Supporting Information

Mechanistic insights into ligand-controlled diastereoselectivity in iridium-catalyzed stereoselective coupling of allylic ethers and alkynes: a DFT perspective

Manzhu Zhao,[1] Lihan Zhu,[1]* Qian Zhang[12]*, and Jingping Zhang[1]*

[1]Jilin Province Key Laboratory of Organic Functional Molecular Design & Synthesis, Department of Chemistry, Northeast Normal University, Changchun 130024, China

[2]State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China

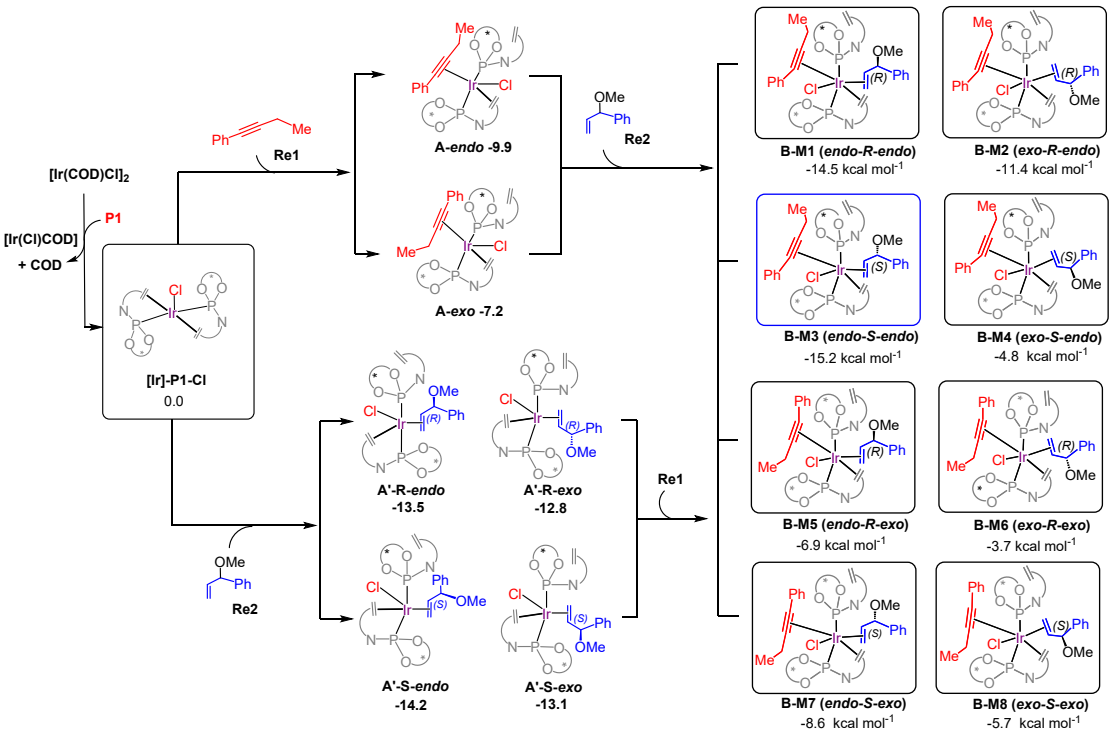
Table of contents

Identification and quantification of Non-Covalent Interactions using AIM

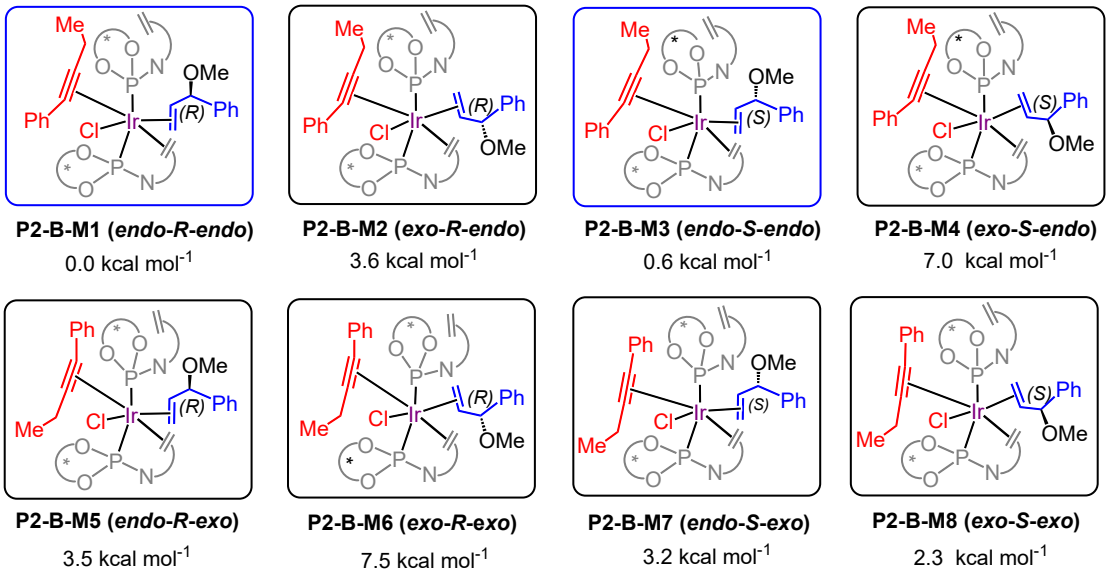
The presence of a bond critical point between a pair of atoms is generally regarded as an indicator of interatomic non-covalent interaction in the AIM. An interacting pair of atoms is characterized by the presence of a bond path and a bond critical point (bcp) along the bond path. The shared electron density shows a minimum at the bcp. The value of the electron density electron densities (ρ), Laplacian of electron density ($\Delta 2\rho$), potential electron density (V) and Kinetic Energy density (K) at such bond critical points provides valuable information about the nature of such interaction and sometime correlates with the strength of such interaction. Summaries of AIM analyses of the stereocontrolling TS structures for the allenyl C(sp2)–H allylation strategy for synthesis of axially chiral tetrasubstituted allenes are presented below.

In general, relatively higher ρbcp values for a given type of interaction imply a stronger interaction. In the present case, ρbcp is employed as an approximate measure of the strength of individual interactions as well as for comparison of the NCIs between the competing transition states.

Scheme S1. Possible routes for the formation of Ir-alkyne-allylic ether complex **B** with substrate using [Ir]-**P1**-Cl catalyst



Scheme S2. Possible routes for the formation of Ir-alkyne-allylic ether complex **P2-B** with substrate using **[Ir]-P2-Cl** catalyst



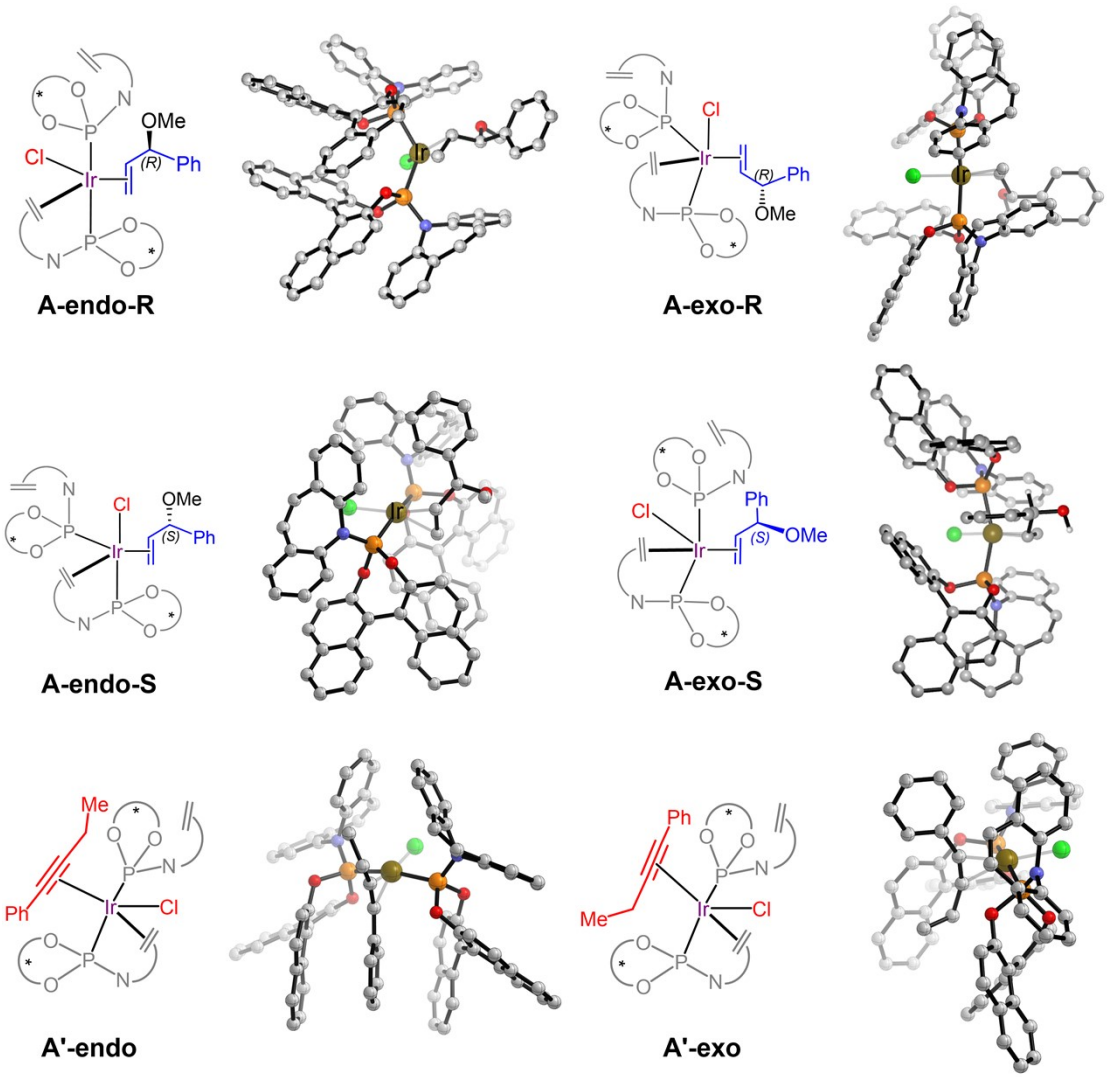


Fig. S1 DFT-optimized structures of intermediates geometries for formation of Ir-alkyne complex or Ir-allylic complex between [Ir(**P1**)$_2$Cl] catalyst and alkyne **Re1** or allylic ether **Re2**.

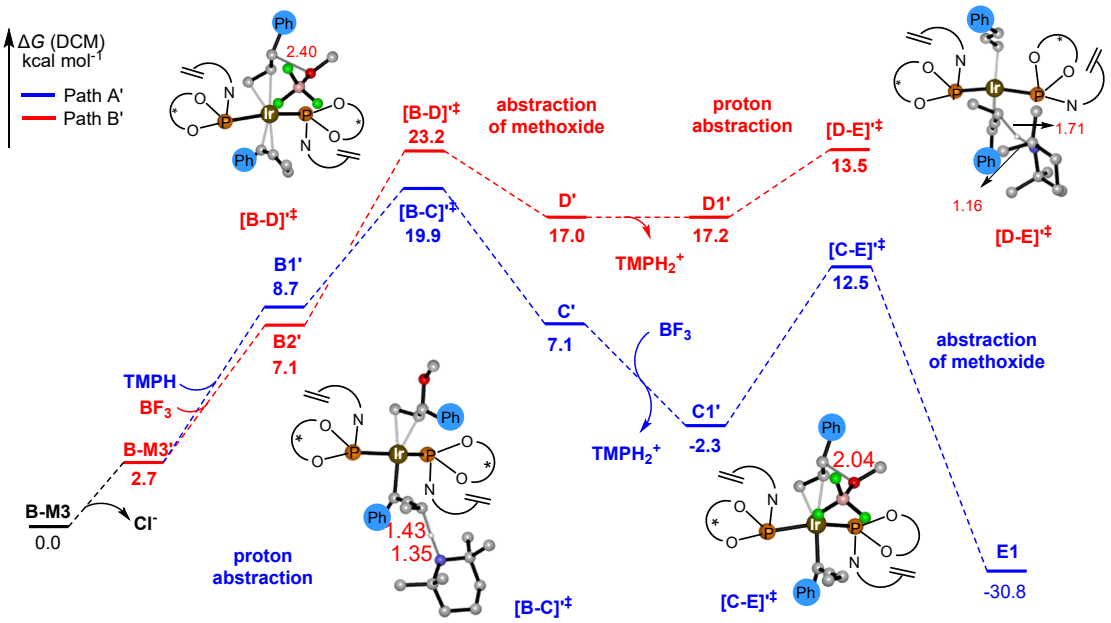


Fig. S2 Relative Gibbs free energy profile diagram for pathway A' and B', and corresponding transition states of the formation of **(*S*,*R*)-Pr1** from Ir-π-alkyne-allylic ether **B-M3**, the distances are in Å.

Our computational results demonstrate that the iridium-catalyzed stereoselective coupling of allylic ethers and alkynes proceeds most favorably via **Path B**, which involves sequential methoxide abstraction, proton abstraction, and enantioselective C–C bond formation. For the methoxide abstraction step, we evaluated the Gibbs free energy profile for interconversion between *R*- and *S*-allylic ethers catalyzed by **[Ir]-P1** (green line) and **[Ir]-P2** (red line) (Fig. S4).

With the Ir-P1-olefin catalyst:

The *S*-allylic ether (**B-M3**, ΔG = 0.0 kcal mol⁻¹) undergoes methoxide abstraction via transition state **[B-D]‡** (ΔG‡ = 2.6 kcal mol⁻¹), yielding the achiral intermediate **D**, exothermic by 3.7 kcal mol^{-1}. Then the **D** species could transfer to the *R*-allylic ether through transition state **[B-D]‡-R** (ΔG‡ = 1.0 kcal mol⁻¹).

With the Ir-P2-olefin catalyst:

A similar trend is observed: the *S*-allylic ethers (**P2-B-M3**) could form the *R*-allylic ethers **P2-B-M1** via transition states **P2-[B-D]‡** (ΔG‡ = 1.2 kcal mol⁻¹) and **P2-[B-D]‡-R** (ΔG‡ = 2.2 kcal mol⁻¹), respectively. Both processes exhibit energy barriers significantly lower than that of the rate-determining step, ensuring smooth progression for interconversion between R- and S-allylic ethers catalyzed by **[Ir]-P1** (green line) and **[Ir]-P2** (red line). This computational outcome corroborates the experimental results, which demonstrated over 50% product yield.

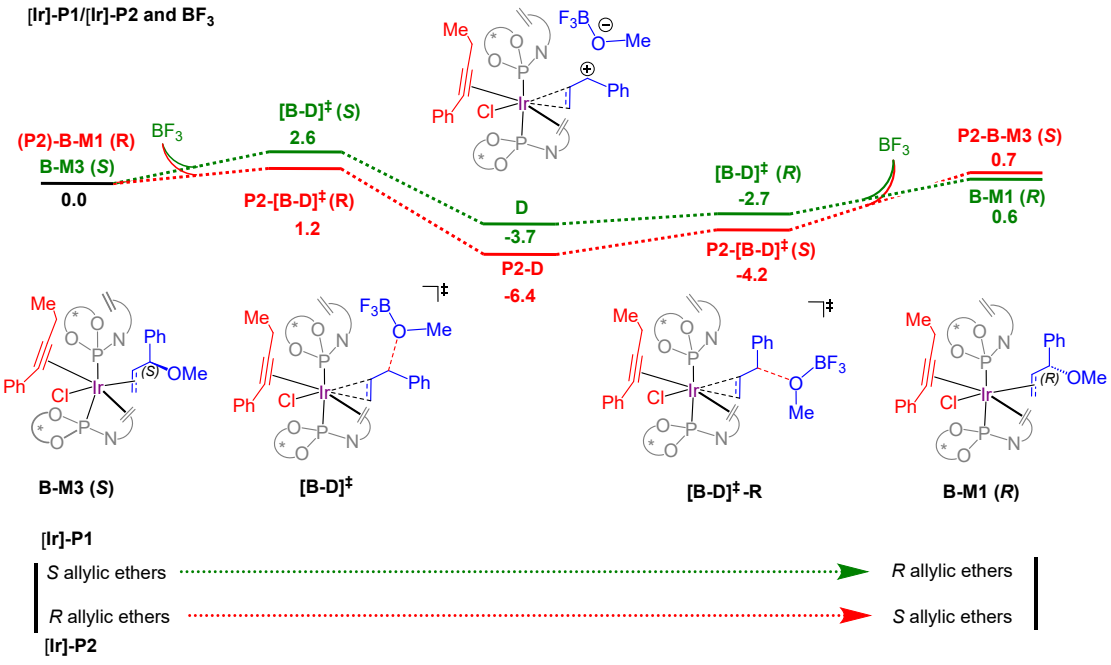


Fig. S3 Gibbs free energy profile for the interconversion between R- and S-allylic ethers catalyzed by **[Ir]-P1** (green line) and **[Ir]-P2** (red line).

To further elucidate the reaction mechanism, we conducted additional computational investigations comparing the pathways in the presence of chloride ions (Path A and Path B, Fig. 1) with those of the cationic species (without Cl^-, Path A' and Path B', Fig. S2). The computational results reveal that for the abstraction of methoxide and proton abstraction processes, the energy barrier of **[D-E]‡** in Path B ($\Delta G^‡$ = 11.8 kcal mol^{-1}) is significantly lower than those of **[B-C]‡** in Path A ($\Delta G^‡$ = 31.2 kcal mol^{-1}), **[B-C]'‡** in Path A' ($\Delta G^‡$ = 19.9 kcal mol^{-1}), and **[B-D]'‡** in Path B' ($\Delta G^‡$ = 23.2 kcal mol^{-1}) by 19.4, 8.1, and 11.4 kcal mol^{-1}. Thus, the chloride-assisted Path B, involving sequential methoxide abstraction ($\Delta G^‡$ = 2.6 kcal mol^{-1}) followed by proton transfer ($\Delta G^‡$ = 11.8 kcal mol^{-1}), represents the most energetically favorable pathway on the potential energy surface. Moreover, for the enantioselective C–C bond formation, our calculations reveal that the departure of chloride from intermediate **E** to form **E1**, followed by C–C bond formation (transition state **(S,R)-[E-F]‡**, $\Delta G^‡$ = 19.7 kcal mol^{-1}), is 3.0 kcal mol^{-1} lower in energy than the direct C–C coupling in the presence of Cl^- (transition state **(S,R)-[E-F]'‡**, $\Delta G^‡$ = 22.7 kcal mol^{-1}). This suggests that chloride dissociation further reduces the reaction barrier of C–C bond formation and facilitates the enantioselective process. The IMGH (Intrinsic Molecular Geometry and Hydrogen-bonding) analysis confirms the presence of stabilizing C–H···Cl^- interactions between the chloride ion and the reactants, which play a crucial role in transition-state stabilization (see Fig. S3).

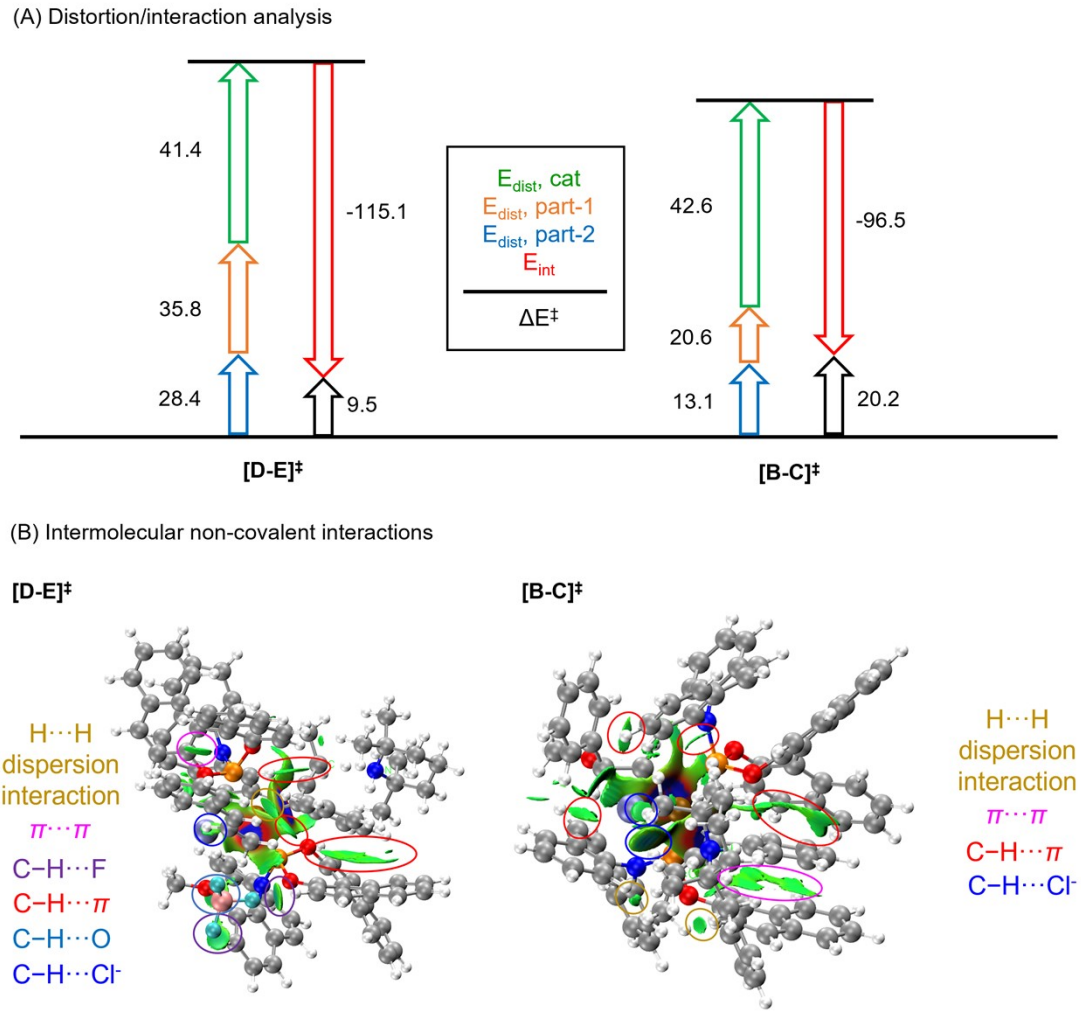
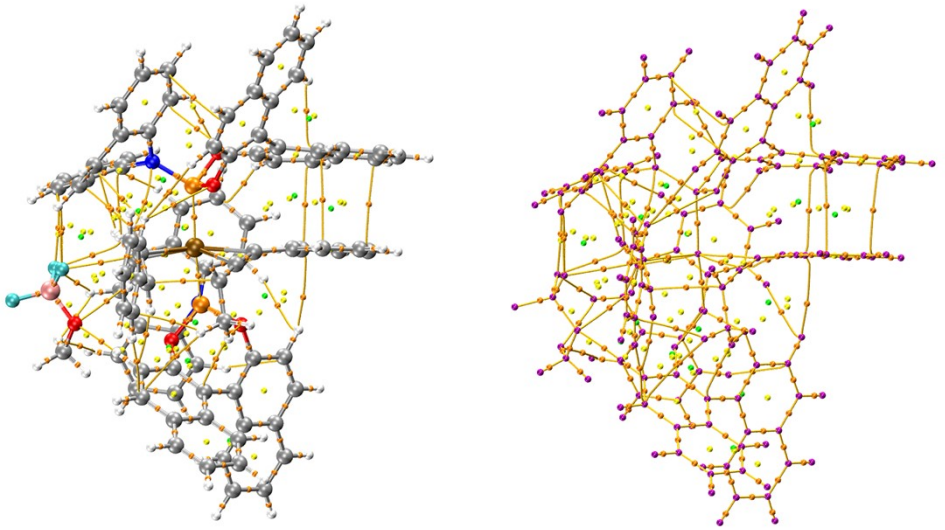
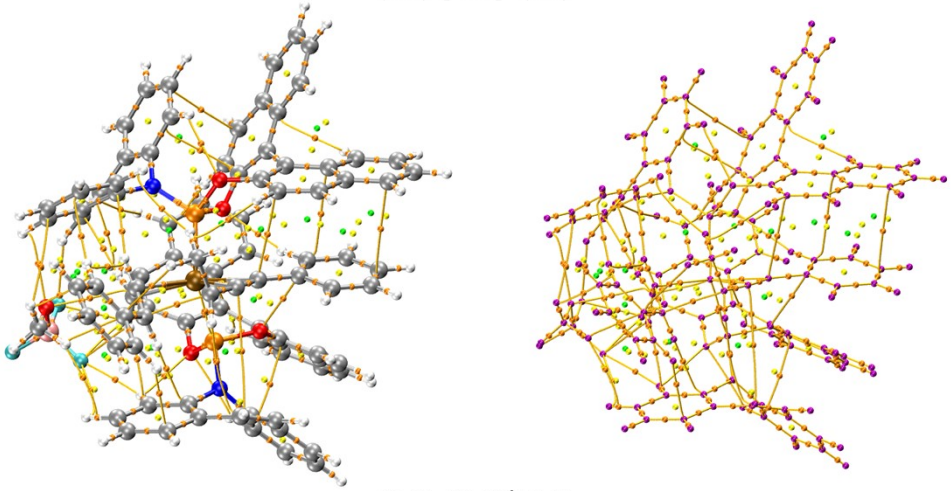


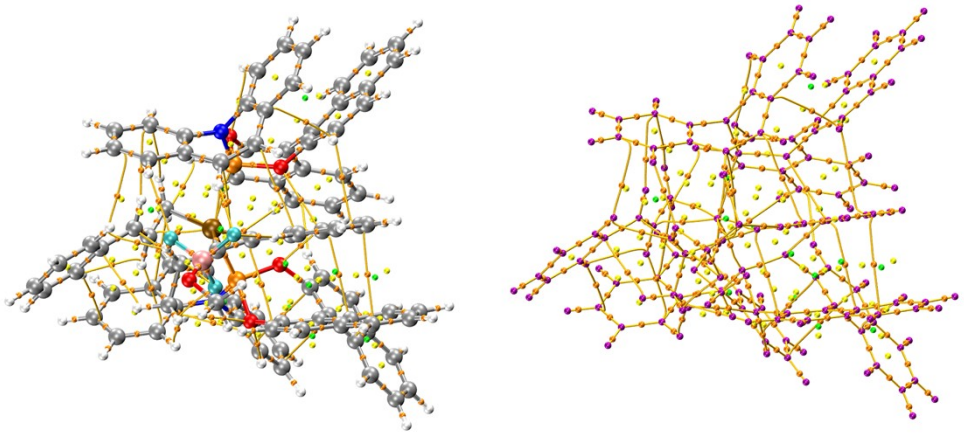
Fig. S4 (A) Distortion/interaction analysis and (B) intermolecular non-covalent interaction analysis for key transition states **[D-E]‡** and **[B-D]‡**.



