3.194350
6	-0.708190	0.400183	-3.120211
7	0.181712	-1.090523	-4.442375
1	1.432188	-1.977257	-2.926115
6	-0.717910	-0.047057	-4.410308
1	-1.273947	1.206819	-2.669154
1	0.425615	-1.647852	-5.248367
1	-1.264582	0.270938	-5.287045
26	0.651398	-0.121670	-0.267960

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**M06-1<sup>OSS</sup>TS(C-D)<sub>Fe(his)</sub>**

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Number of imaginary frequencies: 1    Electronic energy:    HF=-2834.7006627  
Zero-point correction=                    0.876703 (Hartree/Particle)  
Thermal correction to Energy=            0.934675  
Thermal correction to Enthalpy=         0.935619  
Thermal correction to Gibbs Free Energy= 0.785426  
Sum of electronic and zero-point Energies= -2833.823960  
Sum of electronic and thermal Energies= -2833.765988  
Sum of electronic and thermal Enthalpies= -2833.765043  
Sum of electronic and thermal Free Energies= -2833.915236

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Cartesian Coordinates

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6	3.048524	-3.637771	-0.885123
6	1.851470	-2.937515	-0.498335
7	1.986560	-1.586394	-0.684336
6	3.235159	-1.412194	-1.204926
6	3.918925	-2.681878	-1.346670
6	0.703932	-3.568964	-0.054638
6	-0.480035	-2.933702	0.277856
7	-0.677686	-1.582051	0.289604
6	-1.990000	-1.404356	0.628951
6	-2.642333	-2.675891	0.832089
6	-1.690407	-3.634711	0.624706
6	-2.623655	-0.176882	0.712569
6	-2.035173	1.044573	0.433935
7	-0.737692	1.230082	0.052429
6	-0.601479	2.570116	-0.159400
6	-1.838478	3.263327	0.106319
6	-2.738703	2.305559	0.471822
6	0.552217	3.211987	-0.577310
6	1.748226	2.587213	-0.871228
7	1.937454	1.234306	-0.867503
6	3.194204	1.037707	-1.364061
6	3.833038	2.292158	-1.674143
6	2.941919	3.273504	-1.333368
6	3.796887	-0.194249	-1.547391
1	0.510409	4.291825	-0.700091
1	4.796037	-0.200825	-1.979474
1	0.719073	-4.656818	0.002050
1	-3.673819	-0.171502	1.003882
6	-4.207207	2.446018	0.681990
1	-4.567347	1.773550	1.474460
1	-4.473139	3.459828	1.009604
6	-4.936054	2.130696	-0.624642
1	-4.598408	1.170341	-1.042201
1	-4.671013	2.882062	-1.386383
6	-6.425877	2.139673	-0.482320
8	-7.071947	2.759438	0.321379
8	-7.017906	1.337572	-1.413389
1	-7.978473	1.411617	-1.263260
6	-4.093111	-2.904264	1.094108
1	-4.553703	-2.056159	1.620482
1	-4.218340	-3.770961	1.758688
6	-4.882871	-3.191409	-0.200554
1	-4.344910	-3.933910	-0.802499
1	-5.875570	-3.584007	0.053685
6	-5.059876	-1.950914	-1.029940
8	-4.363888	-1.606516	-1.961294
8	-6.101127	-1.229200	-0.588862
1	-6.215400	-0.441565	-1.161588
6	-1.827063	-5.115267	0.710813

1	-2.821851	-5.409078	1.068892
1	-1.673179	-5.602725	-0.263130
1	-1.090995	-5.549758	1.403527
6	-2.033786	4.733679	-0.017614
1	-1.865354	5.087679	-1.044823
1	-3.049561	5.031087	0.271367
1	-1.332896	5.284497	0.627726
6	3.269641	-5.103138	-0.753104
1	2.751992	-5.514125	0.123125
1	2.913104	-5.660934	-1.632469
1	4.339621	-5.324052	-0.645002
6	5.224628	2.438378	-2.179858
1	5.956313	2.068232	-1.446843
1	5.386268	1.873935	-3.109238
1	5.470670	3.487596	-2.380866
6	5.276666	-2.837617	-1.839408
6	5.767494	-3.906772	-2.477053
1	5.951344	-1.995091	-1.663728
1	6.807956	-3.945299	-2.792393
1	5.148366	-4.765279	-2.732492
6	3.164046	4.710250	-1.400298
6	2.714705	5.620886	-0.529163
1	3.792006	5.054798	-2.227244
1	2.942656	6.677460	-0.655398
1	2.139654	5.340360	0.353848
6	1.301464	0.048626	1.612250
6	1.654969	1.400562	2.112857
6	0.553660	-0.782729	2.588994
6	0.711756	2.308060	2.608443
6	2.992229	1.832398	2.070179
8	-0.425587	-0.428574	3.212013
8	1.102301	-2.012647	2.715501
6	1.074933	3.597423	2.983064
1	-0.321235	1.977805	2.693086
6	3.367119	3.120669	2.423428
8	3.985317	0.985433	1.623014
6	2.399969	4.012640	2.873730
1	0.315600	4.279556	3.363862
1	4.416375	3.399341	2.345494
6	3.779613	-0.332973	1.908109
1	2.688904	5.023843	3.157579
1	3.690829	-0.580583	2.972942
1	4.395185	-0.988661	1.291969
1	2.393556	-0.501911	1.466998
7	-0.152959	-0.306802	-2.209191
6	-1.276777	-0.913034	-2.531551
6	0.237054	0.402353	-3.319755
7	-1.626608	-0.625145	-3.804518
1	-1.882584	-1.542282	-1.891318
6	-0.668308	0.217930	-4.325580

1	1.142530	0.997955	-3.310768
1	-2.479045	-0.939992	-4.246962
1	-0.716254	0.594101	-5.337879
6	0.382717	-2.943922	3.526959
1	-0.693842	-2.803642	3.361219
1	0.671864	-3.929560	3.139580
6	0.740543	-2.789486	4.986323
1	0.423005	-1.806828	5.352228
1	0.243847	-3.560163	5.589201
1	1.823874	-2.885692	5.131621
26	0.653308	-0.166869	-0.225989