(*S*,*R*)-**[E-F]‡** (0.0)

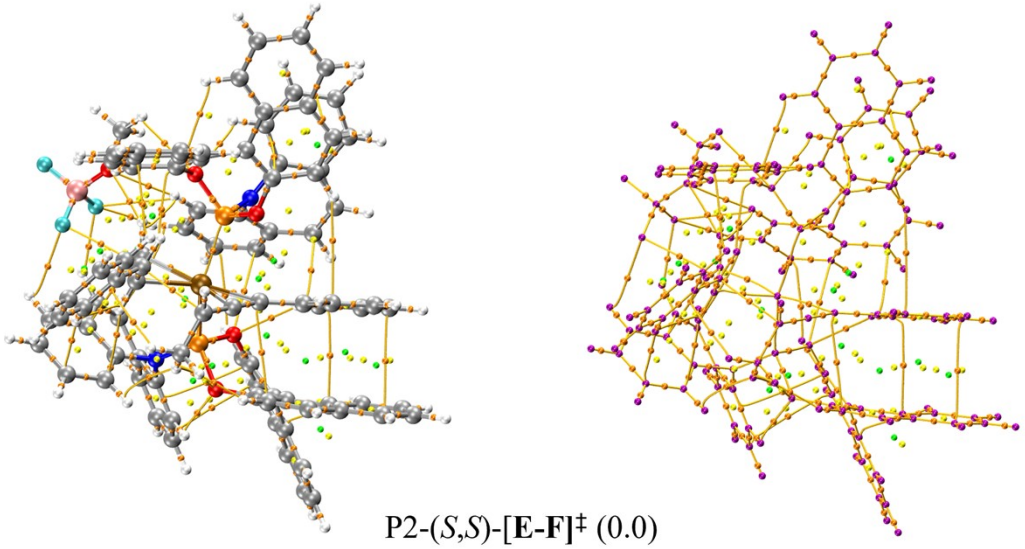


(*R*,*S*)-**[E-F]‡** (1.6)

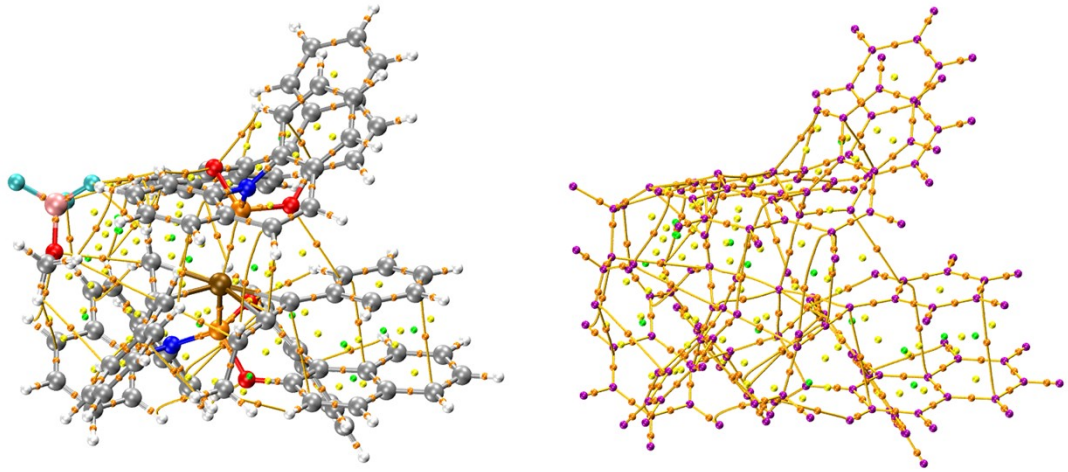


(*S*,*S*)-**[E-F]‡** (2.5)

Fig. S5 Visualization of QTAIM critical points for the transition states (*S*,*R*)-**[E-F]‡**, (*R*,*S*)-**[E-F]‡**, and (*S*,*S*)-**[E-F]‡**. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP), and green to cage critical points (CCP). Yellow lines indicate the bond path.



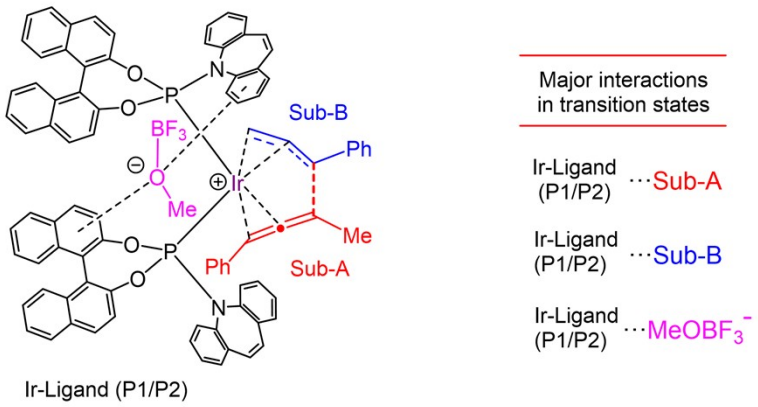
P2-(*S*,*S*)-[**E-F**]‡ (0.0)



P2-(*S*,*R*)-**[E-F]‡** (1.9)

Fig. S6 Visualization of QTAIM critical points for the transition states P2-(*S*,*S*)-**[E-F]‡** and P2-(*S*,*R*)-**[E-F]‡**. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP), and green to cage critical points (CCP). Yellow lines indicate the bond path.

(a) Fragments of enantioselectivity transition states



(b) Distortion/interaction analysis

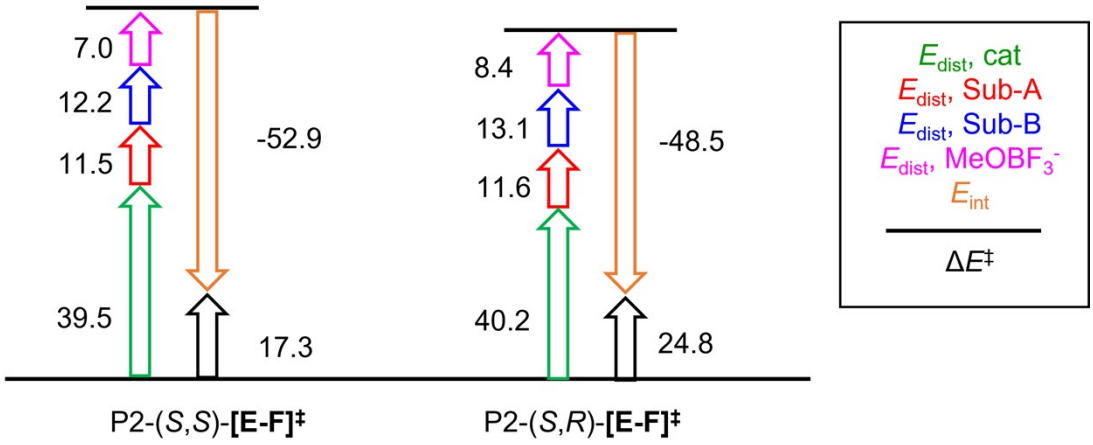
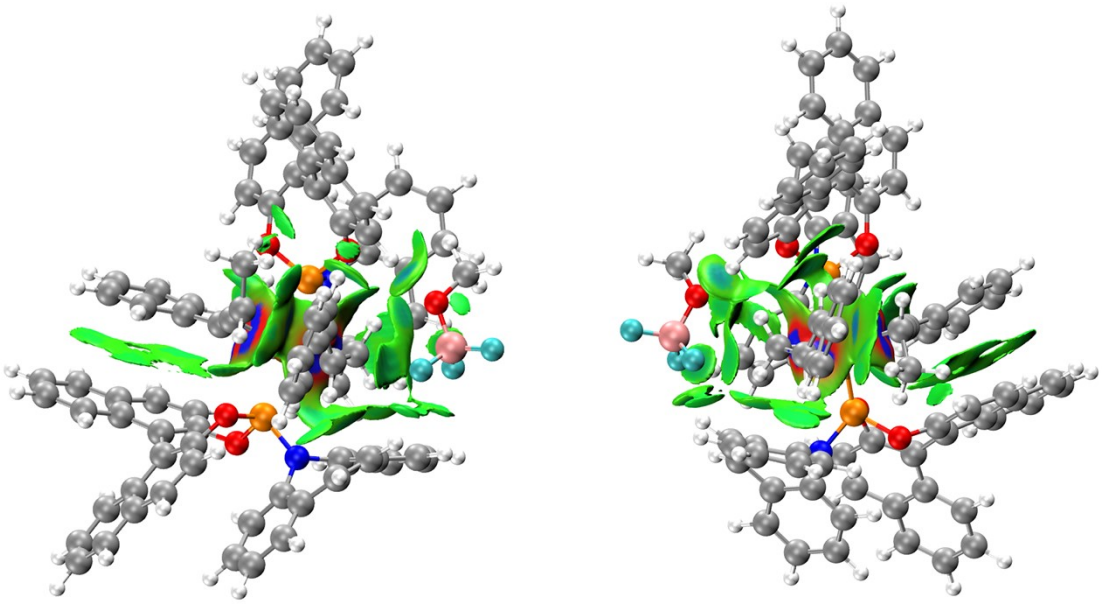


Fig. S7 (a) Fragments of enantioselectivity transition states and classification of various NCIs as identified in the stereocontrolling C-C bond formation TSs. (b) Distortion/interaction analysis for key transition states P2-(*S*,*S*)-**[E-F]‡** and P2-(*S*,*R*)-**[E-F]‡**.



(*S*,*R*)-**[E-F]‡**

P2-(*S*,*S*)-[**E-F**]‡

Fig. S8 NCI plot of (*S*,*R*)-**[E-F]‡** and P2-(*S*,*S*)-**[E-F]‡**. The plot corresponds to a reduced density gradient of 0.60 au.

Table S1. Electron densities at the bond critical points of transition state **(*S*,*R*)-[E-F]‡**.

classification	Bond Id	Noncovalent Interactions	Distance	a.u				E_{NCI}
				ρ	$\Delta_2\rho$	V	K	
[Ir]-P1···SubA	1a	$\pi\cdots\pi$	3.19	0.008	0.023	-0.36 e^{-2}	-0.11 e^{-2}	-1.1
			3.32	0.007	0.017	-0.28 e^{-2}	-0.74 e^{-3}	-0.9
			3.46	0.005	0.013	-0.23 e^{-2}	-0.52 e^{-3}	-0.7
	1b	C−H···O	2.82	0.005	0.020	-0.32 e^{-2}	-0.89 e^{-3}	-1.0
	1c	C−H···π	2.37	0.013	0.042	-0.79 e^{-2}	-0.14 e^{-2}	-2.5
	1d		2.86	0.006	0.017	-0.30 e^{-2}	-0.69 e^{-3}	-0.9
	1e		3.02	0.004	0.011	-0.17 e^{-2}	-0.56 e^{-3}	-0.5
$E_{NCI(IrL1\cdots SubA)}$								-7.6
[Ir]-P1···SubB	1f	C−H···π	2.62	0.010	0.034	-0.57 e^{-2}	-0.14 e^{-2}	-1.8
	1g		2.40	0.013	0.039	-0.77 e^{-2}	-0.98 e^{-3}	-2.4
	1h		3.02	0.003	0.014	-0.18 e^{-2}	-0.80 e^{-3}	-0.6
	1i		2.66	0.009	0.026	-0.43 e^{-2}	-0.11 e^{-2}	-1.3
	1j		2.30	0.015	0.045	-0.90 e^{-2}	-0.12 e^{-2}	-2.8
	1k		2.82	0.006	0.017	-0.26 e^{-2}	-0.85 e^{-3}	-0.8
$E_{NCI(IrL1\cdots SubB)}$								-9.7
[Ir]-P1···MeOBF_3^-	1l	C−H···O	2.03	0.023	0.068	-0.17 e^{-1}	-0.34 e^{-3}	-5.3
	1m	C−H···F	2.40	0.010	0.037	-0.79 e^{-2}	-0.68 e^{-3}	-2.5
	1n	C−H···F	2.50	0.008	0.034	-0.60 e^{-2}	-0.12 e^{-2}	-1.9
	1o	C−F···π	3.00	0.008	0.031	-0.48 e^{-2}	-0.15 e^{-2}	-1.5
	1p		3.25	0.005	0.021	-0.26 e^{-2}	-0.14 e^{-2}	-0.8
	1q	H···H	2.26	0.007	0.024	-0.40 e^{-2}	-0.97 e^{-3}	-1.3
	1r		2.62	0.004	0.015	-0.17 e^{-2}	-0.10 e^{-2}	-0.5
$E_{NCI(IrL1\cdots MeOBF3-)}$								-13.8
$E_{NCI\text{-}Total}$								-31.1

Table S2. Electron densities at the bond critical points of transition state **(*S*,*S*)-[E-F]**‡.

classification	Bond Id	Noncovalent Interactions	Distance	a.u				E_{NCI}
				ρ	$\Delta^2\rho$	V	K	
[Ir]-P1···SubA	2a	C−H···O	2.39	0.011	0.036	-0.87 e^{-2}	-0.15 e^{-3}	-2.7
	2b	$\pi\cdots\pi$	3.28	0.007	0.021	-0.33 e^{-2}	-0.95 e^{-3}	-1.0
			3.55	0.005	0.012	-0.22 e^{-2}	-0.42 e^{-3}	-0.7
$E_{NCI(IrL1\cdots SubA)}$								-4.4
[Ir]-P1···SubB	2c	C−H···π	2.47	0.013	0.039	-0.75 e^{-2}	-0.11 e^{-2}	-2.4
	2d		2.45	0.011	0.038	-0.62 e^{-2}	-0.16 e^{-2}	-1.9
	2e		2.54	0.011	0.031	-0.62 e^{-2}	-0.83 e^{-3}	-1.9
	2f		2.52	0.011	0.031	-0.60 e^{-2}	-0.95 e^{-3}	-1.9
	2g		2.54	0.010	0.029	-0.54 e^{-2}	-0.96 e^{-3}	-1.7
$E_{NCI(IrL1\cdots SubB)}$								-9.8
[Ir]-P1···MeOBF_3^-	2h	C−H···F	2.17	0.015	0.052	-0.12 e^{-1}	0.69 e^{-5}	-3.8
	2i		2.18	0.015	0.048	-0.11 e^{-1}	0.32 e^{-3}	-3.5
	2j		2.36	0.010	0.041	-0.80 e^{-2}	-0.93 e^{-3}	-2.5
	2k		2.39	0.010	0.034	-0.74 e^{-2}	-0.52 e^{-3}	-2.3
$E_{NCI(IrL1\cdots MeOBF3^-)}$								-12.1
$E_{NCI\text{-}Total}$								-26.3

Table S3. Electron densities at the bond critical points of transition state **(*R*,*S*)-[E-F]‡**.

classification	Bond Id	Noncovalent Interactions	Distance	a.u				E_{NCI}
				ρ	$\Delta^2\rho$	V	K	
[Ir]-P1···Sub A	3a	C–H···O	2.48	0.010	0.031	-0.70 e^{-2}	-0.32 e^{-3}	-2.2
	3b		2.80	0.005	0.020	-0.34 e^{-2}	-0.80 e^{-3}	-1.1
	3c	$\pi\cdots\pi$	3.16	0.008	0.026	-0.40 e^{-2}	-0.13 e^{-2}	-1.3
				0.008	0.023	-0.36 e^{-2}	-0.11 e^{-2}	-1.1
				0.006	0.014	-0.24 e^{-2}	-0.52 e^{-3}	-0.8
	3d	C–H···π	3.07	0.005	0.015	-0.19 e^{-2}	-0.91 e^{-3}	-0.6
$E_{NCI(IrL1\cdots SubA)}$								-7.1
[Ir]-P1···Sub B	3e	C–H···π	2.49	0.012	0.036	-0.68 e^{-2}	-0.11 e^{-2}	-2.1
	3f		2.60	0.010	0.030	-0.56 e^{-2}	-0.94 e^{-3}	-1.8
	3g		2.68	0.008	0.024	-0.40 e^{-2}	-0.97 e^{-3}	-1.3
	3h		2.74	0.007	0.023	-0.36 e^{-2}	-0.10 e^{-2}	-1.1
	3i		2.75	0.007	0.024	-0.36 e^{-2}	-0.11 e^{-2}	-1.1
	3j		3.13	0.003	0.011	-0.14 e^{-2}	-0.70 e^{-3}	-0.4
$E_{NCI(IrL1\cdots SubB)}$								-7.8
[Ir]-P1···MeOBF_3^-	3k	C–H···F	2.10	0.018	0.054	-0.14 e^{-1}	0.65 e^{-3}	-4.4
	3l		2.37	0.010	0.043	-0.86 e^{-2}	-0.10 e^{-2}	-2.7
$E_{NCI(IrL1\cdots MeOBF3^-)}$								-7.1
$E_{NCI\text{-}Total}$								-22.0

Table S4. Electron densities at the bond critical points of transition state **P2-(S,S)-[E-F]**‡.

classification	Bond Id	Noncovalent Interactions	Distance	a.u				E_{HB}
				ρ	$\Delta_2\rho$	V	K	
[Ir]-P2···SubA	4a	C−H···O	2.44	0.010	0.032	-0.77 e^{-2}	-0.23 e^{-3}	-2.4
	4b	C−H···π	2.73	0.008	0.030	-0.37 e^{-2}	-0.19 e^{-2}	-1.2
	4c	π···π	3.24	0.008	0.022	-0.34 e^{-2}	-0.10 e^{-2}	-1.1
			3.25	0.008	0.022	-0.34 e^{-2}	-0.10 e^{-2}	-1.1
			3.50	0.005	0.013	-0.23 e^{-2}	-0.48 e^{-3}	-0.7
$E_{NCI(IrP2\cdots SubA)}$								**-6.5**
[Ir]-P2···SubB	4d	C−H···π	2.42	0.013	0.042	-0.77 e^{-2}	-0.14 e^{-2}	-2.4
	4e		2.42	0.013	0.040	-0.76 e^{-2}	-0.12 e^{-2}	-2.4
	4f		2.70	0.008	0.026	-0.42 e^{-2}	-0.11 e^{-2}	-1.3
	4g		2.49	0.012	0.038	-0.71 e^{-2}	-0.12 e^{-2}	-2.2
	4h		2.56	0.010	0.027	-0.52 e^{-2}	-0.76 e^{-2}	-1.6
$E_{NCI(IrP2\cdots SubB)}$								**-9.9**
[Ir]-P2···[BF_3OMe^-]	4i	C−H···O	2.06	0.023	0.064	-0.16 e^{-1}	-0.55 e^{-5}	-5.0
	4j		2.47	0.010	0.028	-0.72 e^{-2}	0.10 e^{-3}	-2.3
	4k		2.91	0.004	0.018	-0.27 e^{-2}	-0.90 e^{-3}	-0.8
	4l	C−H···F	2.17	0.016	0.050	-0.13 e^{-1}	0.34 e^{-3}	-4.1
	4m		2.22	0.014	0.049	-0.12 e^{-1}	-0.32 e^{-3}	-3.8
	4n		2.56	0.007	0.035	-0.55 e^{-2}	-0.16 e^{-2}	-1.7
	4o		2.75	0.005	0.025	-0.34 e^{-2}	-0.15 e^{-2}	-1.1
$E_{NCI(IrP2\cdots MeOBF3^-)}$								**-18.8**
$E_{NCI\text{-}Total}$								-35.2

Table S5. Electron densities at the bond critical points of transition state **P2-(S,R)-[E-F]**‡.

Bond Id	classification	Noncovalent Interactions	Distance	a.u				E_{NCI}
				ρ	$\Delta_2\rho$	V	K	
[Ir]-P2···SubA	5a	C–H···O	2.39	0.011	0.036	-0.87 e^{-2}	-0.15 e^{-3}	-2.7
	5b		2.74	0.012	0.046	-0.78 e^{-2}	-0.18 e^{-2}	-2.4
	5c	$\pi\cdots\pi$	3.28	0.007	0.021	-0.33 e^{-2}	-0.95 e^{-3}	-1.0
			3.55	0.005	0.012	-0.22 e^{-2}	-0.42 e^{-3}	-0.7
$E_{NCI(IrP2\cdots SubA)}$								-6.8
[Ir]-P2···SubB	5d	C–H···π	2.47	0.013	0.039	-0.75 e^{-2}	-0.11 e^{-2}	-2.4
	5e		2.45	0.012	0.038	-0.62 e^{-2}	-0.16 e^{-2}	-1.9
	5f		2.52	0.011	0.031	-0.60 e^{-2}	-0.95 e^{-3}	-1.9
	5g		2.54	0.011	0.032	-0.62 e^{-2}	-0.83 e^{-3}	-1.9
	5h		2.54	0.010	0.029	-0.54 e^{-2}	-0.96 e^{-3}	-1.7
$E_{NCI(IrP2\cdots SubB)}$								-9.8
[Ir]-P2···$MeOBF_3^-$	5i	C–H···F	2.18	0.016	0.051	-0.13 e^{-1}	0.60 e^{-6}	-4.1
	5j		2.17	0.016	0.048	-0.13 e^{-1}	0.31 e^{-3}	-4.1
	5k		2.36	0.010	0.041	-0.83 e^{-2}	-0.93 e^{-3}	-2.6
	5l		2.39	0.010	0.034	-0.75 e^{-2}	-0.52 e^{-3}	-2.4
$E_{NCI(IrP2\cdots MeOBF3^-)}$								-13.2
$E_{NCI\text{-}Total}$								-29.8

S1. The optimized coordinates for key structures in the manuscript.

A-endo-R

Zero-point correction=	1.135779 (Hartree/Particle)
Thermal correction to Energy=	1.206853
Thermal correction to Enthalpy=	1.207797
Thermal correction to Gibbs Free Energy=	1.027968
Sum of electronic and zero-point Energies=	-4735.677931
Sum of electronic and thermal Energies=	-4735.606857
Sum of electronic and thermal Enthalpies=	-4735.605913
Sum of electronic and thermal Free Energies=	-4735.785742

C	-1.99842000	-0.33757500	-2.11640500
C	-1.72744700	0.80661600	-2.89875400
C	-2.63131100	1.83950200	-2.91772000
C	-3.80950100	1.79333800	-2.12559800
C	-4.71091100	2.89162600	-2.08736700
C	-5.81603000	2.87961000	-1.26669300
C	-6.06687400	1.75175200	-0.45020400
C	-5.22438100	0.66100800	-0.48253600
C	-4.07116000	0.63740600	-1.31779600
C	-3.15231100	-0.47347100	-1.35483400
C	-2.42576500	-2.22645800	0.27160000
C	-3.39673100	-1.71886000	-0.58206400
C	-4.62666000	-2.45860800	-0.70179500
C	-5.58846800	-2.17509900	-1.71177600
C	-6.74835300	-2.91358900	-1.82304800
C	-7.01642300	-3.97387300	-0.92419900
C	-6.09616200	-4.28973100	0.05192900
C	-4.88119300	-3.56359000	0.17669700
C	-3.89085500	-3.94086200	1.12352200
C	-2.67714800	-3.30468900	1.14904600
H	-2.43693400	2.72736000	-3.52315200
H	-4.49265200	3.76099600	-2.71155000
H	-6.48863500	3.73926100	-1.23104200
H	-6.93151400	1.74653700	0.21732200
H	-5.43444500	-0.19587200	0.15295900
H	-5.39263400	-1.36734500	-2.41598400
H	-7.46378700	-2.68006300	-2.61506000
H	-7.94258400	-4.54602200	-1.01587900
H	-6.27756800	-5.12155200	0.73767500
H	-4.09232600	-4.77494400	1.79920800

H	-1.87947500	-3.60321500	1.82836300
H	-0.78534500	0.84159800	-3.44368000
O	-1.16133100	-1.67896000	0.33383100
O	-1.08941200	-1.38009200	-2.16929100
N	0.27735700	-3.35149000	-1.20100200
C	1.62936200	-3.67427200	-1.54265700
C	2.37762600	-4.55498800	-0.72698100
C	2.23158200	-3.03236700	-2.63144600
C	3.73814800	-4.75171200	-1.03990300
C	3.57985400	-3.24607700	-2.92112200
H	1.64420900	-2.33409800	-3.22929700
C	4.33426100	-4.11219700	-2.12398100
H	4.33046300	-5.41673800	-0.40695300
H	4.03873000	-2.72002300	-3.76053800
H	5.39224900	-4.27775100	-2.33843900
C	-0.70290500	-4.39740100	-1.21688600
C	-0.61191700	-5.45553900	-0.28406500
C	-1.78534200	-4.33063800	-2.10235700
C	-1.66204000	-6.39321800	-0.23787100
C	-2.81611000	-5.26680800	-2.03105900
H	-1.82871400	-3.50665700	-2.81161900
C	-2.75618500	-6.30077300	-1.09225200
H	-1.60723100	-7.20348700	0.49368900
H	-3.67683200	-5.17437400	-2.69633900
H	-3.56788800	-7.02819400	-1.02401600
C	1.80702200	-5.25073200	0.42363700
H	2.53624400	-5.58697900	1.16739900
C	0.52172400	-5.62665100	0.61961700
H	0.31529500	-6.22955500	1.50981900
C	0.15929100	1.59985400	2.50732700
C	0.63777600	0.79417700	3.56643400
C	-0.20933200	-0.07621000	4.20939700
C	-1.55364100	-0.22071200	3.77196300
C	-2.41182600	-1.21339500	4.32014400
C	-3.70057100	-1.36876300	3.85872900
C	-4.18393600	-0.52870000	2.82775500
C	-3.38324700	0.45499500	2.29027100
C	-2.05005900	0.64632200	2.74237500
C	-1.18942300	1.64704000	2.16892800
C	-1.14476900	3.05848500	0.08116100
C	-1.71594900	2.74159200	1.30692300
C	-2.80244700	3.57571400	1.77204400
C	-3.36809500	3.45389200	3.07295500
C	-4.42762700	4.24115700	3.47466500

C	-4.98265700	5.20571600	2.60189700
C	-4.43021000	5.38492000	1.35247400
C	-3.32921300	4.60062800	0.91652800
C	-2.72265200	4.83319800	-0.34659900
C	-1.64259100	4.09382400	-0.74467600
H	0.15745000	-0.70358400	5.02514000
H	-2.02038300	-1.86333300	5.10712900
H	-4.34550300	-2.14660400	4.27328300
H	-5.19590700	-0.67379100	2.44369600
H	-3.76085500	1.08704900	1.49021000
H	-2.95241400	2.72888800	3.76956300
H	-4.83666100	4.12008500	4.48060000
H	-5.82919200	5.81543900	2.92620900
H	-4.82538200	6.14511900	0.67353500
H	-3.11702800	5.62555500	-0.98654300
H	-1.13347100	4.27129300	-1.69015900
H	1.69194900	0.87195100	3.83575800
O	-0.10389400	2.35147900	-0.45260400
O	1.08204000	2.35540900	1.81464300
N	2.29801000	3.29139600	-0.26030900
C	3.69154800	3.12328100	-0.52492500
C	4.16694000	3.23590800	-1.84948800
C	4.55974900	2.80994800	0.52279100
C	5.53429100	2.99296700	-2.07842700
C	5.91452000	2.59112700	0.27561800
H	4.15054400	2.72768300	1.53119800
C	6.40140600	2.68428700	-1.03113500
H	5.91557700	3.06146700	-3.10037200
H	6.58503100	2.33411700	1.09847000
H	7.46082100	2.51174400	-1.23556600
C	1.72996500	4.58784800	-0.46263400
C	1.64134000	5.10569100	-1.77532000
C	1.19935500	5.29499900	0.62182200
C	0.96219200	6.32792200	-1.95397000
C	0.54034400	6.50716000	0.41879300
H	1.27631100	4.85544200	1.61594200
C	0.41805600	7.02192600	-0.87572500
H	0.87049700	6.73229300	-2.96544700
H	0.10554500	7.03817900	1.26813000
H	-0.10685000	7.96511500	-1.04417800
C	3.30330600	3.61777400	-2.96433200
H	3.63755300	3.27218700	-3.94683700
C	2.22049300	4.42754300	-2.93248800
H	1.76379300	4.68149600	-3.89425100

P	-0.05289500	-1.70391100	-0.90687700
P	1.36657900	1.95587700	0.19130400
Ir	1.57002800	-0.17602300	-0.44002000
C	1.56934000	-1.43206000	1.37973400
H	0.79549200	-1.15770200	2.09116900
H	1.59321400	-2.49290400	1.11818900
C	2.75697000	-0.68311800	1.26067400
H	2.92352700	0.16506500	1.92910400
C	4.03124500	-1.32555500	0.75063400
H	3.75110700	-2.14656400	0.06609500
O	4.76360400	-0.34016800	0.05679600
C	4.81964400	-1.90840300	1.91494000
C	4.53976400	-3.19563600	2.39029800
C	5.79455800	-1.13880500	2.56237200
C	5.22203700	-3.70792500	3.49588300
H	3.77862900	-3.79610300	1.88941500
C	6.48081700	-1.65119300	3.66611100
H	6.01186700	-0.13967600	2.18016900
C	6.19598300	-2.93634400	4.13722700
H	4.99630800	-4.71467100	3.85672900
H	7.24288200	-1.04447800	4.16197800
H	6.73342900	-3.33695500	5.00016800
C	5.69622400	-0.85044600	-0.86459300
H	6.23785600	0.00747400	-1.28269800
H	6.41933500	-1.53727600	-0.38432700
H	5.18851300	-1.38867700	-1.68311900
Cl	1.68925900	0.60747700	-2.69172300

A-exo-R

Zero-point correction=	1.136797 (Hartree/Particle)
Thermal correction to Energy=	1.207552
Thermal correction to Enthalpy=	1.208496
Thermal correction to Gibbs Free Energy=	1.028746
Sum of electronic and zero-point Energies=	-4735.672000
Sum of electronic and thermal Energies=	-4735.601246
Sum of electronic and thermal Enthalpies=	-4735.600301
Sum of electronic and thermal Free Energies=	-4735.780052

C	2.80066700	-2.17867200	-0.95109600
C	1.86196700	-3.17967800	-1.28232800
C	1.90619200	-4.38503200	-0.62634700
C	2.83705500	-4.60770600	0.42483400

C	2.83383900	-5.81890200	1.17026100
C	3.69879600	-6.00681100	2.22661800
C	4.60465900	-4.97928400	2.58454400
C	4.64618600	-3.80004000	1.87043300
C	3.78080500	-3.57965900	0.76265400
C	3.79577000	-2.36042700	-0.00152700
C	4.47145700	0.00118000	0.46443700
C	4.83124900	-1.31359200	0.20350400
C	6.23615000	-1.61296700	0.09422700
C	6.71282700	-2.87695200	-0.35378100
C	8.06370500	-3.13085800	-0.46976600
C	9.01564500	-2.13658600	-0.14016800
C	8.58863300	-0.89509000	0.27870200
C	7.20395400	-0.59645500	0.39304500
C	6.75780200	0.69890400	0.77192200
C	5.41949500	0.99780700	0.78927300
H	1.19222200	-5.16941200	-0.88168300
H	2.12206500	-6.59958200	0.88996700
H	3.68123100	-6.94003700	2.79436100
H	5.27348300	-5.11931900	3.43703200
H	5.34275400	-3.01469200	2.16242600
H	5.99346900	-3.64966200	-0.62160600
H	8.40094400	-4.10755800	-0.82473400
H	10.08291000	-2.35201800	-0.22968700
H	9.31147100	-0.11120200	0.51957900
H	7.49748700	1.46577200	1.01208400
H	5.05228900	1.99478700	1.02985000
H	1.11091700	-2.94967000	-2.03592800
O	3.14887800	0.39481300	0.45054800
O	2.73790800	-0.97522000	-1.63716000
N	2.70489800	1.58562000	-1.89265100
C	1.75448900	2.42190500	-2.57123500
C	1.65535700	3.78811500	-2.22876100
C	0.89388900	1.85948700	-3.51737900
C	0.64481800	4.55157700	-2.84428700
C	-0.09583600	2.63661200	-4.11855600
H	0.97299200	0.79545800	-3.73763400
C	-0.21636200	3.98825900	-3.78301700
H	0.55298100	5.60809600	-2.58099000
H	-0.78104700	2.17785100	-4.83395100
H	-0.98260300	4.60567500	-4.25792800
C	4.09870200	1.84289300	-2.10688900
C	4.65573900	3.05880600	-1.64809700
C	4.91140800	0.86677000	-2.69509000

C	6.04799400	3.23533800	-1.77139000
C	6.28836700	1.06234000	-2.79487200
H	4.45175600	-0.06112900	-3.03087400
C	6.85814900	2.25218900	-2.33141200
H	6.49145700	4.16530100	-1.40643300
H	6.91710400	0.27855300	-3.22202300
H	7.93707900	2.40751300	-2.40056900
C	2.56361500	4.43467700	-1.28553700
H	2.16641200	5.33150900	-0.79976700
C	3.85728400	4.12163500	-1.04019900
H	4.41255200	4.79437300	-0.37844900
C	-2.44915400	-1.83809100	0.97091000
C	-1.27035000	-2.31198400	1.58667400
C	-0.87972300	-3.61295000	1.37834800
C	-1.60841200	-4.45874000	0.49990900
C	-1.19843000	-5.79888400	0.25845100
C	-1.84490300	-6.58512400	-0.67014700
C	-2.92911900	-6.05048100	-1.40722600
C	-3.37213200	-4.76583000	-1.17196700
C	-2.75333400	-3.93940000	-0.19219600
C	-3.20664700	-2.60467300	0.10281600
C	-4.31673500	-0.83558900	-1.27094100
C	-4.40464800	-2.02425500	-0.55349900
C	-5.68446600	-2.68148800	-0.49648500
C	-5.93196800	-3.78058100	0.37345800
C	-7.16954700	-4.38746000	0.42392400
C	-8.22937900	-3.93356100	-0.39763500
C	-8.02874000	-2.86154600	-1.24036800
C	-6.76994800	-2.20497700	-1.30354100
C	-6.55855800	-1.07915800	-2.14467200
C	-5.36710200	-0.40148400	-2.11508400
H	0.02389200	-3.99730800	1.85640200
H	-0.34898800	-6.18872100	0.82393600
H	-1.51660200	-7.61172700	-0.84957700
H	-3.41955600	-6.66018200	-2.16972200
H	-4.20489400	-4.36982100	-1.75090400
H	-5.12760300	-4.13558700	1.01716500
H	-7.33398000	-5.22359900	1.10781600
H	-9.20316100	-4.42699500	-0.35428200
H	-8.84145900	-2.49070100	-1.87062700
H	-7.37009600	-0.73846300	-2.79184100
H	-5.19292500	0.48203000	-2.72562000
H	-0.67992700	-1.62908900	2.19567400
O	-3.20031300	-0.03750800	-1.25786900

O	-2.84441100	-0.52204600	1.21046700
N	-3.33125700	1.90631500	0.47457700
C	-2.77514700	3.20747200	0.71294400
C	-2.55643600	4.07826600	-0.37435800
C	-2.44886500	3.59828700	2.01097300
C	-1.84504700	5.26915200	-0.13329000
C	-1.78221500	4.80187800	2.24192000
H	-2.68629200	2.92576000	2.83105000
C	-1.45184000	5.62208300	1.15739400
H	-1.63021500	5.93293200	-0.97367800
H	-1.48691800	5.07045300	3.25773700
H	-0.90005700	6.55034400	1.32249800
C	-4.74013600	1.90182900	0.22031900
C	-5.22789200	2.57266900	-0.92618900
C	-5.60303100	1.19188100	1.06059500
C	-6.61555800	2.52704300	-1.16869600
C	-6.96920800	1.14992300	0.78716600
H	-5.17545500	0.65205500	1.90561200
C	-7.47651600	1.83358200	-0.32376600
H	-7.01074900	3.03277700	-2.05338800
H	-7.63643100	0.57546100	1.43292100
H	-8.54644100	1.80492100	-0.54163800
C	-3.15533700	3.82864500	-1.68123700
H	-2.66448800	4.30360100	-2.53323100
C	-4.34615500	3.22055500	-1.89790800
H	-4.74007200	3.25628400	-2.91898800
P	2.14006100	0.36531200	-0.86909800
P	-2.37294500	0.57207900	0.03574700
Ir	-0.07443900	0.55721900	-0.30917400
C	0.45977900	2.32055300	0.77043800
H	1.39263500	2.74375300	0.38676200
H	-0.32972700	3.05984400	0.86589900
C	0.52807600	1.21358800	1.66147800
H	1.51509700	0.78510300	1.85049600
C	-0.31321600	1.05719600	2.91109300
H	-1.39320800	1.02266500	2.68414400
O	0.07002700	-0.19665800	3.47998400
C	-0.08093000	2.18755900	3.91322600
C	-1.08488400	2.52790900	4.83115000
C	1.13600700	2.88068800	3.97250300
C	-0.89378900	3.54529300	5.76923000
H	-2.03963300	1.99607400	4.80385200
C	1.33320800	3.89970400	4.90669300
H	1.93255100	2.63183800	3.27037800

C	0.31815800	4.23987800	5.80598300
H	-1.69403500	3.79824800	6.46909500
H	2.28589500	4.43475500	4.93104900
H	0.47178400	5.04083100	6.53319500
C	-0.70240800	-0.64476000	4.56583200
H	-0.38582100	-1.67500200	4.78343600
H	-0.55118300	-0.02978800	5.47093400
H	-1.78315900	-0.65352200	4.32273900
Cl	-0.52485900	-0.93785800	-2.13579600

A-endo-S

Zero-point correction=	1.108678 (Hartree/Particle)
Thermal correction to Energy=	1.177932
Thermal correction to Enthalpy=	1.178876
Thermal correction to Gibbs Free Energy=	1.003647
Sum of electronic and zero-point Energies=	-4696.437355
Sum of electronic and thermal Energies=	-4696.368101
Sum of electronic and thermal Enthalpies=	-4696.367157
Sum of electronic and thermal Free Energies=	-4696.542386

C	-1.37830600	1.91554000	-1.73590200
C	-0.06643600	1.74495500	-2.23173600
C	0.89987000	2.66325200	-1.90078300
C	0.60476400	3.74965600	-1.03291900
C	1.62284600	4.63847800	-0.59412000
C	1.34772200	5.64834900	0.30140200
C	0.03118600	5.81083900	0.79500200
C	-0.98486800	4.97735400	0.37541600
C	-0.73699200	3.92928700	-0.55432000
C	-1.75803600	3.00551700	-0.96876500
C	-3.81281400	2.12649000	0.14933000
C	-3.17545800	3.14629300	-0.54421000
C	-3.93727400	4.32563200	-0.86067400
C	-3.42291900	5.36240800	-1.68917000
C	-4.17467800	6.48114900	-1.98157800
C	-5.48328300	6.62714800	-1.46156900
C	-6.01926300	5.63361200	-0.67129800
C	-5.27509400	4.46316300	-0.36027900
C	-5.83137000	3.41803000	0.42629700
C	-5.12175000	2.26838100	0.66465100
H	1.92389800	2.53375800	-2.25648800
H	2.63895900	4.49084400	-0.96352900
H	2.14703800	6.30640300	0.64539700

H	-0.18146400	6.59853900	1.52180000
H	-1.99116200	5.10595400	0.77308700
H	-2.42052500	5.26020600	-2.10352000
H	-3.75739200	7.25955600	-2.62480500
H	-6.06670800	7.52057000	-1.69603200
H	-7.03376700	5.72601900	-0.27466900
H	-6.84391500	3.53104700	0.82060000
H	-5.53777800	1.44469800	1.24148500
H	0.15305000	0.85696300	-2.82209400
O	-3.17691000	0.93655000	0.43140400
O	-2.30417600	0.89715200	-1.94833000
N	-3.72862600	-1.10592500	-1.10941100
C	-3.60563500	-2.53512900	-1.19222700
C	-4.15410300	-3.33536900	-0.16866700
C	-2.93733200	-3.11360300	-2.27297300
C	-3.95373000	-4.72743600	-0.24046200
C	-2.74863700	-4.49423000	-2.32265200
H	-2.52799600	-2.46370500	-3.04342400
C	-3.25424300	-5.30166000	-1.29869900
H	-4.36048900	-5.35517700	0.55443100
H	-2.19416900	-4.93477400	-3.15390400
H	-3.10543200	-6.38374300	-1.32855500
C	-5.04571400	-0.55848600	-1.26068900
C	-6.01970700	-0.83133900	-0.27336900
C	-5.32775400	0.29726300	-2.33036700
C	-7.27455600	-0.20305300	-0.39902800
C	-6.57701200	0.90945400	-2.42838900
H	-4.54044900	0.50039100	-3.05569000
C	-7.55328400	0.65489000	-1.45958600
H	-8.03458400	-0.39399400	0.36293000
H	-6.78291000	1.59479600	-3.25318000
H	-8.53174000	1.13581200	-1.52785700
C	-4.94188100	-2.77727600	0.92867200
H	-4.93519500	-3.35826300	1.85470800
C	-5.75924700	-1.70056800	0.87373300
H	-6.36568900	-1.49276600	1.76122000
C	3.09615500	0.72382000	1.88219100
C	2.54617200	1.16386500	3.11080200
C	2.75689100	2.44995900	3.53951700
C	3.49885600	3.36467900	2.74383000
C	3.67280100	4.71676700	3.14543900
C	4.37398300	5.60615500	2.36109000
C	4.91399000	5.17538100	1.12608900
C	4.76437600	3.86872800	0.71111000

C	4.07279700	2.91429600	1.50908000
C	3.91267100	1.53856800	1.10677000
C	3.88484100	0.36196300	-1.09821700
C	4.59659900	1.01494200	-0.10431000
C	6.02273500	1.13194000	-0.27588600
C	6.88314000	1.56760000	0.76998300
C	8.24913900	1.63834700	0.58885600
C	8.83073200	1.28706100	-0.65260000
C	8.02755700	0.84390600	-1.68131800
C	6.62051600	0.73662800	-1.51824100
C	5.79988300	0.19859600	-2.54771000
C	4.46210900	-0.01176700	-2.33326800
H	2.33193300	2.79254300	4.48563400
H	3.23055600	5.03902400	4.09141000
H	4.50109900	6.64297000	2.68071300
H	5.44643500	5.88598600	0.48959700
H	5.17514500	3.56011200	-0.24892600
H	6.45252600	1.83347900	1.73459500
H	8.88722300	1.96465000	1.41347000
H	9.91265900	1.35547100	-0.78710700
H	8.46425700	0.54707400	-2.63834300
H	6.25985200	-0.09366000	-3.49403900
H	3.81649200	-0.48378800	-3.07381300
H	1.94385400	0.46021400	3.68533500
O	2.54983400	0.06305800	-0.93239800
O	2.82611500	-0.57641000	1.51037200
N	2.64817000	-2.51082200	-0.17184900
C	1.89293000	-3.70254600	0.08254100
C	1.51196400	-4.52846700	-0.99567700
C	1.52803700	-4.02013900	1.39307100
C	0.69731300	-5.64014600	-0.71413500
C	0.75575500	-5.15198700	1.65354700
H	1.85300000	-3.36410100	2.20256400
C	0.32953800	-5.95560000	0.59228400
H	0.36503200	-6.27052700	-1.54218800
H	0.46715400	-5.38831500	2.67848300
H	-0.29213200	-6.83329800	0.78378900
C	3.99892700	-2.70351800	-0.61510100
C	4.22591400	-3.27447700	-1.88827900
C	5.07258900	-2.30065700	0.18772300
C	5.55859100	-3.37147300	-2.33595500
C	6.38064400	-2.40266000	-0.28210100
H	4.86156000	-1.87094600	1.16556100
C	6.62292100	-2.93874300	-1.55113400

H	5.74703000	-3.79525000	-3.32566700
H	7.20786900	-2.04525500	0.33421600
H	7.64538800	-3.01169900	-1.92843200
C	1.96496900	-4.29175200	-2.36331000
H	1.31020100	-4.68406700	-3.14638500
C	3.14701000	-3.76011600	-2.74693800
H	3.37355800	-3.76828700	-3.81783300
P	-2.45171100	-0.12147200	-0.63086400
P	1.93546400	-1.01814600	0.14954300
Ir	-0.35645500	-0.80271600	0.03362700
C	-0.30938300	0.75329800	1.48776700
H	0.66808800	1.23213900	1.53158200
H	-1.12396300	1.47183100	1.38720400
C	-0.57490200	-0.47959000	2.14834100
H	0.25338900	-0.98838300	2.66137700
C	-1.90314400	-0.67115200	2.86025000
C	-2.29762700	-2.11123800	3.14256600
C	-3.13428700	-2.38453800	4.23835700
C	-1.90524100	-3.17033800	2.31564800
C	-3.56782300	-3.68394600	4.50267800
H	-3.44187500	-1.55651500	4.87865700
C	-2.33725800	-4.47260700	2.58258800
H	-1.27053000	-2.97173000	1.44823200
C	-3.16889800	-4.73688500	3.67191100
H	-4.21987500	-3.87650900	5.35868000
H	-2.02964700	-5.27938500	1.91857900
H	-3.50614400	-5.75687500	3.87344000
Cl	-0.06283700	-1.76293700	-2.15862900
H	-2.69568000	-0.21610800	2.25101400
O	-1.90350400	0.10473900	4.06096100
H	-1.25172000	-0.29094300	4.65715000

A-exo-S

Zero-point correction=	1.136453 (Hartree/Particle)
Thermal correction to Energy=	1.207460
Thermal correction to Enthalpy=	1.208404
Thermal correction to Gibbs Free Energy=	1.028173
Sum of electronic and zero-point Energies=	-4735.676379
Sum of electronic and thermal Energies=	-4735.605373
Sum of electronic and thermal Enthalpies=	-4735.604429
Sum of electronic and thermal Free Energies=	-4735.784660

C	1.80462100	-1.14336600	-1.88448400
C	0.54893900	-1.11216300	-2.53130400
C	-0.17337800	-2.27372400	-2.65677900
C	0.31404700	-3.49570800	-2.11968300
C	-0.46768800	-4.68283900	-2.16395200
C	-0.02429000	-5.84759900	-1.57583300
C	1.22599400	-5.86786100	-0.91198600
C	2.01309600	-4.73675700	-0.86168900
C	1.59524700	-3.52132700	-1.47143200
C	2.37010900	-2.31169200	-1.39697800
C	3.99112800	-1.38582900	0.25648000
C	3.71971000	-2.27121300	-0.77810600
C	4.79164400	-3.11248100	-1.24186000
C	4.67319700	-3.92264500	-2.40599200
C	5.72149800	-4.70729900	-2.83948400
C	6.94725000	-4.72851200	-2.13169700
C	7.10259900	-3.94156100	-1.01108800
C	6.04690200	-3.11107000	-0.54684300
C	6.21491500	-2.26190200	0.58053600
C	5.21480700	-1.40512000	0.96404200
H	-1.15244100	-2.25953100	-3.14162600
H	-1.44218000	-4.64494600	-2.65726400
H	-0.64077500	-6.74891500	-1.60512300
H	1.56426100	-6.78346500	-0.42145500
H	2.95980800	-4.76169900	-0.32413400
H	3.73945300	-3.90939600	-2.96701300
H	5.60570500	-5.31382100	-3.74084500
H	7.76811700	-5.35890000	-2.48141100
H	8.04894200	-3.93502200	-0.46389700
H	7.16547500	-2.27572000	1.11843300
H	5.33242600	-0.71705500	1.79995300
H	0.17670000	-0.15228000	-2.88274100
O	3.05609600	-0.46086000	0.67397900
O	2.49991600	0.05102400	-1.73078800
N	3.70817200	1.90334900	-0.37579700
C	3.41083300	3.28708400	-0.12399100
C	3.85429300	3.89368500	1.07172300
C	2.60194600	3.98598500	-1.02127000
C	3.40983000	5.20076100	1.35274700
C	2.18055500	5.28222200	-0.72471000
H	2.25233100	3.48058500	-1.92045400
C	2.58000700	5.88739400	0.46942800
H	3.72983400	5.67524300	2.28380000
H	1.51556300	5.80268400	-1.41495500

H	2.23937800	6.89535100	0.71533500
C	5.06970500	1.52051100	-0.59838600
C	6.01971700	1.68883800	0.43523300
C	5.42948100	0.90553100	-1.80287200
C	7.32449400	1.20465600	0.21569300
C	6.72422600	0.42219700	-1.98780500
H	4.66675400	0.77748300	-2.56950200
C	7.67621100	0.57659600	-0.97508400
H	8.06443500	1.31643000	1.01230800
H	6.98559700	-0.08505800	-2.91871600
H	8.69058900	0.19568100	-1.11248700
C	4.75981700	3.23034800	2.00550400
H	4.74025900	3.62089600	3.02789300
C	5.69809400	2.29578300	1.72495700
H	6.36479200	2.00704400	2.54417000
C	-3.28187500	-0.59296500	1.93076100
C	-3.15221900	-0.90149900	3.30631900
C	-3.25632700	-2.20026200	3.73579400
C	-3.44677600	-3.25405200	2.80349900
C	-3.41479400	-4.61570600	3.20513800
C	-3.53546500	-5.63031300	2.28126500
C	-3.68937800	-5.31648700	0.90971700
C	-3.75230900	-4.00361200	0.49248600
C	-3.64509800	-2.93203700	1.42186300
C	-3.66740800	-1.55554100	1.00236300
C	-3.34194200	-0.39553300	-1.18300100
C	-4.11935500	-1.19330700	-0.36581100
C	-5.40924000	-1.59996100	-0.86466700
C	-6.37161200	-2.26299000	-0.05342100
C	-7.60980300	-2.61119200	-0.55311800
C	-7.95315300	-2.32267800	-1.89516800
C	-7.05093300	-1.66562800	-2.70379800
C	-5.77552600	-1.27559900	-2.21432900
C	-4.87516400	-0.53199000	-3.02716400
C	-3.68546200	-0.07901200	-2.51632900
H	-3.13915000	-2.43972900	4.79431800
H	-3.26263200	-4.84180300	4.26310500
H	-3.49288500	-6.67436200	2.59995300
H	-3.75167000	-6.12105000	0.17316600
H	-3.85941200	-3.77551300	-0.56774600
H	-6.12773800	-2.48580300	0.98417800
H	-8.33265600	-3.11104900	0.09599500
H	-8.93372500	-2.61002300	-2.28167800
H	-7.30931800	-1.41752600	-3.73654800

H	-5.16430600	-0.29039200	-4.05232300
H	-2.99294400	0.54042100	-3.08661100
H	-2.94390400	-0.09001100	4.00360400
O	-2.15476400	0.11433200	-0.71314000
O	-3.06788200	0.72493700	1.57680100
N	-2.84477600	2.66294800	-0.06660200
C	-2.28118200	3.93150100	0.28418500
C	-1.90141200	4.85011600	-0.71852000
C	-2.04690900	4.21616200	1.63359900
C	-1.24561400	6.02745200	-0.31239300
C	-1.38991400	5.38827200	2.01174600
H	-2.37871100	3.49489200	2.38316000
C	-0.98548300	6.29570400	1.03000100
H	-0.93583200	6.74173800	-1.07926400
H	-1.19247300	5.58669200	3.06731000
H	-0.46772700	7.21517000	1.31145900
C	-4.11775900	2.63735100	-0.72796300
C	-4.24208300	3.19270500	-2.02314400
C	-5.21338100	2.01021100	-0.12192900
C	-5.47065700	3.03124700	-2.69413500
C	-6.41467200	1.85552400	-0.81268900
H	-5.09568000	1.60737500	0.88145000
C	-6.54165700	2.36353000	-2.10829900
H	-5.56902000	3.43970800	-3.70315400
H	-7.24318700	1.32114200	-0.34364400
H	-7.47519500	2.23440500	-2.66034000
C	-2.16633100	4.63384900	-2.13681500
H	-1.50948700	5.18436800	-2.81639100
C	-3.17040800	3.92312200	-2.69460500
H	-3.25360600	3.95942100	-3.78529900
P	2.44926600	0.78850400	-0.24288900
P	-1.97489300	1.29276300	0.41950000
Ir	0.35639900	1.41413800	0.39255000
C	0.79062200	2.14043400	2.32209700
H	1.68683100	2.76695900	2.28015000
H	-0.07611800	2.63394100	2.77121200
C	0.89738800	0.72735200	2.39463100
H	1.89766100	0.28628500	2.38500300
C	-0.06821000	-0.08209300	3.22799000
C	-0.03830100	-1.57123100	2.91783800
C	0.11004400	-2.50810100	3.94830000
C	-0.22672600	-2.03656600	1.60793600
C	0.08500400	-3.87978300	3.67936000
H	0.22040700	-2.15206700	4.97323900

C	-0.28981500	-3.40498200	1.34544300
H	-0.33799500	-1.32316000	0.78925500
C	-0.12468300	-4.33235800	2.37658500
H	0.20702500	-4.59478200	4.49745400
H	-0.48205400	-3.75091500	0.33289600
H	-0.17537400	-5.40109800	2.15918200
Cl	-0.05784100	2.11192300	-1.89553800
H	-1.08002900	0.29484700	3.03876900
O	0.14244500	0.18619100	4.61286800
H	1.06917000	-0.01291100	4.80761500

A'-endo

Zero-point correction=	1.107305 (Hartree/Particle)
Thermal correction to Energy=	1.177298
Thermal correction to Enthalpy=	1.178242
Thermal correction to Gibbs Free Energy=	1.001312
Sum of electronic and zero-point Energies=	-4659.341339
Sum of electronic and thermal Energies=	-4659.271346
Sum of electronic and thermal Enthalpies=	-4659.270402
Sum of electronic and thermal Free Energies=	-4659.447332

C	-2.89463700	-0.61348100	2.06072600
C	-2.28078400	-0.72197500	3.33006100
C	-2.14242100	-1.95303800	3.91872800
C	-2.57227200	-3.13054100	3.24611400
C	-2.35340000	-4.41884700	3.80065400
C	-2.73431500	-5.55823700	3.12508700
C	-3.33766100	-5.44823600	1.85128800
C	-3.57080800	-4.20994400	1.28972300
C	-3.21658100	-3.01398900	1.97133100
C	-3.44322500	-1.70763700	1.40674000
C	-3.75311900	-0.84117000	-0.92491000
C	-4.24792400	-1.53595000	0.16804900
C	-5.59272500	-2.04793400	0.07612000
C	-6.28006400	-2.59127800	1.19747000
C	-7.57666100	-3.04996900	1.08828400
C	-8.25808700	-2.99846100	-0.15094800
C	-7.62850200	-2.46177200	-1.25326700
C	-6.30088400	-1.96284000	-1.16875200
C	-5.67448700	-1.34632200	-2.28648100
C	-4.43411200	-0.77606900	-2.16198900
H	-1.66746800	-2.04725100	4.89774500

H	-1.86000200	-4.48903300	4.77325500
H	-2.55459300	-6.54374400	3.56090500
H	-3.61224000	-6.35134900	1.30108200
H	-4.02060000	-4.14186100	0.30003800
H	-5.77392500	-2.63060700	2.16094000
H	-8.08272500	-3.45260500	1.96891600
H	-9.28193500	-3.37187400	-0.22702000
H	-8.14824600	-2.39642400	-2.21271800
H	-6.21442700	-1.29260000	-3.23429600
H	-3.95114300	-0.24547300	-2.98220600
H	-1.91639500	0.18970300	3.80224700
O	-2.53705100	-0.19443900	-0.86534700
O	-2.97692700	0.64734600	1.50467000
N	-3.13286500	2.36452800	-0.39332300
C	-2.63839100	3.70374100	-0.28729800
C	-2.47205900	4.48227200	-1.45157400
C	-2.28707500	4.20892900	0.96654700
C	-1.92092300	5.76839600	-1.30701300
C	-1.74186500	5.48774400	1.08675200
H	-2.44084000	3.58019100	1.84346900
C	-1.56479300	6.27037100	-0.05674300
H	-1.77281400	6.37809300	-2.20184200
H	-1.44984100	5.86520600	2.06873700
H	-1.13938200	7.27319500	0.02499600
C	-4.48845200	2.20530200	-0.83811400
C	-4.81774900	2.54470200	-2.16992500
C	-5.45862900	1.67528200	0.02111800
C	-6.12756900	2.27533200	-2.61373900
C	-6.74652800	1.41486900	-0.44431400
H	-5.17488600	1.43199900	1.04322100
C	-7.07982600	1.71217800	-1.76941200
H	-6.38858200	2.51702400	-3.64724800
H	-7.48250500	0.96185100	0.22278100
H	-8.08399700	1.49956300	-2.14308600
C	-2.85150500	4.00372000	-2.77848700
H	-2.29709300	4.45100100	-3.60842000
C	-3.86566200	3.16606900	-3.08886800
H	-4.06907600	3.00115900	-4.15176500
C	2.30200200	-0.88430000	-2.10634900
C	1.19165300	-0.89444400	-2.97931800
C	0.64437300	-2.09876600	-3.35153800
C	1.15143800	-3.32214300	-2.83391900
C	0.55385700	-4.56831600	-3.16806400
C	1.00690000	-5.74543800	-2.61278800

C	2.07373700	-5.71866000	-1.68295800
C	2.68303200	-4.52819600	-1.34839100
C	2.26320000	-3.29877900	-1.92654400
C	2.87652100	-2.03965500	-1.59990000
C	4.03928200	-1.14030000	0.41790200
C	4.06658100	-1.94379800	-0.71524000
C	5.28747300	-2.64648400	-1.01154200
C	5.48462600	-3.34565000	-2.23560200
C	6.67036200	-3.99750600	-2.50315500
C	7.72621900	-3.99030500	-1.56029500
C	7.57642200	-3.30675800	-0.37306700
C	6.37305200	-2.61241100	-0.07379500
C	6.22890700	-1.86568000	1.12700100
C	5.09415100	-1.13127600	1.35963400
H	-0.21182600	-2.12608800	-4.02973100
H	-0.28569400	-4.57122300	-3.86807900
H	0.53546700	-6.69563100	-2.87467500
H	2.40996800	-6.64766600	-1.21667000
H	3.48718500	-4.52028300	-0.61423600
H	4.68522700	-3.35221000	-2.97557500
H	6.79692800	-4.51972200	-3.45449900
H	8.65831500	-4.51573000	-1.78092800
H	8.38923600	-3.27780900	0.35743000
H	7.04968500	-1.85607700	1.84778500
H	4.97405000	-0.51880900	2.25219400
H	0.78885900	0.06239900	-3.31034800
O	2.96158500	-0.33357700	0.70449500
O	2.83275600	0.34412900	-1.73292600
N	3.50338600	2.16135400	-0.01139000
C	3.01313000	3.48098200	0.27181200
C	3.16356700	4.02775300	1.56535800
C	2.32025100	4.17832000	-0.71944600
C	2.55080300	5.26757800	1.83304800
C	1.72635900	5.40679600	-0.43227500
H	2.19702200	3.71951100	-1.69947100
C	1.83885500	5.94996000	0.84988800
H	2.64401700	5.69261500	2.83553200
H	1.14822100	5.91747700	-1.20293100
H	1.36348700	6.90419000	1.08632700
C	4.91745100	1.93064900	0.02057600
C	5.62520900	2.08395400	1.23518400
C	5.57155700	1.47216400	-1.12860800
C	6.99064200	1.73725200	1.25128800
C	6.92094600	1.12313200	-1.08136800

H	4.99364100	1.35324800	-2.04356500
C	7.63339200	1.25818100	0.11389400
H	7.54398400	1.83784100	2.18847400
H	7.41145200	0.73416200	-1.97598200
H	8.68867000	0.98020200	0.15903700
C	3.94238800	3.37986500	2.61653900
H	3.69445300	3.69264600	3.63582700
C	5.00367700	2.55230800	2.47157300
H	5.52882000	2.26001400	3.38674900
P	-2.15435200	1.08448800	0.10874600
P	2.39229000	0.91030800	-0.23427300
C	0.25219600	-0.31047100	1.52354600
C	0.40852600	0.80125300	2.12276300
C	0.77915500	1.62939400	3.28726300
H	0.60623200	1.04290000	4.20794200
H	1.86979800	1.80164700	3.23313000
C	0.06032000	2.97699000	3.35841500
H	-1.02465900	2.83866600	3.48407000
H	0.42994600	3.57456700	4.20611100
H	0.22488800	3.54540800	2.43234300
C	0.25361200	-1.74479400	1.42452900
C	0.80767000	-2.51555700	2.46653500
C	-0.29068300	-2.39837100	0.30610100
C	0.79378800	-3.90607400	2.39615000
H	1.24984400	-2.00627800	3.32482000
C	-0.31313000	-3.79043800	0.24953000
H	-0.69537600	-1.79905200	-0.50865900
C	0.22405400	-4.54799300	1.29146200
H	1.22352400	-4.49565600	3.20979900
H	-0.74192500	-4.28867900	-0.62049200
H	0.20355000	-5.63832100	1.24007900
Ir	0.14747500	1.22065400	0.06713300
Cl	-0.05990800	2.25960500	-2.09557000

A'-exo

Zero-point correction=	1.107257 (Hartree/Particle)
Thermal correction to Energy=	1.177479
Thermal correction to Enthalpy=	1.178424
Thermal correction to Gibbs Free Energy=	0.999564
Sum of electronic and zero-point Energies=	-4659.337400
Sum of electronic and thermal Energies=	-4659.267177
Sum of electronic and thermal Enthalpies=	-4659.266233
Sum of electronic and thermal Free Energies=	-4659.445093

C	2.84188100	0.58218300	1.96497600
C	2.25153000	0.67768000	3.24798700
C	2.15397600	1.89944000	3.86483300
C	2.57057700	3.08433600	3.19505400
C	2.34565700	4.37030200	3.75531400
C	2.69053800	5.51438100	3.06769300
C	3.27647000	5.41292100	1.78382300
C	3.52647400	4.17859800	1.22131500
C	3.19349900	2.97824300	1.90678000
C	3.41114900	1.67694800	1.32704500
C	3.73908300	0.83248400	-1.00991100
C	4.22960000	1.50853600	0.09642800
C	5.58451500	1.99718500	0.03323600
C	6.25586500	2.53919300	1.16492400
C	7.56089800	2.97874300	1.07990900
C	8.26860200	2.90618500	-0.14329900
C	7.65517800	2.36954900	-1.25467000
C	6.31798000	1.89276700	-1.19603800
C	5.70487100	1.28398400	-2.32550300
C	4.44720000	0.74650600	-2.23044700
H	1.70809500	1.98203000	4.85864800
H	1.87381600	4.43461600	4.73908400
H	2.50130100	6.49758900	3.50447900
H	3.52649000	6.32027900	1.22914900
H	3.96496100	4.11420600	0.22602600
H	5.73139400	2.59339900	2.11778500
H	8.05347700	3.38166800	1.96801500
H	9.29940900	3.26342500	-0.19981100
H	8.19454400	2.28884600	-2.20201000
H	6.26626400	1.21340700	-3.25966900
H	3.97065300	0.22499200	-3.06027200
H	1.87501500	-0.23568500	3.70862600
O	2.50133100	0.23285200	-0.98053500
O	2.87809300	-0.66332000	1.38166900
N	2.94499600	-2.36900400	-0.52120100
C	2.34115200	-3.66384200	-0.42898800
C	2.14681800	-4.43159900	-1.59701100
C	1.88437300	-4.11971000	0.81062200
C	1.46581300	-5.65584700	-1.47058100
C	1.21179000	-5.33905700	0.91100400
H	2.04528200	-3.49930200	1.69369000
C	1.00666500	-6.10963400	-0.23538400
H	1.29335500	-6.25345800	-2.36919500

H	0.84207800	-5.67434200	1.88172500
H	0.47942600	-7.06363000	-0.16845000
C	4.31139800	-2.28704600	-0.95061600
C	4.63862600	-2.63920800	-2.27977900
C	5.29703900	-1.80450000	-0.08084900
C	5.96273300	-2.42368900	-2.71095200
C	6.59956300	-1.59826500	-0.53353300
H	5.01584000	-1.55440000	0.94015800
C	6.93092800	-1.90287500	-1.85715600
H	6.22257200	-2.67465900	-3.74254800
H	7.34891500	-1.18274200	0.14308800
H	7.94629300	-1.73224800	-2.22208500
C	2.60548200	-3.99728600	-2.91374700
H	2.05081700	-4.42201000	-3.75536600
C	3.67311900	-3.22264600	-3.20861900
H	3.90973600	-3.08650900	-4.26864000
C	-1.84170700	1.46547800	-2.06286400
C	-0.58708500	1.38576000	-2.70951000
C	0.27425100	2.45309200	-2.63783400
C	-0.06955100	3.61995700	-1.90169400
C	0.86969800	4.66865600	-1.70523700
C	0.56482700	5.75762700	-0.91821600
C	-0.70425400	5.84285000	-0.29762000
C	-1.64515700	4.85071800	-0.48175300
C	-1.36483800	3.71268500	-1.28877800
C	-2.27931700	2.60694000	-1.41000100
C	-3.91520900	1.62764900	0.19565800
C	-3.60759000	2.60399300	-0.74420700
C	-4.60657100	3.59209500	-1.04813300
C	-4.43732900	4.54452000	-2.09198400
C	-5.41343100	5.47850800	-2.36976700
C	-6.61322600	5.51259000	-1.61880700
C	-6.81616600	4.59414300	-0.61149100
C	-5.83459700	3.61253100	-0.30643600
C	-6.04433500	2.64256900	0.71141100
C	-5.11167700	1.66455400	0.94933200
H	1.26236600	2.39018300	-3.09889600
H	1.85364400	4.57829600	-2.17230800
H	1.30391600	6.54523800	-0.75708400
H	-0.93786800	6.69699100	0.34228400
H	-2.61009000	4.92146400	0.01868200
H	-3.52194200	4.52333200	-2.68304000
H	-5.26134300	6.19507000	-3.18043200
H	-7.37711000	6.25989900	-1.84580600

H	-7.74344300	4.60088200	-0.03253500
H	-6.97159500	2.67072000	1.28839300
H	-5.25996500	0.89780800	1.70742500
H	-0.31348100	0.45000500	-3.19429700
O	-3.04173100	0.60415400	0.48752300
O	-2.62741600	0.31853400	-1.99715400
N	-3.65800900	-1.68422000	-0.69211600
C	-3.33404000	-3.07086100	-0.49380500
C	-3.64358000	-3.69223700	0.73465300
C	-2.65305300	-3.76599200	-1.49492500
C	-3.21229200	-5.01867600	0.93047300
C	-2.23277600	-5.07769600	-1.27737800
H	-2.40258600	-3.24606500	-2.41798300
C	-2.51373000	-5.70420600	-0.05975000
H	-3.43329200	-5.50533400	1.88317400
H	-1.66119100	-5.59597500	-2.04878700
H	-2.18012800	-6.72836900	0.12064500
C	-5.03873300	-1.30648300	-0.74287100
C	-5.85261400	-1.48288900	0.39968400
C	-5.54148200	-0.68267800	-1.88956000
C	-7.17601500	-1.00308500	0.34310400
C	-6.85249600	-0.20759300	-1.91469600
H	-4.87474100	-0.54413100	-2.73998800
C	-7.67299100	-0.37305300	-0.79427400
H	-7.81299600	-1.12038200	1.22354800
H	-7.22895200	0.30068900	-2.80484800
H	-8.69936500	0.00058400	-0.80577000
C	-4.40111200	-3.02450000	1.78963400
H	-4.22508500	-3.40544400	2.80001500
C	-5.36440400	-2.08683500	1.63865600
H	-5.90691600	-1.78609200	2.54093800
P	2.04081200	-1.03402600	-0.02792800
P	-2.43953600	-0.53056000	-0.57110400
C	-0.51114400	-0.80779200	1.94578400
C	-0.34763800	0.35708800	1.45865600
C	-0.34311000	1.82922300	1.46846400
H	0.69556400	2.19134000	1.43826700
H	-0.78604200	2.17967800	0.53039300
C	-1.09583600	2.43291900	2.65467400
H	-0.64665700	2.12458000	3.61074400
H	-1.06561900	3.53213400	2.60240800
H	-2.14717600	2.10942100	2.64815400
C	-0.74374500	-1.74960700	3.00604000
C	-0.81191400	-1.32235300	4.34997100

C	-0.91401300	-3.11737100	2.71996900
C	-1.04193400	-2.24154500	5.37191700
H	-0.69110000	-0.26088400	4.57544900
C	-1.14390800	-4.03117300	3.74761000
H	-0.87089800	-3.44126900	1.68043700
C	-1.20773800	-3.60072800	5.07688400
H	-1.09443700	-1.89757000	6.40803800
H	-1.27944500	-5.08846100	3.50620300
H	-1.38683600	-4.31865400	5.88081900
Ir	-0.24730800	-1.03792900	-0.13486400
Cl	-0.00690400	-1.98138200	-2.34144400

B-M1

Zero-point correction=	**1.305094 (Hartree/Particle)**
Thermal correction to Energy=	**1.386183**
Thermal correction to Enthalpy=	**1.387127**
Thermal correction to Gibbs Free Energy=	**1.186870**
Sum of electronic and zero-point Energies=	**-5122.318653**
Sum of electronic and thermal Energies=	**-5122.237565**
Sum of electronic and thermal Enthalpies=	**-5122.236621**
Sum of electronic and thermal Free Energies=	**-5122.436878**

C	3.37754500	-1.05911500	-1.99932500
C	3.04508100	-1.28256100	-3.35572800
C	3.09614600	-2.54715500	-3.88282500
C	3.42510500	-3.65815300	-3.05904200
C	3.39616000	-4.98530300	-3.56223500
C	3.66505000	-6.06094000	-2.74337200
C	3.95657000	-5.84368000	-1.37729200
C	4.00592800	-4.56451200	-0.86422300
C	3.77108100	-3.42963500	-1.68744600
C	3.84315800	-2.07980100	-1.17910400
C	3.78343000	-1.03909000	1.10648100
C	4.43170600	-1.81645200	0.16096500
C	5.73482000	-2.32668100	0.51608000
C	6.60943400	-2.91909800	-0.43741600
C	7.86306400	-3.36959600	-0.07768400
C	8.31107100	-3.26392000	1.26022500
C	7.49782500	-2.67702700	2.20565400
C	6.21229800	-2.17978000	1.86141300
C	5.40930300	-1.49944500	2.81844800
C	4.22875900	-0.91453300	2.44206800
H	2.85648600	-2.71769300	-4.93514500

H	3.13952800	-5.13768700	-4.61384900
H	3.63418600	-7.07825400	-3.14048800
H	4.13009000	-6.69664200	-0.71715600
H	4.20989500	-4.41660800	0.19494800
H	6.28638000	-3.00171200	-1.47393500
H	8.51635100	-3.80856900	-0.83548200
H	9.30135300	-3.63379400	1.53589900
H	7.83760400	-2.56641800	3.23873200
H	5.76993200	-1.40777100	3.84526400
H	3.60924500	-0.33604100	3.12740200
H	2.76878500	-0.41942600	-3.95811900
O	2.62497600	-0.36915500	0.80462000
O	3.30428400	0.24739700	-1.56185900
N	3.34671200	2.10682100	0.18007000
C	3.14589300	3.42236700	-0.34474800
C	2.93579400	4.48862600	0.56117100
C	3.12953300	3.63995400	-1.72570700
C	2.64580500	5.75593200	0.02367700
C	2.85031600	4.91022900	-2.23384700
H	3.32008100	2.79583300	-2.38971200
C	2.60034500	5.96776500	-1.35412600
H	2.44946500	6.58270000	0.71045200
H	2.81719300	5.06877200	-3.31388900
H	2.37049900	6.96211600	-1.74354800
C	4.59942200	1.93983500	0.86795900
C	4.73792500	2.52087000	2.14650600
C	5.65335500	1.22383400	0.28942200
C	5.92355800	2.26333300	2.86254500
C	6.82445900	0.99741300	1.01022900
H	5.52683600	0.81658800	-0.71184400
C	6.95120800	1.50565700	2.30749700
H	6.03414600	2.68645000	3.86416100
H	7.62548900	0.40152300	0.56910700
H	7.85913500	1.31301200	2.88348500
C	2.96351000	4.29751400	2.01148100
H	2.32463300	4.97710500	2.57997800
C	3.73128600	3.42425000	2.70287900
H	3.68863700	3.47464000	3.79535100
C	-3.23167500	0.03630600	2.17839800
C	-3.10218500	0.91440700	3.27829700
C	-2.99910000	0.42251100	4.55291800
C	-2.96111000	-0.97943500	4.77966000
C	-2.73802100	-1.51552800	6.07646000
C	-2.65788400	-2.87637200	6.27793200

C	-2.79011100	-3.75599300	5.17731300
C	-3.02812700	-3.26584500	3.91022500
C	-3.13926300	-1.86787400	3.66881700
C	-3.38458400	-1.33332800	2.35163500
C	-3.13675900	-2.25662000	0.03295900
C	-3.79395200	-2.24250600	1.25002000
C	-4.92773900	-3.12256900	1.39568000
C	-5.82447800	-3.03624600	2.49703900
C	-6.92171000	-3.86736600	2.59422700
C	-7.17856600	-4.84165200	1.60066000
C	-6.33939700	-4.94151300	0.51176800
C	-5.21599600	-4.08363600	0.37003200
C	-4.39607900	-4.13274600	-0.79115700
C	-3.39050000	-3.21908000	-0.97063900
H	-2.89793800	1.10390400	5.40087100
H	-2.61520800	-0.82169600	6.91220000
H	-2.47706700	-3.27673300	7.27823200
H	-2.69504500	-4.83368200	5.33008000
H	-3.11218100	-3.95662500	3.07228400
H	-5.64625300	-2.28767400	3.26767200
H	-7.59934900	-3.76926000	3.44566700
H	-8.04448000	-5.50131200	1.69327700
H	-6.53538000	-5.67495100	-0.27481100
H	-4.60619300	-4.88119300	-1.55833200
H	-2.77012100	-3.19685100	-1.86605300
H	-3.07100100	1.98313800	3.08199000
O	-2.15728200	-1.33957200	-0.25042800
O	-3.27361600	0.62536700	0.92683400
N	-3.32320300	0.56730500	-1.63955900
C	-3.35095300	1.83730000	-2.29841800
C	-3.17948000	1.90247800	-3.70038300
C	-3.54516400	3.00236900	-1.55315000
C	-3.08613200	3.17888100	-4.28957500
C	-3.47590800	4.25659000	-2.16082100
H	-3.71803400	2.91691900	-0.48182300
C	-3.22442400	4.34185300	-3.53336400
H	-2.91950700	3.24587400	-5.36772800
H	-3.59096300	5.15527800	-1.55422100
H	-3.14731700	5.31803100	-4.01722600
C	-4.46801300	-0.26186000	-1.91052600
C	-4.59230800	-0.84411500	-3.19246000
C	-5.43886500	-0.50112900	-0.93076000
C	-5.64631100	-1.75531600	-3.40697600
C	-6.48017000	-1.39571700	-1.17159100

H	-5.34348500	-0.01028200	0.03478500
C	-6.57323400	-2.03933500	-2.40933800
H	-5.73543300	-2.22988100	-4.38748300
H	-7.20193000	-1.60957000	-0.38122100
H	-7.37442700	-2.75799300	-2.59476600
C	-3.14573700	0.71510000	-4.54926800
H	-2.67579700	0.85619400	-5.52745500
C	-3.73775800	-0.48186700	-4.31901700
H	-3.69149400	-1.22043500	-5.12563300
P	2.36033500	0.80648200	-0.28960100
P	-2.23927800	0.28460800	-0.35261500
Ir	0.03446700	0.91684800	-0.44476300
C	-0.18831800	3.02180600	-1.06213800
H	0.64673400	3.28138800	-1.70898800
H	-1.16856700	3.24048100	-1.47862800
C	0.00895000	3.00393800	0.33091900
H	1.01454300	3.17585600	0.69561500
C	-0.95988200	3.41778900	1.42320600
H	-1.59193000	2.56950500	1.71373200
O	-0.13224200	3.78913800	2.53125500
C	0.26873500	-0.96006800	-1.47727300
C	0.16392100	-0.02722800	-2.35432000
C	0.08972200	0.32479000	-3.78827100
H	0.54430900	-0.50019700	-4.36477000
H	-0.97232000	0.33187400	-4.07332400
C	0.72017100	1.66128900	-4.17808000
H	1.77024200	1.72038400	-3.85333200
H	0.69003500	1.80102100	-5.27021700
H	0.18007500	2.49615100	-3.71255200
C	0.37589600	-2.36549200	-1.17419200
C	0.25035000	-3.32020400	-2.20192100
C	0.58142300	-2.80753600	0.14657800
C	0.34841100	-4.68206300	-1.91996200
H	0.07897800	-2.97959200	-3.22480100
C	0.67859200	-4.17021800	0.42047400
H	0.63910200	-2.06571900	0.94371500
C	0.56886100	-5.11171800	-0.60852100
H	0.26443400	-5.41233700	-2.72789400
H	0.84002500	-4.50161800	1.44931400
H	0.65701200	-6.17846900	-0.39025700
C	-1.84043200	4.60555800	1.07704900
C	-3.19404700	4.62705300	1.43241900
C	-1.28428700	5.74476400	0.47432200
C	-3.98387600	5.75641600	1.18768300

H	-3.64267800	3.74437500	1.89464800
C	-2.06542900	6.87401500	0.23184600
H	-0.22942700	5.73535900	0.19310100
C	-3.42029300	6.88432500	0.58771200
H	-5.04075100	5.75222600	1.46535400
H	-1.61915500	7.75306200	-0.24036200
H	-4.03305800	7.76831500	0.39482700
C	-0.62704300	3.44176600	3.79745200
H	0.08455800	3.83098400	4.54142500
H	-1.61697700	3.89818300	4.00255200
H	-0.69990700	2.34653000	3.90981100
Cl	-0.08470800	0.23374100	1.99112800

B-M2

Zero-point correction=	**1.305504 (Hartree/Particle)**
Thermal correction to Energy=	**1.386217**
Thermal correction to Enthalpy=	**1.387161**
Thermal correction to Gibbs Free Energy=	**1.189477**
Sum of electronic and zero-point Energies=	**-5122.315412**
Sum of electronic and thermal Energies=	**-5122.234699**
Sum of electronic and thermal Enthalpies=	**-5122.233755**
Sum of electronic and thermal Free Energies=	**-5122.431440**

C	3.50298300	-0.89868200	-1.66904600
C	3.32117700	-1.08715900	-3.06058800
C	3.52933700	-2.31484800	-3.63310000
C	3.85366300	-3.43993200	-2.82966200
C	3.96688000	-4.74023300	-3.38788800
C	4.20798800	-5.83679700	-2.58880900
C	4.32699700	-5.66838800	-1.19010900
C	4.24064100	-4.41399200	-0.62320800
C	4.03019000	-3.25563600	-1.42076300
C	3.95673300	-1.92915300	-0.85173900
C	3.55691400	-1.04158200	1.45542300
C	4.36956700	-1.71414900	0.55909500
C	5.64469300	-2.17696000	1.05063100
C	6.67062000	-2.65073200	0.18612200
C	7.89374900	-3.05555700	0.68037200
C	8.15673400	-3.02160300	2.07029200
C	7.19124400	-2.55170800	2.93471700
C	5.93173700	-2.10302400	2.45475100
C	4.96639900	-1.54320600	3.33782800
C	3.81045300	-0.99614900	2.84551700
H	3.40599600	-2.44795400	-4.71049300

H	3.83876400	-4.85585800	-4.46730900
H	4.28580400	-6.83413800	-3.02797500
H	4.47672800	-6.54045900	-0.54930200
H	4.31479200	-4.30701100	0.45762000
H	6.48842200	-2.67731200	-0.88731400
H	8.66664100	-3.40249200	-0.00959200
H	9.12478200	-3.35481400	2.45154700
H	7.38636800	-2.49880600	4.00903400
H	5.18116700	-1.51292000	4.40830300
H	3.06477700	-0.51144300	3.47581500
H	3.02092600	-0.23240000	-3.65971700
O	2.41233900	-0.42006200	1.03876200
O	3.29603900	0.38103400	-1.18847600
N	3.05663000	2.11944400	0.68943800
C	2.88602500	3.46168700	0.23105100
C	2.54607200	4.46321300	1.17087600
C	3.09010700	3.78437600	-1.11395200
C	2.38329700	5.77921100	0.69807700
C	2.91779600	5.09635200	-1.55842300
H	3.38506600	2.99166100	-1.79987800
C	2.56537800	6.09678500	-0.64729100
H	2.11517700	6.56245700	1.41150200
H	3.06353100	5.33579400	-2.61393600
H	2.42784400	7.12562600	-0.98657200
C	4.21896000	1.95281700	1.51984500
C	4.16266600	2.43407000	2.84473000
C	5.37682100	1.33776200	1.03166000
C	5.26009000	2.17799400	3.68958000
C	6.45956300	1.11334400	1.87996800
H	5.39966200	1.00600500	-0.00487900
C	6.39244400	1.52038400	3.21695300
H	5.21893500	2.52354900	4.72559100
H	7.34359500	0.59498400	1.50444400
H	7.23088000	1.32609900	3.88946700
C	2.36491000	4.16667100	2.59331800
H	1.65898500	4.81340300	3.12363000
C	3.05249600	3.25770200	3.32300500
H	2.86061100	3.22543200	4.39999400
C	-3.53044100	0.69379500	1.74101600
C	-3.45883800	1.99782200	2.27713300
C	-3.37989600	2.17102700	3.63707900
C	-3.31708300	1.04624600	4.50246000
C	-3.13615300	1.20432800	5.90359900
C	-3.02215100	0.11034900	6.73275500

C	-3.07422000	-1.19354200	6.18398800
C	-3.26926200	-1.37961000	4.83198000
C	-3.41898000	-0.27382600	3.94944800
C	-3.61508600	-0.44006500	2.53315100
C	-3.09699900	-2.32509900	0.93539600
C	-3.87029700	-1.78801000	1.95581600
C	-4.95728300	-2.59826600	2.45071500
C	-5.95086300	-2.08126700	3.32917900
C	-6.99417300	-2.86702400	3.77355200
C	-7.10026200	-4.21985300	3.37227400
C	-6.16445600	-4.74912800	2.50981700
C	-5.08938800	-3.96028200	2.01898300
C	-4.15229700	-4.48730000	1.08862400
C	-3.19053200	-3.68074900	0.53974700
H	-3.32818200	3.17522300	4.06436300
H	-3.07352500	2.21770200	6.30882600
H	-2.87516200	0.24478600	7.80702600
H	-2.94992200	-2.06129100	6.83616100
H	-3.28974000	-2.38889400	4.42380200
H	-5.88974900	-1.03984500	3.64238300
H	-7.74742700	-2.43799900	4.43870500
H	-7.92598700	-4.83512400	3.73722500
H	-6.24072900	-5.78762000	2.17676300
H	-4.23641400	-5.53267200	0.78302900
H	-2.48894400	-4.03623800	-0.21464000
H	-3.45948000	2.84387100	1.58920200
O	-2.16006300	-1.59808900	0.25292900
O	-3.52844200	0.57781600	0.36118800
N	-3.05859700	-0.51560200	-1.90175800
C	-3.01066300	0.28216100	-3.08346800
C	-2.55895700	-0.30711600	-4.28745200
C	-3.43118200	1.61374500	-3.05834200
C	-2.51584900	0.49855300	-5.44005300
C	-3.38660500	2.39015400	-4.21572500
H	-3.78970900	2.03137800	-2.11685800
C	-2.92703800	1.83013700	-5.41052200
H	-2.15059900	0.06089900	-6.37241500
H	-3.70043300	3.43513100	-4.18299500
H	-2.88791600	2.43307400	-6.32066700
C	-4.02015800	-1.58734400	-1.93796600
C	-3.74185300	-2.71800400	-2.73488900
C	-5.18879400	-1.52828100	-1.17018600
C	-4.62394500	-3.81377600	-2.66178400
C	-6.05643400	-2.61893000	-1.12592600

H	-5.38279500	-0.63681500	-0.57653000
C	-5.76430800	-3.76990800	-1.86442400
H	-4.40464900	-4.70400400	-3.25659700
H	-6.94458000	-2.57910800	-0.49247600
H	-6.42962800	-4.63486200	-1.81623600
C	-2.12942200	-1.70149600	-4.36579100
H	-1.38249100	-1.91502000	-5.13706200
C	-2.62273800	-2.75253900	-3.67283400
H	-2.23554300	-3.74583600	-3.91602700
P	2.19082200	0.82108000	0.00992300
P	-2.25589100	-0.13700700	-0.45867900
Ir	-0.14379200	0.77476200	-0.36994000
C	-0.49400500	2.68794200	0.80318800
H	-1.02890200	2.34485600	1.68455000
H	0.44235000	3.20664700	0.99934600
C	-1.13115700	2.87196800	-0.41964100
H	-2.19739700	2.64338800	-0.47503100
C	-0.74438100	3.98539200	-1.36243700
H	0.32163200	4.23592600	-1.22457300
O	-0.98548500	3.60126200	-2.70093600
C	0.33358000	-0.85351000	-1.65923800
C	0.26294800	0.21905400	-2.37279200
C	0.40019600	0.91213300	-3.67206700
H	0.57208000	0.16279000	-4.46536200
H	-0.55141900	1.40963700	-3.89517900
C	1.48891500	1.98820800	-3.69818800
H	2.49633600	1.57845900	-3.55058900
H	1.47275400	2.52586700	-4.65861000
H	1.30566600	2.71070100	-2.89684100
C	0.48926500	-2.27975700	-1.50405200
C	0.55635700	-3.13181500	-2.62306900
C	0.56465700	-2.84414000	-0.21447300
C	0.69652100	-4.50898800	-2.45926700
H	0.50124600	-2.69923800	-3.62122800
C	0.71037000	-4.22098900	-0.05888400
H	0.48817000	-2.18720700	0.65314800
C	0.77734300	-5.05941700	-1.17692600
H	0.76042000	-5.15669400	-3.33674800
H	0.77263600	-4.64405400	0.94667500
H	0.90416900	-6.13705100	-1.05090000
C	-1.59969100	5.18748300	-0.96507300
C	-1.11746700	6.15878200	-0.08168200
C	-2.92282700	5.28384600	-1.42060700
C	-1.93716200	7.20974100	0.33805700

H	-0.09238000	6.08337200	0.28080700
C	-3.74382300	6.33374300	-1.00496800
H	-3.30042000	4.52724500	-2.11023700
C	-3.25336900	7.30153300	-0.12243800
H	-1.54517200	7.96160600	1.02783700
H	-4.77206600	6.39697100	-1.36995400
H	-3.89495600	8.12348300	0.20412800
C	-0.61896300	4.55851200	-3.66230600
H	-0.77018200	4.09834600	-4.64889100
H	-1.23260500	5.47537200	-3.59682600
H	0.44392000	4.84822600	-3.56312600
Cl	-0.29359900	-0.08365400	2.06585700

B-M3

Zero-point correction= 1.304432 (Hartree/Particle)
Thermal correction to Energy= 1.385785
Thermal correction to Enthalpy= 1.386729
Thermal correction to Gibbs Free Energy= 1.186287
Sum of electronic and zero-point Energies= -5122.320107
Sum of electronic and thermal Energies= -5122.238754
Sum of electronic and thermal Enthalpies= -5122.237810
Sum of electronic and thermal Free Energies= -5122.438253

C	-2.28265200	1.65488300	-2.38229400
C	-1.47507500	2.05391400	-3.47266000
C	-1.20874100	3.38161000	-3.68728100
C	-1.70158600	4.37264800	-2.79405800
C	-1.37406000	5.74414600	-2.95597000
C	-1.83146000	6.69335400	-2.06667400
C	-2.62203600	6.29543700	-0.96488400
C	-2.96096900	4.97042800	-0.78599100
C	-2.53858600	3.97057500	-1.70348500
C	-2.90438900	2.58199700	-1.55736900
C	-3.76950600	1.15231600	0.32024600
C	-3.95730500	2.17928400	-0.59142500
C	-5.25180500	2.82040000	-0.61020100
C	-5.65238900	3.69915600	-1.65601700
C	-6.90267100	4.28206700	-1.66244700
C	-7.82358800	4.02877400	-0.61820600
C	-7.47823800	3.16527200	0.39845600
C	-6.20725500	2.53024400	0.41915900
C	-5.87943000	1.57476200	1.41753000
C	-4.70113300	0.87894900	1.34983300

H	-0.59529600	3.69023800	-4.53712500
H	-0.73924600	6.03181900	-3.79805500
H	-1.57050400	7.74576600	-2.20042500
H	-2.95404500	7.04034200	-0.23795300
H	-3.54958700	4.67771200	0.08197900
H	-4.96255500	3.90004400	-2.47377600
H	-7.18503900	4.94228200	-2.48583100
H	-8.80682800	4.50469100	-0.62931800
H	-8.18582600	2.93846800	1.20017600
H	-6.60143500	1.35929800	2.20798300
H	-4.47326600	0.09200900	2.06391300
H	-1.09330800	1.27911400	-4.13311800
O	-2.63334300	0.37087100	0.30411200
O	-2.50450600	0.30198200	-2.23035800
N	-3.22957400	-1.83953800	-1.01944600
C	-2.94569700	-3.04975600	-1.73661500
C	-3.08084200	-4.28364900	-1.06636900
C	-2.52635800	-2.99562100	-3.06660900
C	-2.70210500	-5.44931500	-1.75636700
C	-2.16994400	-4.16583800	-3.73356100
H	-2.44943500	-2.02391700	-3.55448600
C	-2.24927900	-5.39453500	-3.07145600
H	-2.76724600	-6.41008500	-1.23990600
H	-1.80910900	-4.11537500	-4.76315400
H	-1.95370200	-6.31320600	-3.58321500
C	-4.62421600	-1.65111300	-0.73235600
C	-5.20752500	-2.44567200	0.28074300
C	-5.39044300	-0.71285900	-1.43359600
C	-6.54235300	-2.17219600	0.64374300
C	-6.71670500	-0.48002900	-1.07424000
H	-4.92039700	-0.14588800	-2.23505000
C	-7.28640300	-1.19843400	-0.01720300
H	-6.99905400	-2.76248100	1.44247400
H	-7.29549700	0.28077800	-1.60105700
H	-8.31886200	-1.00463300	0.28249100
C	-3.59892200	-4.38282700	0.29396900
H	-3.27844000	-5.26799800	0.85251800
C	-4.51149700	-3.57750200	0.89033000
H	-4.86391200	-3.87391600	1.88155000
C	2.78696600	0.79559400	1.98212300
C	1.89101000	0.99382000	3.05698700
C	1.73319100	2.25046000	3.58776500
C	2.38282000	3.37246600	3.01087800
C	2.16384200	4.68735800	3.50215500

C	2.73978600	5.77858500	2.89069400
C	3.54575700	5.59326700	1.74263500
C	3.79157800	4.32804300	1.25414700
C	3.24758300	3.17504300	1.88532900
C	3.52281100	1.83590600	1.42892000
C	4.33462900	0.84182300	-0.73088000
C	4.57873800	1.58851500	0.41346400
C	5.91224100	2.11237500	0.58758300
C	6.35557500	2.67246400	1.81865100
C	7.64257200	3.14651400	1.96768000
C	8.55920900	3.09737500	0.89070900
C	8.16958700	2.54393200	-0.30987700
C	6.85830600	2.02644900	-0.48711000
C	6.47367500	1.39358100	-1.70045100
C	5.24892800	0.78942700	-1.80946000
H	1.07204900	2.40815600	4.44272600
H	1.50884800	4.81638300	4.36767900
H	2.55815900	6.78564700	3.27337100
H	3.96936600	6.46113700	1.23176200
H	4.40175500	4.20448800	0.36085100
H	5.66730300	2.71049500	2.66171700
H	7.95725500	3.55939400	2.92905400
H	9.57288100	3.48440400	1.01777400
H	8.87150600	2.47855300	-1.14539500
H	7.18697500	1.34817200	-2.52623300
H	4.95512800	0.23707000	-2.70119900
H	1.33125600	0.14474400	3.44383600
O	3.16620700	0.14737400	-0.91284600
O	2.98151200	-0.49936700	1.53983400
N	3.53844200	-2.32565600	-0.15163600
C	3.17451800	-3.70096300	0.02207900
C	3.11871200	-4.53488900	-1.11210900
C	2.90429600	-4.20250600	1.29598400
C	2.68513300	-5.85925700	-0.93581500
C	2.48715000	-5.52513500	1.45170600
H	3.00284500	-3.53575300	2.15382600
C	2.36414700	-6.34854100	0.32816200
H	2.59564200	-6.50592600	-1.81181200
H	2.24879600	-5.90850200	2.44636600
H	2.02258700	-7.38007000	0.44100500
C	4.93021900	-2.14554400	-0.45247500
C	5.38792900	-2.53550100	-1.73088300
C	5.80579900	-1.59072200	0.48746900
C	6.74147000	-2.29973200	-2.04364800

C	7.14181500	-1.37437800	0.15584100
H	5.41209600	-1.30135100	1.46118600
C	7.60773500	-1.72832300	-1.11573200
H	7.10905100	-2.58181000	-3.03363000
H	7.81362600	-0.91045500	0.88052600
H	8.65192000	-1.55095700	-1.38334700
C	3.51046300	-4.05706100	-2.43568300
H	3.01011500	-4.53946700	-3.28046900
C	4.50980700	-3.18433100	-2.70690000
H	4.76908500	-3.02273400	-3.75836500
P	-2.06168900	-0.61870700	-0.89317700
P	2.47745800	-1.02144500	0.02561100
Ir	0.18454700	-1.05738800	-0.44968700
C	0.26962000	-2.33274900	1.86665700
H	0.72029100	-3.17897900	1.35574700
H	0.88188500	-1.72330500	2.52984300
C	-1.07373700	-2.18478800	1.82136100
H	-1.66745400	-2.89097900	1.23805600
C	-1.86504100	-1.28375500	2.72541900
O	-1.03039000	-0.26380500	3.23928000
C	0.40353100	0.99768900	-0.88098600
C	0.65700700	0.28847300	-1.93347400
C	1.19748300	0.10264800	-3.29728300
H	1.14644400	1.06101800	-3.84364600
H	2.27139400	-0.12779700	-3.18570000
C	0.52753600	-1.02926100	-4.08163200
H	-0.53792000	-0.81732800	-4.25971900
H	1.01599600	-1.17069500	-5.05840100
H	0.58069400	-1.96849600	-3.51081400
C	0.32069200	2.31205700	-0.29970200
C	0.89330300	3.42500400	-0.94580600
C	-0.35993400	2.50845200	0.91632000
C	0.76104000	4.70108200	-0.40327700
H	1.44038500	3.27260700	-1.87776700
C	-0.50199700	3.78811100	1.44461500
H	-0.76550000	1.63457700	1.42264600
C	0.05099300	4.88939400	0.78540300
H	1.20661400	5.55768500	-0.91256800
H	-1.03827500	3.92874500	2.38649100
H	-0.05900500	5.89181600	1.20245200
C	-1.73049000	0.76859700	3.89111400
H	-0.99095800	1.51632300	4.20479500
H	-2.45424700	1.25710700	3.21343000
H	-2.27435500	0.40295900	4.78166600

C	-2.49970400	-2.10585300	3.84438100
C	-1.68922400	-2.73258300	4.80062000
C	-3.88935800	-2.22551900	3.94926200
C	-2.25929400	-3.46945900	5.83876400
H	-0.60410500	-2.63724500	4.72199500
C	-4.46542400	-2.96902700	4.98455600
H	-4.52960300	-1.73817200	3.21090000
C	-3.65072400	-3.59357900	5.93113500
H	-1.61774700	-3.95428600	6.57880300
H	-5.55273200	-3.05531100	5.05326100
H	-4.09697400	-4.17421100	6.74210600
H	-2.67525300	-0.83476200	2.13916200
Cl	0.16856100	-3.45108200	-1.15365800

B-M4

Zero-point correction=	**1.305420 (Hartree/Particle)**
Thermal correction to Energy=	**1.386097**
Thermal correction to Enthalpy=	**1.387041**
Thermal correction to Gibbs Free Energy=	**1.189469**
Sum of electronic and zero-point Energies=	**-5122.305129**
Sum of electronic and thermal Energies=	**-5122.224452**
Sum of electronic and thermal Enthalpies=	**-5122.223508**
Sum of electronic and thermal Free Energies=	**-5122.421080**

C	3.06189300	-0.78726300	-2.13581800
C	2.80432000	-0.34890600	-3.45732800
C	2.65394800	-1.25068400	-4.47812600
C	2.69254100	-2.64617900	-4.21940700
C	2.44032400	-3.59492300	-5.24497400
C	2.42054100	-4.94562200	-4.97322900
C	2.63475400	-5.39320400	-3.64946600
C	2.89614300	-4.49436500	-2.63658900
C	2.96275500	-3.09570700	-2.88680500
C	3.24898300	-2.13534300	-1.84477300
C	3.09261100	-2.20173600	0.65061600
C	3.71102900	-2.61486700	-0.51680800
C	4.82006300	-3.52701500	-0.38244500
C	5.69507800	-3.82857800	-1.46287700
C	6.76761500	-4.68100400	-1.29869600
C	7.01851400	-5.29067300	-0.04654200
C	6.19946400	-5.00802000	1.02569000
C	5.10208400	-4.11517700	0.89590000

C	4.30073900	-3.76577000	2.01907600
C	3.33004100	-2.80498300	1.90688300
H	2.46852400	-0.90309000	-5.49717800
H	2.24566700	-3.22781100	-6.25600700
H	2.22006300	-5.66687000	-5.76897100
H	2.57989100	-6.46034000	-3.42176000
H	3.03470000	-4.85890000	-1.62051300
H	5.51939800	-3.36264900	-2.43174700
H	7.43059500	-4.88371900	-2.14316300
H	7.86473000	-5.97183500	0.06941600
H	6.39234300	-5.45510400	2.00443100
H	4.50306200	-4.23820800	2.98276600
H	2.72775400	-2.46463900	2.74917100
H	2.73798700	0.71943600	-3.63925900
O	2.15325800	-1.20911200	0.63414100
O	3.20200800	0.19753600	-1.17591500
N	3.44216100	1.00282300	1.25393400
C	3.67134800	2.40932200	1.36235000
C	3.51733700	3.01799400	2.62712600
C	4.08307100	3.14956000	0.24789300
C	3.74255100	4.40364300	2.71944900
C	4.31575800	4.51909500	0.36990100
H	4.20632500	2.63616800	-0.70566700
C	4.14724100	5.14260400	1.61141800
H	3.59229600	4.89915300	3.68040000
H	4.61306000	5.10154800	-0.50426000
H	4.32104900	6.21608100	1.71169900
C	4.46841500	0.22999200	1.89476700
C	4.45085900	0.15761000	3.30342700
C	5.46545300	-0.41124800	1.15240500
C	5.40015400	-0.67278100	3.93129200
C	6.41068800	-1.20610700	1.79718600
H	5.46454800	-0.30597300	0.06834300
C	6.36469500	-1.34926300	3.18909400
H	5.38521200	-0.76083900	5.02056000
H	7.16454400	-1.73590700	1.21222500
H	7.09140100	-1.98849600	3.69561500
C	3.15487000	2.24556500	3.81683600
H	2.59172600	2.79240100	4.57939300
C	3.54565600	0.98131600	4.10660400
H	3.27436400	0.57965700	5.08784100
C	-3.33795500	0.24853000	2.47296000
C	-3.04754800	1.01433100	3.62346200
C	-2.92593600	0.39832200	4.84353800

C	-3.04105100	-1.01351100	4.94770100
C	-2.81679700	-1.68068100	6.18267200
C	-2.87774800	-3.05400100	6.26955300
C	-3.15738100	-3.81679900	5.11049100
C	-3.40036200	-3.19759900	3.90284000
C	-3.37258900	-1.77995600	3.78075300
C	-3.61287400	-1.10945600	2.52855200
C	-3.44249600	-1.86241200	0.12531400
C	-4.09819800	-1.87572600	1.34805900
C	-5.29323200	-2.68004800	1.43964300
C	-6.17778300	-2.60171900	2.55190200
C	-7.32662500	-3.36349500	2.60914400
C	-7.65280100	-4.25646800	1.56093900
C	-6.82628000	-4.34688700	0.46159700
C	-5.64683700	-3.56057200	0.36311000
C	-4.82226400	-3.60927900	-0.79441900
C	-3.75618000	-2.75873300	-0.92392000
H	-2.70311100	0.98190300	5.73980200
H	-2.57791800	-1.07831000	7.06304800
H	-2.69497600	-3.55585000	7.22263400
H	-3.17276600	-4.90765900	5.17028600
H	-3.59719100	-3.80174000	3.01868300
H	-5.94553900	-1.91468400	3.36464800
H	-7.99198100	-3.27283300	3.47106000
H	-8.56050800	-4.86144400	1.62107700
H	-7.07230900	-5.01948000	-0.36438000
H	-5.07676100	-4.30066900	-1.60081900
H	-3.13856300	-2.72871100	-1.82089300
H	-2.91844700	2.09086800	3.50665300
O	-2.41279000	-1.00240500	-0.14648500
O	-3.35953500	0.92403500	1.26612800
N	-3.24302600	1.16185000	-1.27198900
C	-3.23445000	2.50856200	-1.73685400
C	-2.97539200	2.74349300	-3.10550300
C	-3.56248900	3.56275100	-0.87547400
C	-3.04543300	4.07236000	-3.56731000
C	-3.63335600	4.86833100	-1.35971300
H	-3.77831500	3.33431000	0.16962000
C	-3.38675000	5.11879800	-2.71319900
H	-2.84556600	4.27299100	-4.62302500
H	-3.88066500	5.68932500	-0.68381800
H	-3.44583500	6.13862700	-3.09818400
C	-4.34390600	0.39121200	-1.78583900
C	-4.27332300	-0.05795300	-3.12069500

C	-5.45160500	0.08836300	-0.98668100
C	-5.29177200	-0.91216700	-3.58629100
C	-6.46242500	-0.73699200	-1.47699800
H	-5.48827600	0.47332600	0.03113000
C	-6.37061000	-1.25271100	-2.77427500
H	-5.23528500	-1.28960700	-4.61036200
H	-7.30485300	-1.00175800	-0.83546300
H	-7.14838900	-1.91923500	-3.15366800
C	-2.68955800	1.65394100	-4.04285500
H	-2.03926300	1.91554000	-4.88337300
C	-3.24058100	0.41793000	-4.03973300
H	-3.00028600	-0.24767600	-4.87375300
P	2.26477100	0.36086900	0.22146100
P	-2.29074100	0.61016200	0.01419400
Ir	-0.00867000	1.00954200	0.15284000
C	-0.10397800	2.25235600	2.00422500
H	-0.94655100	1.84558800	2.55570800
H	0.84082500	2.22866900	2.54978700
C	-0.27526300	3.18229200	0.97306600
H	-1.29341600	3.44584300	0.67602200
C	0.74801500	4.29664500	0.86224400
O	0.82770400	5.00616400	2.11132600
C	0.00955700	-0.05266400	-1.70967700
C	0.19056000	1.19566400	-1.96504000
C	0.52997300	2.24040900	-2.95892900
H	0.60249800	1.76364900	-3.95281700
H	-0.30209700	2.95615000	-3.02404100
C	1.81511700	3.01412700	-2.64204700
H	2.70712900	2.38011600	-2.72299700
H	1.92865400	3.87394500	-3.31853500
H	1.78729000	3.39860400	-1.61737900
C	-0.19349400	-1.40902400	-2.15591500
C	-0.47935200	-1.67820400	-3.50814800
C	-0.13521100	-2.48177400	-1.24437200
C	-0.69118900	-2.98758700	-3.94005200
H	-0.53130200	-0.84763200	-4.21258200
C	-0.33894400	-3.78662700	-1.68528700
H	0.04227900	-2.26583100	-0.19069500
C	-0.61637200	-4.04715900	-3.03176000
H	-0.90063700	-3.18529800	-4.99409500
H	-0.28546500	-4.61043100	-0.96976400
H	-0.76501600	-5.07353000	-3.37424900
C	-0.35491500	5.64151600	2.52881400
H	-0.10339800	6.24244700	3.41523500

H	-0.76490400	6.31540200	1.75269600
H	-1.14180600	4.91744400	2.81202600
C	0.60820800	5.29261400	-0.27723800
C	1.41937200	6.44069400	-0.24293800
C	-0.23193800	5.10237200	-1.37508700
C	1.41831200	7.35333100	-1.29527500
H	2.05217300	6.60285800	0.62900800
C	-0.22208900	6.00805500	-2.44239500
H	-0.87470600	4.22596700	-1.41447100
C	0.60333900	7.13122800	-2.41103700
H	2.05932800	8.23762100	-1.25050900
H	-0.86297300	5.82595900	-3.30473100
H	0.60876700	7.83441200	-3.24760900
H	1.73824000	3.83948000	0.77904500
Cl	-0.30642500	-0.73666100	2.02188800

B-M5

Zero-point correction=	**1.305462 (Hartree/Particle)**
Thermal correction to Energy=	**1.386348**
Thermal correction to Enthalpy=	**1.387293**
Thermal correction to Gibbs Free Energy=	**1.189069**
Sum of electronic and zero-point Energies=	**-5122.319223**
Sum of electronic and thermal Energies=	**-5122.238336**
Sum of electronic and thermal Enthalpies=	**-5122.237392**
Sum of electronic and thermal Free Energies=	**-5122.435615**

C	-3.34598900	-1.24892500	1.89650400
C	-2.98219400	-1.36872000	3.25809400
C	-2.97390600	-2.59978800	3.86229600
C	-3.26553000	-3.77291000	3.11140400
C	-3.14227500	-5.06794900	3.68273900
C	-3.36831400	-6.20038700	2.93032300
C	-3.72127900	-6.07649700	1.56567300
C	-3.87048300	-4.83258400	0.98854000
C	-3.66545500	-3.64257300	1.73995600
C	-3.80747200	-2.33056300	1.15556400
C	-3.87902800	-1.43018500	-1.19586100
C	-4.45872800	-2.16396700	-0.17262700
C	-5.76456000	-2.72565100	-0.42837200
C	-6.56941600	-3.28945400	0.60105900
C	-7.82607300	-3.79305200	0.33415900
C	-8.34799400	-3.77126900	-0.98059700

C	-7.60406900	-3.21443200	-1.99845400
C	-6.31684000	-2.66619600	-1.75174600
C	-5.58378700	-2.02301900	-2.78716800
C	-4.39912800	-1.39357500	-2.50974100
H	-2.69919200	-2.69360300	4.91555500
H	-2.84702800	-5.14786300	4.73217100
H	-3.26121000	-7.19090100	3.37841800
H	-3.87009800	-6.97379600	0.96056000
H	-4.13022800	-4.75405900	-0.06640000
H	-6.19095600	-3.30700700	1.62183600
H	-8.42447600	-4.20838300	1.14847300
H	-9.34007900	-4.18192400	-1.18183800
H	-8.00102600	-3.16940500	-3.01592800
H	-6.00074600	-1.99763200	-3.79625100
H	-3.83450900	-0.84221500	-3.26145800
H	-2.70939400	-0.46328700	3.79633200
O	-2.71984100	-0.72192700	-1.00004500
O	-3.31176600	0.01951400	1.36410600
N	-3.42558400	1.77534100	-0.45478600
C	-3.24128600	3.10007200	0.05267400
C	-3.07024800	4.15628900	-0.87221300
C	-3.19846800	3.33438900	1.43114100
C	-2.78399400	5.43441300	-0.35793400
C	-2.92466500	4.61505900	1.91468400
H	-3.34692800	2.49613400	2.11285300
C	-2.70801700	5.66427600	1.01544500
H	-2.62060700	6.25699000	-1.05854700
H	-2.86653200	4.78642900	2.99172600
H	-2.48060600	6.66614500	1.38637000
C	-4.69663300	1.57541700	-1.09732000
C	-4.87855900	2.12713000	-2.38329400
C	-5.72673900	0.86584000	-0.47008900
C	-6.07826800	1.83508100	-3.06198000
C	-6.91467500	0.60921700	-1.15233900
H	-5.56941600	0.48844300	0.53838500
C	-7.08081200	1.07925900	-2.45973100
H	-6.22228500	2.23312500	-4.06960000
H	-7.69820500	0.01965000	-0.67293000
H	-8.00162900	0.86201100	-3.00578700
C	-3.13898400	3.94292500	-2.31855400
H	-2.53495400	4.62477200	-2.92277600
C	-3.90461700	3.04218200	-2.97765400
H	-3.88598000	3.07607000	-4.07122300
C	3.29409700	-0.42808800	-2.27767700

C	3.05216400	0.15085900	-3.54452400
C	3.03172800	-0.62725400	-4.67201900
C	3.19718900	-2.03514000	-4.57767900
C	3.07068900	-2.87514100	-5.71647800
C	3.19010500	-4.24358600	-5.60618000
C	3.43358300	-4.82512700	-4.33940900
C	3.58039400	-4.03382000	-3.21916700
C	3.48464100	-2.61642800	-3.29931300
C	3.63167700	-1.76783100	-2.14217400
C	3.46281900	-2.15464600	0.32806000
C	4.13969100	-2.33177400	-0.86572300
C	5.38763100	-3.05426200	-0.81783300
C	6.28294900	-3.10428700	-1.92269600
C	7.48335200	-3.77962700	-1.84120700
C	7.85296200	-4.45333600	-0.65289400
C	7.01769800	-4.41026500	0.44252400
C	5.78622900	-3.70331000	0.39768600
C	4.96265200	-3.58883000	1.55096000
C	3.83797700	-2.80591500	1.52583600
H	2.84233200	-0.17627900	-5.64889900
H	2.86054100	-2.41174100	-6.68394100
H	3.08219100	-4.88008400	-6.48751400
H	3.49827600	-5.91170600	-4.24504500
H	3.75427900	-4.49983800	-2.25013000
H	6.01822900	-2.58567000	-2.84293900
H	8.15573800	-3.79074500	-2.70229400
H	8.80155400	-4.99298200	-0.60345200
H	7.29835700	-4.90694600	1.37498700
H	5.26586200	-4.09074300	2.47221500
H	3.22689200	-2.64112800	2.41268600
H	2.86688600	1.22005700	-3.59800400
O	2.34810400	-1.35219200	0.39872000
O	3.25566400	0.42310600	-1.18695500
N	3.24688000	0.94551900	1.32245200
C	3.07637700	2.29697000	1.76574000
C	2.70594800	2.53992300	3.10471000
C	3.28994300	3.35400500	0.87853800
C	2.42476200	3.86994900	3.47404100
C	3.04006800	4.66842600	1.27313300
H	3.61523200	3.13172000	-0.13589900
C	2.58261500	4.92030100	2.57146400
H	2.09180100	4.06822400	4.49529700
H	3.17191200	5.47925800	0.55572800
H	2.35928300	5.94300300	2.88402200

C	4.44409300	0.32851800	1.81930600
C	4.50512400	0.00412800	3.19347600
C	5.52091400	0.04921500	0.96972800
C	5.64861800	-0.67710700	3.65768300
C	6.64223100	-0.61985700	1.45534000
H	5.44665100	0.32835400	-0.07985700
C	6.70106900	-0.99084000	2.80348100
H	5.70150500	-0.95143900	4.71437900
H	7.45931600	-0.87197700	0.77680400
H	7.57256600	-1.52751800	3.18509600
C	2.67327700	1.48141400	4.10792700
H	2.02746800	1.66597100	4.96887000
C	3.45690100	0.37774100	4.14143400
H	3.38565600	-0.25210700	5.03403300
P	-2.41312300	0.49986500	0.03026700
P	2.23878300	0.26405300	0.14135600
Ir	-0.10193200	0.67985100	0.11755800
C	-0.00065000	2.88547500	0.25598500
H	-0.82062400	3.25054300	0.86757700
H	0.97781900	3.24089500	0.56423700
C	-0.23681800	2.55697800	-1.09011500
H	-1.25832300	2.58511800	-1.45817300
C	0.69637400	2.78391000	-2.26430000
H	1.34993500	1.91396200	-2.40097200
O	-0.16211600	2.90373000	-3.40216900
C	-0.18480500	0.11438300	2.16850000
C	-0.16957800	-0.98021900	1.48866300
C	-0.14583300	-2.46392300	1.49554700
H	0.84352300	-2.77496600	1.87239800
H	-0.87211700	-2.81156100	2.24839100
C	-0.41025700	-3.13809100	0.15084700
H	0.32789900	-2.82294500	-0.59741000
H	-0.37933900	-4.23299100	0.26213300
H	-1.39738700	-2.86082500	-0.24064700
C	-0.30766700	0.69182200	3.48269100
C	-0.19124900	-0.13502300	4.62339900
C	-0.57701300	2.05811800	3.67527700
C	-0.34662000	0.38917300	5.90366200
H	0.02578300	-1.19537000	4.48290600
C	-0.73238400	2.58090800	4.96005700
H	-0.64881200	2.70420200	2.80425100
C	-0.61812200	1.75328700	6.08107600
H	-0.25089700	-0.26575300	6.77365300
H	-0.93729200	3.64726700	5.08612400

H	-0.73786100	2.16454500	7.08609900
C	1.54161700	4.04131400	-2.15704300
C	2.91026400	4.02290600	-2.44671500
C	0.93915700	5.26722900	-1.83338100
C	3.66835400	5.19949500	-2.41221500
H	3.39635800	3.07387800	-2.68267000
C	1.68758000	6.44261100	-1.80126900
H	-0.12601700	5.28840100	-1.59588400
C	3.05796000	6.41317900	-2.09144100
H	4.73762300	5.16450000	-2.63498900
H	1.20478900	7.38901400	-1.54417700
H	3.64578400	7.33401200	-2.06429100
C	0.37803700	2.41323600	-4.60060600
H	-0.35414400	2.61624900	-5.39664000
H	1.32743600	2.91793300	-4.87294600
H	0.55089500	1.32402300	-4.54263800
Cl	0.12887000	-0.47625100	-2.11043500

B-M6

Zero-point correction=	**1.305515 (Hartree/Particle)**
Thermal correction to Energy=	**1.386121**
Thermal correction to Enthalpy=	**1.387065**
Thermal correction to Gibbs Free Energy=	**1.188859**
Sum of electronic and zero-point Energies=	**-5122.322996**
Sum of electronic and thermal Energies=	**-5122.242389**
Sum of electronic and thermal Enthalpies=	**-5122.241445**
Sum of electronic and thermal Free Energies=	**-5122.439651**

C	2.86538100	-1.55277700	-1.88092200
C	2.27257900	-1.67567000	-3.15465500
C	2.01110800	-2.92690000	-3.65542800
C	2.25138400	-4.08704900	-2.87236700
C	1.90211300	-5.38021600	-3.34575100
C	2.06981100	-6.49621700	-2.55689100
C	2.57724500	-6.35559500	-1.24327300
C	2.94517300	-5.11724400	-0.76156800
C	2.82165600	-3.94823200	-1.56353200
C	3.22529700	-2.64469600	-1.10217500
C	3.69777800	-1.60522500	1.15610600
C	4.03188100	-2.49291700	0.14051200
C	5.24481500	-3.25897700	0.31734600
C	5.83759400	-3.99995800	-0.74406200

C	7.00781200	-4.70697600	-0.55963300
C	7.65038400	-4.72442400	0.70083200
C	7.11734900	-4.00045200	1.74514500
C	5.92747900	-3.24165800	1.57916900
C	5.42112800	-2.43116900	2.63098000
C	4.34932200	-1.60691200	2.41241600
H	1.56013200	-3.04165300	-4.64312100
H	1.47229500	-5.46646200	-4.34640600
H	1.78861500	-7.48359300	-2.93034800
H	2.67483200	-7.23530800	-0.60255600
H	3.32789300	-5.02525200	0.25415000
H	5.36464400	-3.99269000	-1.72456800
H	7.44374500	-5.25499000	-1.39825500
H	8.57059300	-5.29702900	0.83771300
H	7.61279400	-3.98312400	2.71943700
H	5.93074900	-2.43193300	3.59701000
H	3.98575100	-0.91641100	3.17323400
H	2.00581000	-0.76054300	-3.68192400
O	2.68890200	-0.68224000	1.03690900
O	3.16146300	-0.27605400	-1.44042700
N	3.57749100	1.60041200	0.22081700
C	3.58027400	2.92101400	-0.32355300
C	3.67159100	4.01345000	0.57062800
C	3.53484700	3.12293900	-1.70680000
C	3.65643200	5.31218400	0.02683500
C	3.56118500	4.41928400	-2.21862700
H	3.44916700	2.25803800	-2.36559500
C	3.61453600	5.51471700	-1.34977100
H	3.68248500	6.16756700	0.70495700
H	3.51252100	4.57556700	-3.29786200
H	3.61231300	6.53132500	-1.74844700
C	4.85268600	1.22824400	0.78285200
C	5.20279200	1.76144100	2.04134000
C	5.72686700	0.36909400	0.10667800
C	6.39210900	1.30859600	2.64666400
C	6.91081300	-0.04616300	0.71395100
H	5.44790900	0.00262900	-0.87896400
C	7.23314800	0.40993000	1.99651200
H	6.66157800	1.69731600	3.63201500
H	7.56707600	-0.74775900	0.19576900
H	8.14909800	0.06926400	2.48445800
C	3.79522100	3.83718400	2.01744500
H	3.41766400	4.66705400	2.62158200
C	4.43611600	2.83634300	2.66789100

H	4.52687000	2.91903700	3.75570500
C	-3.14890600	0.83600300	2.16318200
C	-2.63083500	1.76941600	3.09215300
C	-2.47017400	1.41343200	4.40885300
C	-2.77031000	0.09249900	4.83973700
C	-2.50578600	-0.32548300	6.17257900
C	-2.74138300	-1.62358900	6.56921100
C	-3.24654800	-2.56070300	5.63638600
C	-3.53108700	-2.18109900	4.34180800
C	-3.32144700	-0.84380900	3.90178400
C	-3.58923700	-0.42589200	2.54699800
C	-3.73198800	-1.66929000	0.37130700
C	-4.28422500	-1.33998700	1.60063800
C	-5.55437300	-1.93540200	1.93309600
C	-6.32361200	-1.51472900	3.05362100
C	-7.54534300	-2.08903000	3.33859100
C	-8.06371200	-3.12272400	2.52314600
C	-7.35104600	-3.54432600	1.42097000
C	-6.09825300	-2.96156500	1.08978200
C	-5.37978000	-3.36386500	-0.07069200
C	-4.22931800	-2.71692900	-0.43838300
H	-2.07654300	2.13244800	5.13099600
H	-2.09622700	0.40477600	6.87517200
H	-2.52717300	-1.93492600	7.59413900
H	-3.40590800	-3.59737800	5.94182700
H	-3.90524500	-2.91929700	3.63451100
H	-5.94382200	-0.71332800	3.68665000
H	-8.11975300	-1.73763700	4.19901300
H	-9.02904400	-3.57466500	2.76241600
H	-7.74568200	-4.33086100	0.77245800
H	-5.78035900	-4.16880800	-0.69078300
H	-3.67980800	-2.96394500	-1.34664600
H	-2.36917200	2.76409200	2.73018800
O	-2.61770900	-1.03856300	-0.10258100
O	-3.23818600	1.23783200	0.84784800
N	-3.17597300	0.93421400	-1.69111600
C	-3.02073300	2.12004400	-2.48230300
C	-2.69041800	1.97117400	-3.84483800
C	-3.28726700	3.37566600	-1.93791100
C	-2.59119000	3.13393100	-4.62731300
C	-3.21269700	4.51395500	-2.73913000
H	-3.55123900	3.44828800	-0.88192900
C	-2.86333300	4.39038800	-4.08651400
H	-2.31962200	3.03881700	-5.68150900

H	-3.40997900	5.49661700	-2.30600000
H	-2.79985200	5.27881200	-4.71949300
C	-4.36128400	0.19447900	-2.03301500
C	-4.34858200	-0.55409700	-3.22969300
C	-5.49264500	0.21989500	-1.21000500
C	-5.47206200	-1.35702000	-3.51088100
C	-6.60354600	-0.56025000	-1.52528900
H	-5.47170700	0.82957600	-0.30751900
C	-6.58301300	-1.36376500	-2.67105400
H	-5.46943300	-1.96376800	-4.41997000
H	-7.47209900	-0.56186900	-0.86398900
H	-7.44254500	-1.99349000	-2.91230300
C	-2.52593500	0.65537300	-4.46367300
H	-1.81649000	0.61030100	-5.29481800
C	-3.25281000	-0.45403900	-4.19421800
H	-3.10033500	-1.32854300	-4.83346500
P	2.40292300	0.42794000	-0.14422300
P	-2.26008100	0.53530800	-0.34014300
Ir	0.08929200	0.72441100	-0.21780000
C	0.29304500	2.14191700	1.42635400
H	-0.27922300	1.80872500	2.29240600
H	1.34881100	2.32786400	1.64404500
C	-0.33484500	2.86317000	0.38231500
H	-1.41951500	2.97905100	0.46727000
C	0.24929600	4.05033800	-0.34778100
H	1.31461700	3.87023300	-0.53797000
O	-0.45076600	4.21381900	-1.56003900
C	0.01074600	-1.46177900	-0.16217300
C	0.02799700	-0.99992800	1.03141400
C	-0.00947400	-1.16904900	2.49466600
H	0.92991000	-0.76978300	2.91449200
H	-0.80726500	-0.53133500	2.90546500
C	-0.22123000	-2.61863400	2.93623400
H	0.61750600	-3.25487700	2.61269200
H	-0.30502100	-2.68271300	4.03187200
H	-1.14714600	-3.02646800	2.50408700
C	-0.34311300	-2.55401500	-1.03839600
C	-0.33055500	-3.88213200	-0.56671700
C	-0.83268800	-2.30134800	-2.33208400
C	-0.82668400	-4.91984500	-1.35186500
H	0.06388500	-4.08940600	0.42807000
C	-1.33136000	-3.34422400	-3.11195600
H	-0.82492200	-1.27680400	-2.70557200
C	-1.33743300	-4.65536900	-2.62690600

H	-0.80402300	-5.94330900	-0.97148600
H	-1.71548000	-3.13009200	-4.11201200
H	-1.72422100	-5.47056900	-3.24329800
C	0.11852200	5.31994400	0.50384600
C	-0.55612900	6.44246800	0.00836800
C	0.66311700	5.38637900	1.79480200
C	-0.65994200	7.61034200	0.77128400
H	-1.00645200	6.38624000	-0.98241400
C	0.56234600	6.54973600	2.55899400
H	1.16413700	4.51337000	2.21086600
C	-0.09682300	7.67260400	2.04735900
H	-1.18894700	8.47639400	0.36467800
H	0.99525500	6.57858600	3.56271700
H	-0.17789000	8.58461900	2.64389500
C	0.31883700	4.59594100	-2.67189300
H	-0.38459300	4.80449400	-3.48801000
H	0.91463400	5.50518400	-2.47002300
H	0.98491300	3.77874600	-2.98740400
Cl	0.31883700	1.14855400	-2.69596200

B-M7

Zero-point correction=	**1.305930 (Hartree/Particle)**
Thermal correction to Energy=	**1.386445**
Thermal correction to Enthalpy=	**1.387389**
Thermal correction to Gibbs Free Energy=	**1.189647**
Sum of electronic and zero-point Energies=	**-5122.335092**
Sum of electronic and thermal Energies=	**-5122.254577**
Sum of electronic and thermal Enthalpies=	**-5122.253632**
Sum of electronic and thermal Free Energies=	**-5122.451374**

C	4.04635600	1.17706000	1.09043300
C	4.14331700	2.28762500	1.95898700
C	4.87276100	3.38869000	1.58930200
C	5.44464100	3.46811200	0.29180000
C	6.07362600	4.65546400	-0.17008300
C	6.57120100	4.74315900	-1.45204700
C	6.45538900	3.63630400	-2.32771700
C	5.87186200	2.46219400	-1.89999200
C	5.35818300	2.33406800	-0.57912000
C	4.74588000	1.11648600	-0.10899200
C	3.90658700	-1.00728100	-1.15809300

C	4.95364400	-0.15950400	-0.84067500
C	6.28761100	-0.60219600	-1.17732600
C	7.45699700	0.04925300	-0.69417500
C	8.71829200	-0.41488100	-1.00738400
C	8.88504100	-1.55280400	-1.83107100
C	7.77460500	-2.22294500	-2.29681100
C	6.46340000	-1.78541800	-1.96943200
C	5.32221700	-2.53358600	-2.36702800
C	4.07075600	-2.17123800	-1.94233600
H	4.96484000	4.23919200	2.26506800
H	6.13312500	5.50911500	0.50965600
H	7.04247700	5.66565000	-1.79924800
H	6.82764900	3.71408500	-3.35198700
H	5.78567300	1.61857800	-2.58476300
H	7.35330700	0.92010100	-0.04961000
H	9.59585100	0.10068000	-0.61020700
H	9.88861800	-1.90464100	-2.08106100
H	7.88431200	-3.11994100	-2.91186200
H	5.45962000	-3.43386800	-2.97013300
H	3.18691200	-2.76171100	-2.17664300
H	3.63197800	2.22791100	2.91804500
O	2.61982000	-0.73439000	-0.74472800
O	3.31581900	0.10609200	1.56029600
N	2.31087100	-2.22643600	1.43931700
C	1.43873200	-2.77037800	2.44038900
C	0.74959000	-3.97728900	2.17337900
C	1.22343500	-2.07274800	3.62904400
C	-0.18177600	-4.42776300	3.12677400
C	0.28879200	-2.53592600	4.55631100
H	1.74709700	-1.13244000	3.79653300
C	-0.41198800	-3.71779000	4.30445200
H	-0.74399300	-5.34143400	2.91979100
H	0.09318000	-1.95314200	5.45788600
H	-1.14886900	-4.08306300	5.02362200
C	3.49397900	-3.00042600	1.16137200
C	3.35254900	-4.23408500	0.48796000
C	4.76385600	-2.52942300	1.51447700
C	4.52134400	-4.92825900	0.12098600
C	5.90650900	-3.23406800	1.13802100
H	4.84482200	-1.58589700	2.04956100
C	5.78431900	-4.43443400	0.43157400
H	4.41949600	-5.87204000	-0.42049600
H	6.89279800	-2.83258000	1.37861100
H	6.67780800	-4.98035200	0.12090400

C	0.92814300	-4.72563200	0.93206700
H	0.06665500	-5.32287300	0.62015600
C	2.05071700	-4.82294700	0.18542700
H	2.02087100	-5.48834300	-0.68177500
C	-3.87340300	-0.41876800	1.67316500
C	-3.47278300	-0.97897900	2.90625700
C	-3.78666300	-2.28657700	3.17948700
C	-4.46776600	-3.08608800	2.22055100
C	-4.69618800	-4.47056000	2.45012800
C	-5.29766400	-5.26086700	1.49533600
C	-5.69344800	-4.69049800	0.26161800
C	-5.50034300	-3.34774800	0.01485800
C	-4.89569300	-2.49773500	0.98236700
C	-4.63781300	-1.10243800	0.73760600
C	-4.23724100	0.23068200	-1.36427400
C	-5.10617200	-0.43071600	-0.50672300
C	-6.50531900	-0.43160400	-0.85696400
C	-7.50955100	-0.89980700	0.03663500
C	-8.84371500	-0.88156200	-0.31316100
C	-9.25098700	-0.39892400	-1.57980800
C	-8.30726500	0.07940900	-2.46280700
C	-6.92668700	0.09018200	-2.12557900
C	-5.95596700	0.63738400	-3.00796800
C	-4.64432900	0.72920600	-2.62317400
H	-3.46164600	-2.74551700	4.11553700
H	-4.37006100	-4.89902300	3.40142000
H	-5.46063900	-6.32494000	1.68185700
H	-6.15127800	-5.32029800	-0.50486600
H	-5.80569600	-2.92801500	-0.94201900
H	-7.21404100	-1.26631600	1.01887200
H	-9.59300600	-1.23824500	0.39745100
H	-10.30995100	-0.39576300	-1.84807600
H	-8.60741300	0.47285000	-3.43750700
H	-6.27641500	1.02835500	-3.97604600
H	-3.89198400	1.20837800	-3.24930000
H	-2.85015800	-0.37327100	3.56460600
O	-2.90128700	0.40330700	-1.07400000
O	-3.43332200	0.85420400	1.37749300
N	-2.49763000	2.76430700	-0.01308800
C	-1.92761200	3.79151600	0.80967400
C	-1.33135800	4.89741900	0.16573200
C	-2.03960200	3.74343300	2.20233000
C	-0.86167000	5.95333400	0.96671100
C	-1.57733200	4.81005500	2.97141500

H	-2.47761900	2.86397100	2.67270000
C	-1.00220500	5.92273900	2.35080900
H	-0.37900900	6.80567000	0.48459800
H	-1.65738400	4.76443400	4.05966500
H	-0.63310500	6.75657500	2.95137700
C	-3.65914900	3.23410700	-0.72896800
C	-3.44970800	4.02658200	-1.87778300
C	-4.95740000	2.94806300	-0.28973600
C	-4.57369500	4.38797300	-2.64676000
C	-6.05744300	3.34818100	-1.04633400
H	-5.08911300	2.38088600	0.62927100
C	-5.86212500	4.04658500	-2.24269500
H	-4.42209700	4.97897800	-3.55373200
H	-7.06494600	3.09035700	-0.71450800
H	-6.71990700	4.34149100	-2.85160200
C	-1.21819400	4.98838700	-1.29083900
H	-0.34015800	5.52915200	-1.65744000
C	-2.13405500	4.58005500	-2.20009700
H	-1.95313900	4.82072100	-3.25251100
P	2.05469800	-0.67288100	0.80427200
P	-2.22795300	1.11652800	0.24733100
Ir	-0.13393200	0.22599100	0.59900400
C	-1.18500900	-1.74425300	0.78112000
H	-0.83390500	-2.20100100	1.69808900
H	-2.26121800	-1.72218700	0.66401100
C	-0.43537100	-1.77723300	-0.40674000
H	0.53790800	-2.26362900	-0.36744200
C	-1.06982300	-1.97704900	-1.78353000
O	-2.43408500	-2.31992300	-1.63250700
C	0.83573500	2.07799300	0.04959300
C	0.65604600	1.37738200	-1.01090500
C	0.83086000	1.20661900	-2.46880700
H	1.65728200	1.86040400	-2.80090000
H	1.16053500	0.17427200	-2.66176900
C	-0.43574600	1.51745100	-3.27671000
H	-0.73053600	2.56752900	-3.14706200
H	-0.27150500	1.32518300	-4.34912500
H	-1.27909600	0.90158700	-2.93462300
C	1.39929900	3.28232200	0.61113300
C	2.03861600	4.21460400	-0.23427700
C	1.33624400	3.54986500	1.98961100
C	2.58931800	5.38172700	0.28605800
H	2.10350800	4.00556100	-1.30368100
C	1.88889400	4.72259400	2.50272900

H	0.84229300	2.82419500	2.63738700
C	2.51487200	5.64298300	1.65971500
H	3.09348300	6.08592200	-0.38018300
H	1.82245000	4.92239400	3.57502800
H	2.94494100	6.56143200	2.06745500
C	-3.13939800	-2.38415900	-2.84686400
H	-4.19887600	-2.53444200	-2.60353600
H	-3.04302400	-1.44571300	-3.42303400
H	-2.79357400	-3.21805300	-3.48520300
C	-0.30457000	-3.08754900	-2.49486100
C	0.74190700	-2.79848200	-3.37549500
C	-0.61410700	-4.42734900	-2.22284200
C	1.48061000	-3.82913100	-3.96658300
H	0.98655000	-1.75691600	-3.59691800
C	0.11350000	-5.45821800	-2.81850300
H	-1.43935000	-4.64385500	-1.54120700
C	1.16951300	-5.16239500	-3.68819600
H	2.29793100	-3.58739700	-4.65058200
H	-0.14024600	-6.49920400	-2.60185100
H	1.74110000	-5.96885100	-4.15401400
H	-0.99357200	-1.05713500	-2.38541300
Cl	-0.41786400	0.66799000	3.08333100

B-M8

Zero-point correction=	**1.305818 (Hartree/Particle)**
Thermal correction to Energy=	**1.386525**
Thermal correction to Enthalpy=	**1.387469**
Thermal correction to Gibbs Free Energy=	**1.190127**
Sum of electronic and zero-point Energies=	**-5122.328691**
Sum of electronic and thermal Energies=	**-5122.247984**
Sum of electronic and thermal Enthalpies=	**-5122.247040**
Sum of electronic and thermal Free Energies=	**-5122.444382**

C	3.77633500	0.75465500	-0.19931400
C	3.84916200	2.11476400	0.16962200
C	4.32052000	3.04762300	-0.71966900
C	4.64986100	2.67447300	-2.04760000
C	5.01796000	3.64569100	-3.01823800
C	5.25739000	3.28691000	-4.32594300
C	5.12977900	1.93101400	-4.71616500
C	4.79720700	0.96261500	-3.79311400
C	4.56220100	1.29473200	-2.42806200

C	4.20303900	0.30645800	-1.44346600
C	3.17234400	-1.96134000	-1.56967300
C	4.27120100	-1.14034900	-1.76351700
C	5.47354600	-1.74404400	-2.27821000
C	6.71738200	-1.05468900	-2.31567100
C	7.85916200	-1.66640800	-2.79096800
C	7.81897600	-2.99962200	-3.26395900
C	6.63308300	-3.70143600	-3.22746600
C	5.44468000	-3.10664400	-2.72546100
C	4.23256400	-3.84437200	-2.63077600
C	3.12356900	-3.29194500	-2.04357300
H	4.37712400	4.09772800	-0.42964400
H	5.08055900	4.69082400	-2.70606900
H	5.52928500	4.04360200	-5.06568800
H	5.29103800	1.64983300	-5.75956700
H	4.69533100	-0.07364700	-4.11239600
H	6.76631600	-0.03058900	-1.94740200
H	8.80358300	-1.11702900	-2.79773300
H	8.72784100	-3.47109300	-3.64504400
H	6.59051500	-4.73796200	-3.57216200
H	4.20955700	-4.87470000	-2.99252600
H	2.19425400	-3.84408700	-1.90892500
H	3.52138900	2.40308300	1.16356300
O	2.03619500	-1.49033800	-0.95851500
O	3.31865100	-0.13894200	0.75411400
N	2.19833500	-2.29530300	1.56594200
C	1.46072800	-2.61836500	2.75546000
C	0.49446600	-3.64713500	2.71717100
C	1.72596000	-1.93654100	3.94244900
C	-0.27722800	-3.86761200	3.87145200
C	0.97216500	-2.19448600	5.08869800
H	2.49770100	-1.16955900	3.95751500
C	-0.04795200	-3.14781600	5.04408300
H	-1.04544600	-4.64342100	3.84510100
H	1.16776500	-1.62484000	5.99815200
H	-0.65701500	-3.34308700	5.93007900
C	3.18814700	-3.27359700	1.20534900
C	2.76780600	-4.57184300	0.83030900
C	4.54562400	-2.93195500	1.19909700
C	3.76104400	-5.49154900	0.43718500
C	5.50369500	-3.85681900	0.78889300
H	4.82787700	-1.91935800	1.48314500
C	5.10753800	-5.14463300	0.41174800
H	3.45041300	-6.49370000	0.13088700

H	6.55615600	-3.56875500	0.75107600
H	5.85316200	-5.87288400	0.08478200
C	0.35468300	-4.54741900	1.57667300
H	-0.63093900	-5.00097800	1.44382500
C	1.36399000	-4.97829300	0.78766600
H	1.13272800	-5.77103300	0.06900000
C	-3.82125200	-1.29078900	1.15088200
C	-3.51978600	-1.93935400	2.36801400
C	-3.59451700	-3.30639400	2.44587300
C	-3.91896000	-4.07702200	1.29810600
C	-3.87793500	-5.49748200	1.32932500
C	-4.13954900	-6.24077800	0.19885100
C	-4.45271000	-5.58343600	-1.01506500
C	-4.51960500	-4.20718900	-1.07227800
C	-4.26925300	-3.40830700	0.07789300
C	-4.29210700	-1.97040200	0.03861600
C	-3.95906200	-0.31100700	-1.82597500
C	-4.75375300	-1.24387800	-1.17503200
C	-6.06871200	-1.48351100	-1.71704500
C	-7.04031500	-2.26573100	-1.03128700
C	-8.29809700	-2.46887000	-1.55989100
C	-8.65542300	-1.90705200	-2.80886100
C	-7.74472800	-1.13136000	-3.49298300
C	-6.44658600	-0.88942000	-2.96750100
C	-5.52102400	-0.05017100	-3.64509500
C	-4.31158700	0.25073700	-3.07502900
H	-3.35835300	-3.81737600	3.38112600
H	-3.61951800	-5.99015500	2.27054100
H	-4.09506600	-7.33186300	0.23285700
H	-4.63490400	-6.17118600	-1.91788100
H	-4.74558400	-3.71756000	-2.01861000
H	-6.78400400	-2.69903400	-0.06537500
H	-9.02638700	-3.06606400	-1.00610500
H	-9.65217600	-2.08113000	-3.22072700
H	-8.01047700	-0.67771500	-4.45141700
H	-5.80334000	0.38792900	-4.60491000
H	-3.60930100	0.94255500	-3.53945800
H	-3.20562200	-1.33936900	3.22045300
O	-2.74885500	0.10352700	-1.32008200
O	-3.62966000	0.08021900	1.08584900
N	-3.00991700	2.31859500	0.02207300
C	-2.59251900	3.37737100	0.88515600
C	-2.01945200	4.53186800	0.31175700
C	-2.79685500	3.28546300	2.26740400

C	-1.62733400	5.57045400	1.17852800
C	-2.41711700	4.33525500	3.10356300
H	-3.26167500	2.38370200	2.66965300
C	-1.83375300	5.48298400	2.55267500
H	-1.15917400	6.45911700	0.75062200
H	-2.57111200	4.25645400	4.18187000
H	-1.53236100	6.30827100	3.20170200
C	-4.14265200	2.64176000	-0.80299200
C	-3.94273800	3.51570400	-1.89301600
C	-5.40257500	2.08971700	-0.54666000
C	-5.02720900	3.74020200	-2.76392100
C	-6.46545700	2.34173600	-1.41281000
H	-5.52314300	1.43111900	0.31196300
C	-6.27144500	3.15926500	-2.53129300
H	-4.88233800	4.39806300	-3.62462800
H	-7.43673700	1.87897000	-1.22813600
H	-7.09662100	3.34565700	-3.22241100
C	-1.84774800	4.68242300	-1.13370900
H	-1.00271300	5.30252300	-1.44353300
C	-2.67945900	4.22501000	-2.09771200
H	-2.45570700	4.51328600	-3.12964600
P	1.85829200	-0.95848600	0.59049700
P	-2.40922600	0.74504000	0.14653200
Ir	-0.19878500	0.16023400	0.61507700
C	-0.73171600	0.07157500	2.70619400
H	-1.81128200	0.16798300	2.82729500
H	-0.30730800	-0.75384800	3.27169900
C	0.02855800	1.26913000	2.52332700
H	-0.53957500	2.19575600	2.45165000
C	1.36389700	1.40143700	3.25557200
O	1.28182300	0.89655000	4.60282500
C	0.47111000	1.55587600	-0.94586100
C	0.14002200	0.47693100	-1.53312800
C	-0.04590100	-0.38577400	-2.71478600
H	-0.04804300	-1.43359100	-2.38148500
H	-1.06005700	-0.20068500	-3.10688900
C	0.99943200	-0.15397400	-3.81030300
H	2.01871000	-0.28409700	-3.42261100
H	0.85456200	-0.86711400	-4.63736200
H	0.93166400	0.86224300	-4.22901300
C	0.94071300	2.91445000	-1.07075500
C	1.27638700	3.42232300	-2.34399700
C	1.07960600	3.75773600	0.03934500
C	1.73519200	4.72860900	-2.48816900

H	1.18726100	2.77324800	-3.21513800
C	1.54551600	5.06295700	-0.10235800
H	0.82225100	3.36705600	1.01659500
C	1.87314300	5.55866000	-1.36755200
H	2.00363800	5.09816400	-3.48057700
H	1.65661300	5.68834300	0.78551600
H	2.24113700	6.58126400	-1.48246500
C	0.36789000	1.52688400	5.46237900
H	0.40032800	0.98205100	6.41739500
H	0.62854200	2.58450700	5.65441200
H	-0.66701900	1.48646200	5.07535100
C	1.97779700	2.79018500	3.32540100
C	3.36789000	2.89559900	3.48560700
C	1.21502400	3.96260100	3.37227300
C	3.98416300	4.13822100	3.63966100
H	3.97189500	1.98490700	3.48243900
C	1.82444900	5.20978300	3.53372200
H	0.13321700	3.91445300	3.26880100
C	3.21206300	5.30424000	3.65929000
H	5.07013000	4.19751500	3.74496100
H	1.20647500	6.11080500	3.55813300
H	3.69056000	6.27936800	3.77786000
H	2.10833700	0.73825300	2.79933800
Cl	-0.95800700	-2.17745300	0.09258900

[B-C]‡

Zero-point correction= 1.571224 (Hartree/Particle)
Thermal correction to Energy= 1.664611
Thermal correction to Enthalpy= 1.665555
Thermal correction to Gibbs Free Energy= 1.442515
Sum of electronic and zero-point Energies= -5530.936504
Sum of electronic and thermal Energies= -5530.843117
Sum of electronic and thermal Enthalpies= -5530.842173
Sum of electronic and thermal Free Energies= -5531.065213

C	3.20988100	0.10348200	2.01280400
C	2.74680000	0.40656500	3.31610900
C	3.02322300	1.61996700	3.88969600
C	3.71602600	2.61979700	3.15578400
C	3.88460200	3.93253200	3.67039400
C	4.46710100	4.92366600	2.91107100
C	4.90363700	4.63306200	1.59661400
C	4.78451400	3.35896700	1.08326100

C	4.20405300	2.30735800	1.84582400
C	4.03677600	0.97773300	1.31359200
C	4.08896700	-0.03222500	-0.98235800
C	4.74800800	0.57716200	0.07363300
C	6.17558700	0.75494600	-0.04622400
C	6.99369900	1.14268500	1.05165000
C	8.36070000	1.27480100	0.91660100
C	8.98930800	1.03707400	-0.32834900
C	8.23034500	0.63894500	-1.40768500
C	6.82497000	0.46856300	-1.29259700
C	6.05755000	-0.03607200	-2.37768500
C	4.72433700	-0.30986900	-2.21609300
H	2.66232700	1.85229200	4.89385500
H	3.50843900	4.14929600	4.67327000
H	4.57397800	5.93490900	3.31035400
H	5.32682600	5.42707200	0.97763000
H	5.11157200	3.15461200	0.06476500
H	6.53145300	1.32072100	2.02108300
H	8.96271600	1.56155500	1.78214400
H	10.07108900	1.15409700	-0.42601700
H	8.70255500	0.42488000	-2.37006000
H	6.55596000	-0.25197400	-3.32531600
H	4.12550400	-0.75978400	-3.00844600
H	2.15953500	-0.35189400	3.82797300
O	2.75783300	-0.35062500	-0.90342700
O	2.86656400	-1.12876300	1.51782400
N	2.80924300	-2.93819500	-0.28499000
C	2.10330600	-4.15913500	-0.04974400
C	2.02425200	-5.13429900	-1.07148800
C	1.45924500	-4.36522200	1.17448300
C	1.30125300	-6.31275300	-0.79931800
C	0.71306000	-5.51932600	1.40284700
H	1.52715200	-3.59072800	1.93713500
C	0.64885800	-6.50669400	0.41597900
H	1.24707000	-7.08158600	-1.57289000
H	0.17481400	-5.63655000	2.34442300
H	0.07839100	-7.42216100	0.58794800
C	4.22122500	-3.07097900	-0.53607700
C	4.65305700	-3.61742700	-1.76551000
C	5.16639800	-2.64159100	0.40437600
C	6.03114400	-3.61002700	-2.05505300
C	6.52686100	-2.64979100	0.09922900
H	4.81769400	-2.25905800	1.35997700
C	6.96069600	-3.12031500	-1.14322800

H	6.36461100	-4.00925700	-3.01645300
H	7.24500500	-2.26305800	0.82496800
H	8.02343200	-3.10733300	-1.39499800
C	2.62177400	-4.95143900	-2.39170200
H	2.13500900	-5.50351000	-3.19805700
C	3.73867500	-4.25772700	-2.70630800
H	4.07891000	-4.29898600	-3.74597100
C	0.03228800	2.25825400	-2.11519700
C	1.36743200	1.96891400	-2.47967200
C	2.33401500	2.93496500	-2.35769300
C	2.00820700	4.21982100	-1.84561200
C	3.02003900	5.19474000	-1.63069200
C	2.72719000	6.40827200	-1.04900300
C	1.39800300	6.68931500	-0.65260900
C	0.39112000	5.77085400	-0.86204500
C	0.65059000	4.51352900	-1.47778900
C	-0.36434400	3.50569700	-1.65315800
C	-2.40993200	2.94307000	-0.30909400
C	-1.77222700	3.75988100	-1.23858400
C	-2.49831200	4.90509700	-1.71892600
C	-2.05904900	5.65477600	-2.84564100
C	-2.77355100	6.74266100	-3.30084800
C	-3.96035200	7.15096600	-2.64442500
C	-4.41896000	6.44161600	-1.55536900
C	-3.71877400	5.30066600	-1.07621600
C	-4.21191600	4.52384300	0.00583600
C	-3.59714700	3.34512400	0.34667900
H	3.37049700	2.71154800	-2.62045500
H	4.04528900	4.94890900	-1.91824600
H	3.51637600	7.14377300	-0.87722100
H	1.16762100	7.63875500	-0.16350000
H	-0.61578600	5.99753400	-0.51904700
H	-1.15015200	5.34425900	-3.36099600
H	-2.42365900	7.29156900	-4.17831800
H	-4.51361800	8.01947700	-3.00933800
H	-5.34220200	6.73673100	-1.04960600
H	-5.12361500	4.84175800	0.51739400
H	-4.00281300	2.68169800	1.10984300
H	1.60761500	0.96539200	-2.82270100
O	-1.89637700	1.72700900	0.06352100
O	-0.89466500	1.26434900	-2.26085400
N	-3.06987700	0.23687500	-1.87157900
C	-4.22240600	-0.28839500	-1.20038600
C	-5.37735300	0.51805800	-1.02780900

C	-4.18871500	-1.57707100	-0.66415300
C	-6.45714700	-0.01846700	-0.29608700
C	-5.27410700	-2.09091600	0.04409800
H	-3.29284600	-2.17993000	-0.75233500
C	-6.41735900	-1.30978800	0.22753200
H	-7.34709900	0.60060200	-0.15483400
H	-5.19851600	-3.09871400	0.45394400
H	-7.27513700	-1.70101200	0.78054500
C	-3.22253900	0.63175900	-3.24723100
C	-4.03515500	1.73206200	-3.59959000
C	-2.50862600	-0.04248100	-4.24621800
C	-4.02907000	2.17101900	-4.93986300
C	-2.53531900	0.39057700	-5.57057700
H	-1.88091500	-0.88738600	-3.97009600
C	-3.28935500	1.51571100	-5.91849300
H	-4.63442300	3.04211200	-5.20290400
H	-1.94942900	-0.14008100	-6.32450800
H	-3.30194300	1.87679300	-6.94947700
C	-5.51386200	1.86707600	-1.56883400
H	-6.24721500	2.49283800	-1.05195300
C	-4.92297900	2.40204400	-2.65931500
H	-5.21650900	3.41824300	-2.93713900
P	2.01546400	-1.46302900	0.09745000
P	-1.59670000	0.45679400	-0.97296500
Ir	-0.21858000	-1.17760300	-0.10952200
C	-0.10848100	-0.02882400	1.74893400
C	-0.31332000	-0.90692700	2.66096700
C	-0.62962500	-1.79783900	3.65338200
H	-1.71624300	-1.11104100	4.25918100
H	-1.36020400	-2.52382900	3.24569900
C	0.44506800	-2.41640500	4.53992500
H	1.03210500	-1.65258700	5.07395600
H	-0.01346600	-3.06640500	5.30135500
H	1.15452600	-3.03522400	3.96676600
C	0.07931300	1.41988500	1.96842600
C	-0.49806800	2.05054400	3.08454100
C	0.92237600	2.17954500	1.14723900
C	-0.26105400	3.39474300	3.36529100
H	-1.13152300	1.46589100	3.74955800
C	1.19729900	3.51259300	1.45089800
H	1.38604600	1.70702700	0.28420000
C	0.59629300	4.13356500	2.54618900
H	-0.73517500	3.86158000	4.23295700
H	1.90347700	4.06809100	0.83866700

H	0.81252400	5.18111300	2.76499700
C	0.37075600	-1.67876700	-2.19985400
H	0.39982700	-0.74442200	-2.75956600
H	1.26821300	-2.29424500	-2.28355000
C	-0.85384100	-2.31902500	-1.95594100
H	-1.75314400	-1.79813900	-2.27791100
C	-1.01999800	-3.82866100	-2.03548600
C	-2.48293000	-4.23654300	-2.08905500
C	-3.02492600	-5.12550100	-1.15531500
C	-3.30457400	-3.75129900	-3.11705200
C	-4.36851700	-5.50228400	-1.23204500
H	-2.39315000	-5.49131200	-0.34570600
C	-4.64711900	-4.12303600	-3.19577300
H	-2.88791200	-3.07395600	-3.86525600
C	-5.18519700	-4.99808300	-2.24791600
H	-4.78163400	-6.18872500	-0.48827500
H	-5.27636100	-3.72222500	-3.99404700
H	-6.23839400	-5.28505700	-2.30097300
O	-0.35184700	-4.19471200	-3.25873400
C	-0.56315600	-5.51197100	-3.70099500
H	-1.58312600	-5.66765700	-4.09525300
H	0.15628900	-5.69847000	-4.51322600
H	-0.39748300	-6.25430800	-2.89998900
H	-0.53607800	-4.33070200	-1.18691300
C	-5.18796500	0.15396000	4.45961200
C	-4.01557700	-0.61933600	3.82479500
C	-2.90689800	-0.65384400	6.19946400
C	-4.13856300	0.09964800	6.73774400
C	-5.40877900	-0.18101100	5.93420300
H	-4.98336500	1.23621600	4.36607000
H	-6.09473500	-0.04278800	3.86667400
H	-4.27460900	-0.15623400	7.80108300
H	-3.92787100	1.18360000	6.70094700
H	-5.70927400	-1.23548200	6.04579600
H	-6.24163400	0.41720600	6.33641900
N	-2.80298700	-0.45823400	4.71526100
H	-2.50099300	0.50855200	4.57704300
C	-1.62311000	-0.05502300	6.79063000
H	-1.65598400	-0.10228700	7.88892700
H	-0.73369800	-0.60330800	6.44830800
H	-1.50694900	1.00288100	6.50311500
C	-2.96474200	-2.14650000	6.55476600
H	-2.19992100	-2.71272500	6.00574600
H	-2.77384900	-2.26765100	7.63122800

H	-3.94022200	-2.59758500	6.34078100
C	-3.64960700	0.00691300	2.47428300
H	-2.90529800	-0.59510400	1.93845200
H	-4.54528500	0.06464900	1.84203700
H	-3.25244100	1.02609100	2.59715300
C	-4.36876900	-2.09370800	3.59986200
H	-5.20685400	-2.13360300	2.89087200
H	-3.53755500	-2.63662600	3.12903800
H	-4.68048600	-2.61322600	4.51335400
Cl	-1.77236500	-3.08726200	1.03627900

C

Zero-point correction= 1.576085 (Hartree/Particle)
Thermal correction to Energy= 1.670621
Thermal correction to Enthalpy= 1.671566
Thermal correction to Gibbs Free Energy= 1.441769
Sum of electronic and zero-point Energies= -5530.986029
Sum of electronic and thermal Energies= -5530.891492
Sum of electronic and thermal Enthalpies= -5530.890547
Sum of electronic and thermal Free Energies= -5531.120344

C	4.12015100	-0.90076200	1.22978100
C	4.13800800	-1.92988500	2.20116100
C	4.31788600	-1.62625700	3.52655500
C	4.41710000	-0.27361600	3.94834700
C	4.45827000	0.07246200	5.32603000
C	4.49708300	1.38977800	5.72805600
C	4.50178300	2.42011100	4.75652600
C	4.48536500	2.11483800	3.41191300
C	4.44286300	0.76530900	2.96109400
C	4.38531100	0.42367900	1.56273100
C	3.75012500	1.65531000	-0.52689100
C	4.63792800	1.45076000	0.51872600
C	5.84712900	2.23701700	0.53206200
C	6.92601600	1.96683500	1.42001900
C	8.08133300	2.72107900	1.39470500
C	8.22206000	3.79491100	0.48423200
C	7.20458900	4.07200500	-0.40352900
C	6.01162300	3.30100600	-0.41623500
C	4.99101800	3.54076600	-1.37717100
C	3.89540400	2.72122400	-1.44662600
H	4.31877300	-2.41833100	4.27749200
H	4.43489700	-0.73370900	6.06346800
H	4.51501600	1.64284000	6.79068000

H	4.51310400	3.46555100	5.07365300
H	4.49258300	2.91644500	2.67425100
H	6.84082900	1.13796900	2.12127100
H	8.89662900	2.48228300	2.08183600
H	9.13782700	4.39059900	0.47885600
H	7.30536400	4.88491600	-1.12747200
H	5.11344100	4.36160200	-2.08724600
H	3.12248100	2.84690800	-2.20446500
H	3.97819500	-2.95178600	1.86329900
O	2.64598800	0.86540900	-0.68752700
O	3.90709500	-1.26695400	-0.07662000
N	3.27623000	-0.93316800	-2.52351200
C	2.93195100	-2.05595000	-3.33307600
C	2.43134500	-1.85189900	-4.63887000
C	3.05106200	-3.35074300	-2.81503200
C	2.05113200	-2.98588500	-5.38596900
C	2.65965600	-4.45489100	-3.56993900
H	3.43464600	-3.47410900	-1.80394300
C	2.16047800	-4.27149200	-4.86395600
H	1.65455300	-2.84003000	-6.39345600
H	2.73058700	-5.45679700	-3.14189600
H	1.84701600	-5.13104000	-5.46011700
C	4.37464600	-0.13343500	-2.98729600
C	4.19731200	0.67106900	-4.13564000
C	5.59300700	-0.11224200	-2.29696200
C	5.23536100	1.54960500	-4.50226600
C	6.60922400	0.76112100	-2.68197600
H	5.71163400	-0.75598200	-1.42848100
C	6.42490000	1.60430000	-3.78184700
H	5.09474600	2.19079600	-5.37628800
H	7.53614700	0.79909900	-2.10636100
H	7.21124800	2.30307700	-4.07585700
C	2.26029100	-0.51979100	-5.21636800
H	1.47828800	-0.43974500	-5.97791000
C	3.00756200	0.58314100	-4.98013600
H	2.78242400	1.47552700	-5.57298500
C	-1.30659300	2.40674900	0.73187400
C	-0.03351100	1.84786700	0.98205700
C	0.94030800	2.60446400	1.58662300
C	0.66672400	3.93698500	1.99930300
C	1.64690100	4.71378500	2.67564900
C	1.36780200	5.99189300	3.10764000
C	0.08123300	6.54095800	2.88877100
C	-0.88910300	5.81737300	2.22743500

C	-0.62919400	4.50352900	1.74367200
C	-1.61772600	3.72163100	1.04767400
C	-4.10131000	3.62163500	1.18840300
C	-2.96140800	4.26970500	0.72511300
C	-3.13274900	5.47192300	-0.04170800
C	-2.05572200	6.07932200	-0.74537200
C	-2.25234900	7.20960900	-1.51025300
C	-3.53491500	7.80342900	-1.60235000
C	-4.60029300	7.23911000	-0.93450800
C	-4.43561800	6.06279700	-0.15415200
C	-5.53331600	5.44414200	0.50242400
C	-5.37540200	4.23611800	1.13625500
H	1.93040100	2.18185600	1.76543400
H	2.62502900	4.26472900	2.85691200
H	2.12967500	6.57698600	3.62830900
H	-0.14836000	7.54565200	3.25216900
H	-1.87674500	6.25160600	2.07826900
H	-1.06711700	5.62375300	-0.68877800
H	-1.41238000	7.64814900	-2.05440800
H	-3.67703700	8.70201200	-2.20745600
H	-5.59758200	7.68148300	-1.00640300
H	-6.51638600	5.91944700	0.45390600
H	-6.21139700	3.70942300	1.59480500
H	0.15096600	0.82223000	0.64921000
O	-4.02685400	2.37042200	1.74527700
O	-2.23514400	1.61832300	0.09515800
N	-4.54489000	0.84443400	-0.49608100
C	-5.50333100	-0.22063300	-0.51512900
C	-6.88393100	0.05650300	-0.36883600
C	-5.05515200	-1.54320500	-0.60638100
C	-7.76959200	-1.03520200	-0.26016400
C	-5.95406100	-2.60669000	-0.50466500
H	-3.98842100	-1.72973400	-0.72663500
C	-7.31651000	-2.35120300	-0.32244500
H	-8.83582400	-0.83179000	-0.13068200
H	-5.58183700	-3.63091200	-0.56529200
H	-8.02709500	-3.17686000	-0.23625800
C	-4.58500900	1.80732100	-1.55967700
C	-5.68903200	2.68126800	-1.68322300
C	-3.49538500	1.92475800	-2.42942700
C	-5.60262900	3.73422600	-2.61501700
C	-3.44350100	2.96239000	-3.36029700
H	-2.67742100	1.21363100	-2.35351000
C	-4.48992000	3.88620200	-3.43692100

H	-6.43333300	4.44056500	-2.68445500
H	-2.57230300	3.05530200	-4.01235400
H	-4.44005400	4.72178900	-4.13834100
C	-7.42773700	1.41143000	-0.34399400
H	-8.42262700	1.49789900	0.10476000
C	-6.91526400	2.53100700	-0.90714800
H	-7.53690400	3.42985700	-0.86180000
P	2.55993800	-0.77643100	-0.97494800
P	-3.55789300	0.96518900	0.90613800
Ir	0.54880500	-1.45068900	-0.53874600
C	1.20078800	-2.68645800	1.01135500
C	1.60818200	-3.88342700	0.65057600
C	2.04613600	-5.07190500	0.28363100
H	-1.94082800	-2.93581900	2.04955000
H	1.31170600	-5.87378500	0.11491000
C	3.49655600	-5.43693000	0.07169100
H	3.67071700	-5.83638000	-0.94268400
H	4.15225000	-4.56426400	0.20637900
H	3.82389900	-6.22037700	0.77798200
C	1.12297700	-2.32494200	2.45055000
C	1.20794000	-3.29286900	3.47518200
C	1.03994500	-0.97784100	2.84296100
C	1.23301400	-2.92338500	4.82324500
H	1.32166800	-4.34277700	3.19587100
C	1.08598400	-0.60258400	4.18415700
H	0.97982800	-0.22302900	2.06555600
C	1.18111100	-1.57250400	5.18660800
H	1.31807500	-3.69461400	5.59432200
H	1.05880000	0.45808300	4.44388900
H	1.22450000	-1.27927900	6.23799200
C	0.12914100	0.21187600	-2.09428600
H	-0.09689100	1.12239500	-1.54001900
H	0.93649100	0.28701300	-2.82528600
C	-0.81598000	-0.79438700	-2.20437300
H	-1.77270800	-0.64030500	-1.70433000
C	-0.88574900	-1.78273800	-3.34218300
C	-1.49564400	-3.10218100	-2.89379500
C	-0.68338700	-4.10755900	-2.35496600
C	-2.87961900	-3.30028500	-2.94849900
C	-1.24513800	-5.29752600	-1.88971100
H	0.39181700	-3.94611500	-2.28432200
C	-3.44354700	-4.49391700	-2.48863100
H	-3.51118900	-2.50905400	-3.35702700
C	-2.62738500	-5.49761800	-1.95904000

H	-0.59604500	-6.07289600	-1.47557600
H	-4.52469300	-4.64064300	-2.55114700
H	-3.06687500	-6.43470400	-1.60687400
O	-1.66321100	-1.15309900	-4.35868800
C	-1.60131200	-1.78462500	-5.61122700
H	-1.95747800	-2.83150200	-5.57585800
H	-2.24494100	-1.21702900	-6.29951700
H	-0.57100600	-1.79291400	-6.01552800
H	0.13090000	-1.97347100	-3.71700600
C	-3.41503900	-3.56204200	5.03642100
C	-3.09082800	-2.69172100	3.81304800
C	-2.48838100	-4.92079700	2.52277800
C	-2.85438400	-5.68679100	3.80303800
C	-3.89292100	-4.96855300	4.66779700
H	-2.50758600	-3.63987000	5.66162600
H	-4.16816100	-3.03533700	5.64256400
H	-3.20407900	-6.69056700	3.51567100
H	-1.93411900	-5.83421600	4.39615900
H	-4.85939800	-4.91792600	4.14168800
H	-4.07535300	-5.55025000	5.58475600
N	-2.14364100	-3.49578000	2.93006600
H	-1.22864300	-3.51863500	3.40580900
C	-1.22393600	-5.48843600	1.87382400
H	-1.41587500	-6.51865700	1.54247000
H	-0.93119800	-4.88891200	1.00060900
H	-0.38163400	-5.50941500	2.57863800
C	-3.61151900	-4.92611500	1.48003400
H	-3.38383100	-4.22783300	0.66352900
H	-3.67207100	-5.93380300	1.04640200
H	-4.59500800	-4.68225400	1.89368000
C	-2.31218600	-1.43631300	4.20994900
H	-2.07033200	-0.83231700	3.32393300
H	-2.92596300	-0.82552900	4.88714300
H	-1.37536200	-1.68656200	4.72607500
C	-4.34382200	-2.27005600	3.03806100
H	-4.84905200	-1.47900900	3.60976100
H	-4.08181700	-1.84664800	2.06054700
H	-5.06527600	-3.08002900	2.88912900
Cl	-1.70226500	-1.93480700	0.41910500

C1

Zero-point correction= **1.306410 (Hartree/Particle)**

Thermal correction to Energy=	**1.390709**
Thermal correction to Enthalpy=	**1.391653**
Thermal correction to Gibbs Free Energy=	**1.187265**
Sum of electronic and zero-point Energies=	**-5446.119347**
Sum of electronic and thermal Energies=	**-5446.035049**
Sum of electronic and thermal Enthalpies=	**-5446.034105**
Sum of electronic and thermal Free Energies=	**-5446.238492**

C	3.40339800	-1.02430600	-2.40167800
C	3.03172500	-1.30246700	-3.73877800
C	3.00170500	-2.59649300	-4.19645400
C	3.27397200	-3.67678900	-3.31304500
C	3.11308500	-5.02804500	-3.72237700
C	3.31201900	-6.06744600	-2.83909800
C	3.67593000	-5.78822100	-1.50043400
C	3.86008000	-4.48880800	-1.08004500
C	3.68310100	-3.39226100	-1.96822000
C	3.84074200	-2.02545500	-1.53987600
C	3.90986000	-0.93736100	0.77171600
C	4.47541900	-1.73520300	-0.22323800
C	5.78413400	-2.29143400	0.04214500
C	6.57315500	-2.89708700	-0.97761600
C	7.82970100	-3.40482900	-0.71535700
C	8.37413200	-3.34726700	0.58865300
C	7.64800000	-2.74881800	1.59671600
C	6.36318500	-2.19759500	1.35054400
C	5.64612700	-1.51484400	2.37003200
C	4.47074800	-0.88159800	2.07781100
H	2.71560200	-2.81335900	-5.22899400
H	2.80665800	-5.22553300	-4.75353400
H	3.17153700	-7.10185700	-3.16333200
H	3.79243100	-6.60758000	-0.78698000
H	4.10657500	-4.28701100	-0.03903600
H	6.18030900	-2.94307200	-1.99196200
H	8.40977500	-3.85088700	-1.52744200
H	9.36614300	-3.76004600	0.78890400
H	8.05894400	-2.67131600	2.60734200
H	6.07318300	-1.45497700	3.37407400
H	3.93430500	-0.28598300	2.81661600
H	2.74988500	-0.45788200	-4.36724600
O	2.80786200	-0.16735200	0.63848900
O	3.32001300	0.27131500	-1.97863600
N	3.22985400	2.10270800	-0.27394300
C	2.90236600	3.39437600	-0.73560900

C	2.80660700	4.47100200	0.18845600
C	2.64927000	3.62583100	-2.09414900
C	2.45769200	5.74520300	-0.30297500
C	2.28909600	4.89126100	-2.55181600
H	2.71536400	2.78228700	-2.78099000
C	2.20162400	5.96037800	-1.65582000
H	2.39653100	6.57947900	0.40162800
H	2.05534200	5.03524800	-3.60865100
H	1.92568400	6.95732400	-2.00891500
C	4.53442700	1.98897000	0.29676000
C	4.77875800	2.51547300	1.58801600
C	5.57287900	1.32352500	-0.37290600
C	6.01316700	2.25072700	2.21106300
C	6.79606500	1.08463100	0.25343100
H	5.38222800	0.95251500	-1.37682500
C	7.01226100	1.53237800	1.55976100
H	6.18132600	2.63359800	3.22171700
H	7.56902900	0.51785700	-0.27052300
H	7.95753500	1.32115500	2.06580800
C	3.01428100	4.29040400	1.62405900
H	2.48690800	4.99804400	2.26644800
C	3.82705900	3.40542600	2.24421700
H	3.88173400	3.45665000	3.33607300
C	-2.31168500	-0.88254600	2.16575800
C	-1.71123000	-0.33778700	3.32821700
C	-1.24793200	-1.17145000	4.31474000
C	-1.33843700	-2.58258700	4.17412800
C	-0.77875700	-3.45649700	5.14566400
C	-0.82524200	-4.82428600	4.98381100
C	-1.43060900	-5.36962200	3.82670100
C	-1.98952000	-4.54738700	2.87159700
C	-1.98144500	-3.13131400	3.01531200
C	-2.53219300	-2.24630500	2.01916300
C	-2.85127800	-2.49204800	-0.44869000
C	-3.25226700	-2.80340800	0.84528300
C	-4.34802200	-3.72031600	0.99888300
C	-5.00964300	-3.90527200	2.24458400
C	-6.08531900	-4.75918500	2.36265100
C	-6.54941200	-5.49171400	1.24236900
C	-5.93128700	-5.33587800	0.02041200
C	-4.83563800	-4.44432800	-0.13990900
C	-4.22526300	-4.23283800	-1.40543600
C	-3.27962700	-3.25018700	-1.56390400
H	-0.78006100	-0.75129300	5.20824800

H	-0.29540400	-3.01557900	6.02158200
H	-0.38340600	-5.48505900	5.73381400
H	-1.43887500	-6.45212900	3.67696700
H	-2.41306800	-4.98584900	1.97093200
H	-4.66720300	-3.33647700	3.10871700
H	-6.58789300	-4.86702300	3.32713300
H	-7.39905900	-6.17101100	1.34828900
H	-6.28660300	-5.88558300	-0.85576300
H	-4.56002400	-4.82329100	-2.26225400
H	-2.83948300	-3.01012300	-2.53091700
H	-1.63117800	0.74450000	3.42183800
O	-1.97867800	-1.47869100	-0.69558800
O	-2.74499400	0.01111600	1.22394900
N	-3.74895800	0.54864200	-0.98489200
C	-3.89716100	1.41696700	-2.11764900
C	-4.33649300	0.89605700	-3.35857400
C	-3.59353000	2.77146300	-1.99337100
C	-4.39999800	1.76892100	-4.46092900
C	-3.67663600	3.62089300	-3.09674900
H	-3.25240300	3.14564700	-1.03297800
C	-4.07498100	3.11722700	-4.33553000
H	-4.71514600	1.36799100	-5.42796100
H	-3.39084500	4.66609200	-2.98342200
H	-4.12372200	3.77394100	-5.20779000
C	-4.96348700	-0.03361300	-0.48402000
C	-5.65567300	-1.00550400	-1.24321700
C	-5.43481400	0.32425300	0.78572000
C	-6.72776700	-1.68774300	-0.63297200
C	-6.51442700	-0.34607000	1.35865400
H	-4.90787200	1.10407000	1.33241400
C	-7.14759400	-1.37678800	0.65564300
H	-7.23038200	-2.47828800	-1.19466000
H	-6.84488200	-0.07952300	2.36540800
H	-7.96540500	-1.93790900	1.11286500
C	-4.76033800	-0.48662800	-3.54292200
H	-4.70456500	-0.85315200	-4.57337200
C	-5.32941500	-1.30884100	-2.63157000
H	-5.68829200	-2.27747800	-2.98817600
P	2.21413600	0.65194900	-0.71536700
P	-2.19673000	0.14050600	-0.35989800
Ir	-0.12180400	1.11253400	-0.65797400
C	0.43150900	1.46414500	1.46447600
H	0.26341300	0.57129800	2.06440700
H	1.43800800	1.87668000	1.53781200

C	-0.64157700	2.33328900	1.18746100
H	-1.62528500	2.01044400	1.51851200
C	-0.52137600	3.81250800	1.08956400
C	0.95131300	-0.72372300	-1.11262600
C	0.23135600	-0.23053900	-2.22153600
C	-0.11356100	-0.46187800	-3.48709200
H	0.35707800	-1.32133200	-3.98282500
C	-1.08686400	0.33164900	-4.30678400
H	-0.64448100	0.62616400	-5.27599400
H	-1.98848200	-0.26222500	-4.54076900
H	-1.39281300	1.24565500	-3.78282800
C	0.77758000	-2.06043400	-0.50755800
C	0.50734800	-3.15349900	-1.35237200
C	0.90958200	-2.31345000	0.86917700
C	0.39143200	-4.44730300	-0.84689600
H	0.38967200	-2.97593200	-2.42064300
C	0.80577300	-3.60922900	1.37358200
H	1.08134600	-1.48218100	1.54874200
C	0.54657100	-4.68607100	0.52086900
H	0.19209200	-5.27597000	-1.53106700
H	0.90641400	-3.77592600	2.44809000
H	0.45922800	-5.69825100	0.92299000
C	-1.79170500	4.51789200	0.68458400
C	-2.98575800	4.29219400	1.38576800
C	-1.77633100	5.45152000	-0.35921800
C	-4.15138000	4.97581300	1.03304600
H	-2.99369100	3.59008500	2.21997000
C	-2.94027000	6.14217700	-0.70352300
H	-0.85309500	5.60448700	-0.91864700
C	-4.13212700	5.90158600	-0.01432100
H	-5.07856900	4.78298800	1.57824100
H	-2.91821600	6.86393800	-1.52407000
H	-5.04559400	6.43223200	-0.29476400
B	-0.29883400	3.64506000	3.89662500
F	0.78881100	2.83738100	4.04722200
F	-1.49412400	2.95718300	3.83818600
F	-0.33876700	4.67956600	4.79837500
O	-0.12348900	4.39470900	2.46091800
C	-0.00510600	5.82352600	2.47027700
H	-0.98607900	6.29301600	2.62700700
H	0.67469100	6.09801100	3.28250900
H	0.40628600	6.13704300	1.50417100
H	0.31393800	4.10955600	0.44891400
Cl	-0.49415900	3.08565000	-2.15458700

[C-E]‡

Zero-point correction=	1.304712 (Hartree/Particle)
Thermal correction to Energy=	1.389554
Thermal correction to Enthalpy=	1.390498
Thermal correction to Gibbs Free Energy=	1.183777
Sum of electronic and zero-point Energies=	-5446.131837
Sum of electronic and thermal Energies=	-5446.046995
Sum of electronic and thermal Enthalpies=	-5446.046051
Sum of electronic and thermal Free Energies=	-5446.252772

C	-3.54478300	-0.28991600	2.16682100
C	-3.16629400	-0.21915600	3.52732000
C	-3.37559000	-1.30340500	4.33988400
C	-3.88043600	-2.52314600	3.80755700
C	-3.98168400	-3.69018400	4.61199400
C	-4.39533500	-4.89177800	4.07724700
C	-4.71527100	-4.97063600	2.70119800
C	-4.64197600	-3.85143300	1.89871500
C	-4.24554300	-2.59050600	2.42228300
C	-4.14883500	-1.40640100	1.60529200
C	-3.93871600	-0.93162800	-0.87055400
C	-4.68070900	-1.38663200	0.21585300
C	-6.03617200	-1.80888700	-0.05090100
C	-6.98042600	-2.03182900	0.99158600
C	-8.27942400	-2.40913300	0.71911400
C	-8.71125400	-2.59655700	-0.61532100
C	-7.83070200	-2.36776800	-1.65101600
C	-6.49477600	-1.95357900	-1.40262200
C	-5.61137800	-1.63682800	-2.46985900
C	-4.37566300	-1.11031100	-2.20668000
H	-3.10052200	-1.26427800	5.39672100
H	-3.70132800	-3.61849300	5.66644700
H	-4.45665900	-5.78405200	4.70551300
H	-5.00497900	-5.92961800	2.26434200
H	-4.85486200	-3.93725000	0.83468600
H	-6.66963700	-1.88300700	2.02441900
H	-8.98106000	-2.55946700	1.54352600
H	-9.73929900	-2.90558900	-0.82051600
H	-8.15230100	-2.48325900	-2.68984700
H	-5.95092700	-1.76741000	-3.49999200
H	-3.69858600	-0.79187500	-2.99903500
H	-2.67235500	0.69500300	3.86073900
O	-2.72359000	-0.32314100	-0.75062900

O	-3.36265000	0.83876300	1.40943500
N	-3.01642800	2.25957200	-0.65089500
C	-2.64766100	3.62000100	-0.44049900
C	-2.32366400	4.41019000	-1.56840000
C	-2.61401000	4.16235300	0.85037700
C	-1.99487300	5.76127200	-1.35669600
C	-2.27961900	5.50426200	1.03084700
H	-2.79788900	3.51280800	1.70615000
C	-1.98779600	6.30950700	-0.07612300
H	-1.72730200	6.37575200	-2.21887900
H	-2.23839700	5.91796700	2.04086000
H	-1.73050100	7.36222400	0.06394100
C	-4.25832100	2.10175100	-1.35458400
C	-4.27771700	2.34396700	-2.74578400
C	-5.42548900	1.70527000	-0.68959700
C	-5.46450500	2.06992600	-3.45270000
C	-6.59515200	1.45780900	-1.40661400
H	-5.38558700	1.55261800	0.38694600
C	-6.60858800	1.62479800	-2.79528100
H	-5.47923800	2.22845400	-4.53441600
H	-7.48607000	1.10446400	-0.88372100
H	-7.51624100	1.40821600	-3.36392700
C	-2.28719200	3.85634600	-2.92462200
H	-1.52205900	4.27743100	-3.58199200
C	-3.12905700	2.93057300	-3.43745300
H	-3.02020400	2.67811800	-4.49721800
C	2.33420900	-1.23240900	-2.23008000
C	1.79233600	-0.74649100	-3.44686700
C	1.33764700	-1.62636500	-4.39710400
C	1.36681000	-3.02742900	-4.15752000
C	0.78193700	-3.94787400	-5.06859900
C	0.76252300	-5.29963200	-4.79911800
C	1.33070200	-5.78211100	-3.59596600
C	1.92411800	-4.91570500	-2.70256700
C	1.97505400	-3.51676700	-2.95447800
C	2.54927800	-2.58834700	-2.01617900
C	3.02240300	-2.71041900	0.44359600
C	3.34256700	-3.07587800	-0.85768900
C	4.46049700	-3.96241600	-1.05101900
C	5.00233500	-4.23638500	-2.33859600
C	6.07648100	-5.08658000	-2.49793000
C	6.66738100	-5.71924600	-1.37762200
C	6.17950100	-5.46328000	-0.11431100
C	5.08554000	-4.57762100	0.08572300

C	4.60596100	-4.27266400	1.38800700
C	3.62123600	-3.33410400	1.56453500
H	0.92042000	-1.25437400	-5.33602600
H	0.32778100	-3.55640300	-5.98293300
H	0.29691500	-5.99575300	-5.50121100
H	1.28570800	-6.84899000	-3.36416100
H	2.33180600	-5.29877200	-1.76832200
H	4.56488500	-3.74842800	-3.20874000
H	6.47834600	-5.26764200	-3.49798200
H	7.51368100	-6.39682100	-1.51606000
H	6.63586100	-5.93057700	0.76279900
H	5.06439500	-4.76149800	2.25131700
H	3.26943400	-3.04273700	2.55313300
H	1.76346000	0.33194700	-3.60488600
O	2.05616000	-1.78458800	0.70028400
O	2.70700500	-0.30509200	-1.30153800
N	3.57897400	0.42922300	0.87556500
C	3.62755300	0.76977400	2.26776800
C	4.51440800	0.09738000	3.14847000
C	2.72299400	1.70337000	2.77527600
C	4.45935300	0.42118700	4.51902500
C	2.66512800	1.98321400	4.14002100
H	2.01829300	2.18533600	2.10685100
C	3.55096800	1.35331800	5.01565800
H	5.13985100	-0.09591700	5.20123700
H	1.89856600	2.67336500	4.49190100
H	3.51856800	1.56708900	6.08716700
C	4.77929200	0.57002800	0.09548700
C	5.91111800	-0.23767600	0.34822500
C	4.80943200	1.47620800	-0.97190000
C	7.00444200	-0.16180700	-0.54025300
C	5.90796100	1.55364000	-1.82520600
H	3.94101600	2.09114600	-1.18675200
C	7.01030000	0.71856800	-1.61723400
H	7.86527200	-0.81074800	-0.35815500
H	5.87860200	2.25359000	-2.66318700
H	7.86926500	0.75408000	-2.29212100
C	5.45440700	-0.93377500	2.72260700
H	5.75898500	-1.62605300	3.51467800
C	6.03212800	-1.10375600	1.51404200
H	6.75335600	-1.92043400	1.41459000
P	-2.24530500	0.96700200	0.17214300
P	2.08339100	-0.18291800	0.25170600
Ir	0.03816300	0.79468800	0.47870400

C	0.15700500	1.60859000	-1.48806000
H	0.57805700	0.93911200	-2.23158100
H	-0.78086600	2.05034000	-1.82530500
C	1.05886700	2.42210100	-0.72496700
H	2.11521600	2.18216500	-0.82214800
C	0.83691000	3.78988100	-0.30843100
C	-0.52393500	-1.07354600	1.37138000
C	-0.30809100	-1.16679100	2.66164200
C	0.03040800	-1.28192600	3.92627900
H	-0.73814600	-1.14527300	4.69727700
C	1.43544300	-1.54577200	4.40287300
H	1.74771300	-0.79623100	5.14722900
H	1.52913500	-2.54052900	4.87797700
H	2.14687800	-1.49229000	3.56901200
C	-0.86923300	-2.28923800	0.58636400
C	-1.30863500	-3.45971200	1.23519200
C	-0.75704500	-2.33042500	-0.81509000
C	-1.61862400	-4.61544700	0.51975100
H	-1.41400200	-3.44821100	2.32105800
C	-1.07284900	-3.48208300	-1.53558200
H	-0.42727900	-1.43227300	-1.33383400
C	-1.50537200	-4.63491400	-0.87415700
H	-1.96582300	-5.50143600	1.05781200
H	-0.97459100	-3.48104000	-2.62290100
H	-1.74919400	-5.53737000	-1.44102800
C	1.75958800	4.32996200	0.73468000
C	3.14719000	4.36208800	0.52567700
C	1.23847900	4.78143100	1.95451200
C	4.00037000	4.81907000	1.52881500
H	3.54884200	4.04597200	-0.43572600
C	2.09643100	5.23977000	2.95696900
H	0.16755700	4.70767700	2.13609000
C	3.47719800	5.25720000	2.74961500
H	5.07944900	4.82518800	1.35758600
H	1.68056300	5.56605500	3.91349900
H	4.14730500	5.60219100	3.54122400
B	1.78071400	4.31870300	-2.97750900
F	0.90112100	3.45534100	-3.59613900
F	2.97001900	3.68670200	-2.61934200
F	2.02381700	5.44504200	-3.73879400
O	1.09185000	4.83030800	-1.66920500
C	1.26395800	6.20759300	-1.35086300
H	2.32505400	6.45138100	-1.19129400
H	0.86803200	6.81206800	-2.17627400

H	0.70576000	6.42320200	-0.43333700
H	-0.20452800	4.04665700	-0.13430700
Cl	-0.57731400	2.12040400	2.77918800

[B-D]‡

Zero-point correction=	1.320109 (Hartree/Particle)
Thermal correction to Energy=	1.404581
Thermal correction to Enthalpy=	1.405525
Thermal correction to Gibbs Free Energy=	1.200371
Sum of electronic and zero-point Energies=	-5446.654552
Sum of electronic and thermal Energies=	-5446.570080
Sum of electronic and thermal Enthalpies=	-5446.569135
Sum of electronic and thermal Free Energies=	-5446.774290

C	3.61659700	-0.95360700	-2.06785000
C	3.17104100	-1.01164600	-3.40714700
C	3.25804100	-2.19682000	-4.09542700
C	3.70707200	-3.37954700	-3.44557100
C	3.68983900	-4.63592200	-4.11093200
C	4.03851600	-5.79446600	-3.45215100
C	4.41081100	-5.74091800	-2.08746400
C	4.45931400	-4.53577000	-1.41917300
C	4.13097900	-3.31540800	-2.07414400
C	4.16678200	-2.04036900	-1.40086700
C	4.11610800	-1.30109300	1.01634000
C	4.77435700	-1.90680900	-0.04702000
C	6.11012000	-2.39559000	0.20614600
C	6.98231100	-2.80354900	-0.84194300
C	8.26214000	-3.24641800	-0.57807700
C	8.74193800	-3.31650500	0.75099300
C	7.93150800	-2.91022500	1.78911100
C	6.61727000	-2.42735800	1.54787800
C	5.80584400	-1.94255800	2.61007200
C	4.59277600	-1.36440000	2.34629000
H	2.92846600	-2.25603300	-5.13514300
H	3.37427900	-4.66505100	-5.15695100
H	4.01249600	-6.75430800	-3.97302500
H	4.65671000	-6.66327200	-1.55619500
H	4.73954500	-4.51368800	-0.36694100
H	6.63623300	-2.74762100	-1.87297100
H	8.91211400	-3.54050800	-1.40550900
H	9.75373900	-3.67778000	0.94846800

H	8.29374700	-2.93724600	2.82005500
H	6.18381700	-1.99051200	3.63356600
H	3.97377900	-0.92457200	3.12749500
H	2.74288100	-0.10717900	-3.83840200
O	2.92641700	-0.63172900	0.86445600
O	3.54864700	0.26847500	-1.43300200
N	3.32834800	1.91061500	0.48042700
C	3.07875400	3.26248900	0.09041800
C	2.79343200	4.19853100	1.10925800
C	3.15855200	3.64940600	-1.25260100
C	2.59135900	5.53797100	0.72984400
C	2.95715700	4.98504800	-1.59869200
H	3.35224400	2.89300900	-2.01280500
C	2.68503800	5.93136400	-0.60271000
H	2.34886100	6.26979800	1.50237400
H	3.01459000	5.28820000	-2.64640000
H	2.53290700	6.97911900	-0.87128300
C	4.55985100	1.75962400	1.21702600
C	4.56925900	2.16136200	2.56887700
C	5.71026200	1.24128200	0.61283300
C	5.73417900	1.91478900	3.32129900
C	6.86106400	1.03109200	1.37090400
H	5.67811400	0.97325000	-0.44170700
C	6.86402900	1.35151600	2.73291000
H	5.74840600	2.19809700	4.37668900
H	7.74502800	0.59274400	0.90409300
H	7.75698900	1.16898000	3.33509000
C	2.68262900	3.80950800	2.51795200
H	1.94048900	4.36046400	3.10058400
C	3.44697500	2.89411700	3.15796800
H	3.30204100	2.77816000	4.23651800
C	-3.27606500	0.13232200	1.81503100
C	-2.97110600	1.09990500	2.80168000
C	-3.05832500	0.76314300	4.13020400
C	-3.41251900	-0.55488400	4.52479100
C	-3.39986200	-0.94379100	5.89229200
C	-3.67965200	-2.24101000	6.26333700
C	-3.97854600	-3.20477900	5.27081000
C	-4.02091000	-2.85277600	3.93818400
C	-3.75706500	-1.51873400	3.51943600
C	-3.76080400	-1.12786600	2.13123500
C	-3.40482100	-2.42942100	0.02618200
C	-4.22530400	-2.07620700	1.08755200
C	-5.52032300	-2.69594700	1.16430300

C	-6.52713100	-2.23670500	2.05776700
C	-7.77419600	-2.82361700	2.08620400
C	-8.07751100	-3.91448300	1.23503100
C	-7.12525800	-4.38348600	0.35670100
C	-5.83766000	-3.78455100	0.28538900
C	-4.86229800	-4.22740900	-0.64768400
C	-3.68213900	-3.54099600	-0.80080500
H	-2.82115100	1.50831800	4.89260800
H	-3.14608900	-0.19163700	6.64343600
H	-3.65775200	-2.53082900	7.31638700
H	-4.16976000	-4.24037600	5.56130800
H	-4.23631500	-3.61258500	3.18876200
H	-6.30874100	-1.39125800	2.70960400
H	-8.53699600	-2.44085500	2.76824800
H	-9.06711400	-4.37571300	1.27275800
H	-7.35013400	-5.21784600	-0.31286600
H	-5.08466300	-5.09085700	-1.27935100
H	-2.94400700	-3.81734000	-1.55252800
H	-2.68176700	2.10573700	2.50192900
O	-2.23941700	-1.74535100	-0.22176400
O	-3.13454600	0.52314600	0.49968100
N	-3.16068600	0.15171500	-1.95207400
C	-2.72282300	0.38198200	-3.30527100
C	-2.89558000	-0.62528700	-4.28384100
C	-2.15925400	1.60682300	-3.64921300
C	-2.39219700	-0.38446100	-5.57654700
C	-1.70156900	1.83822700	-4.94600500
H	-2.05335200	2.36340400	-2.88110400
C	-1.80214100	0.83291700	-5.90818200
H	-2.49790700	-1.16639400	-6.33268700
H	-1.23417800	2.79419400	-5.18320800
H	-1.42599300	0.99846300	-6.92050500
C	-4.59369600	0.04679600	-1.79531700
C	-5.27737000	-1.08083500	-2.30286000
C	-5.29005000	1.03952000	-1.09729100
C	-6.63509300	-1.24009200	-1.95696900
C	-6.64059200	0.87472300	-0.79483500
H	-4.74451800	1.91707500	-0.75564600
C	-7.30812800	-0.28598300	-1.20175100
H	-7.15993000	-2.13405100	-2.30043700
H	-7.16452900	1.64130400	-0.21981300
H	-8.35541500	-0.44221400	-0.93512100
C	-3.62855300	-1.86256300	-4.04600000
H	-3.38530100	-2.68461000	-4.72652200

C	-4.66171200	-2.05670900	-3.19379500
H	-5.17673800	-3.01831700	-3.24772800
P	2.52263300	0.57427500	-0.16557400
P	-2.12557100	-0.14320000	-0.63736800
Ir	0.20324700	0.42523300	-0.45171700
C	0.05989500	1.58204000	1.40060400
H	-0.47715800	1.04755900	2.17998500
H	1.04454400	1.92805900	1.71537300
C	-0.69387400	2.35541100	0.48362700
H	-1.76961100	2.21899000	0.51582000
C	-0.30423800	3.57584200	-0.16882400
C	0.39239700	-1.47702800	0.51032400
C	0.54194300	-1.66901600	-0.74607800
C	0.59545200	-2.66533900	-1.83746100
H	1.64063900	-2.84129300	-2.11783600
H	0.23251000	-3.62082700	-1.41713200
C	-0.21233100	-2.28061300	-3.07439400
H	0.09391900	-1.29418000	-3.45038800
H	-0.07753000	-3.02279600	-3.87667400
H	-1.28294900	-2.22717200	-2.83711900
C	0.45415700	-2.07272100	1.82238000
C	1.34692000	-3.14754300	2.02492600
C	-0.34568300	-1.65123200	2.89792000
C	1.42317600	-3.78254000	3.26270600
H	1.98439700	-3.46699900	1.19844200
C	-0.27311100	-2.29444000	4.13373700
H	-1.04093200	-0.82891300	2.75691300
C	0.61207200	-3.35957300	4.32222100
H	2.12242100	-4.61072800	3.40343800
H	-0.91959200	-1.96507900	4.94915900
H	0.66972900	-3.85926400	5.29227500
C	-1.18251400	4.09978100	-1.23424900
C	-2.57875200	4.15119200	-1.06574700
C	-0.61653600	4.56833200	-2.42978000
C	-3.38864800	4.65542100	-2.08121100
H	-3.01463000	3.83717300	-0.11717900
C	-1.43222100	5.06953300	-3.44576700
H	0.46300700	4.51008800	-2.56288000
C	-2.81813800	5.11237300	-3.27511100
H	-4.47130000	4.69396500	-1.94236700
H	-0.98363700	5.42359000	-4.37677700
H	-3.45622300	5.50105400	-4.07209000
B	-1.18963800	4.65720800	2.43167500
F	-0.46785900	3.71854700	3.14617900

F	-2.45060200	4.15676700	2.06938200
F	-1.30684200	5.84895700	3.11152800
O	-0.41380700	4.94390000	1.13174700
C	-0.60661900	6.23847900	0.58127500
H	-1.66402400	6.42212400	0.33459800
H	-0.27252200	6.98551800	1.31341500
H	-0.00614700	6.32815500	-0.33150800
H	0.75682500	3.73565400	-0.32648200
Cl	0.73924100	1.40251900	-2.71180100

[B-D]‡-R

Zero-point correction=	1.319236 (Hartree/Particle)
Thermal correction to Energy=	1.404091
Thermal correction to Enthalpy=	1.405035
Thermal correction to Gibbs Free Energy=	1.196419
Sum of electronic and zero-point Energies=	-5446.658760
Sum of electronic and thermal Energies=	-5446.573905
Sum of electronic and thermal Enthalpies=	-5446.572961
Sum of electronic and thermal Free Energies=	-5446.781577

C	3.67286300	-0.91327000	-2.08952000
C	3.26152300	-0.98706100	-3.43859000
C	3.35931300	-2.18291300	-4.10706200
C	3.77139500	-3.36059200	-3.42347100
C	3.75421500	-4.62870100	-4.06607800
C	4.06421200	-5.77997500	-3.37569700
C	4.39741300	-5.70717700	-2.00181200
C	4.44671200	-4.49057300	-1.35457600
C	4.15545800	-3.27864000	-2.04132300
C	4.19810700	-1.99225300	-1.39163300
C	4.16020900	-1.19870600	1.01293000
C	4.80617200	-1.83615500	-0.03915600
C	6.13598000	-2.33849700	0.22208600
C	6.99871300	-2.78758300	-0.81724200
C	8.27072200	-3.24721200	-0.54496200
C	8.75280100	-3.29319100	0.78429900
C	7.95294000	-2.84604000	1.81354200
C	6.64660800	-2.34592400	1.56329600
C	5.84617900	-1.82410000	2.61600400
C	4.64019400	-1.23601100	2.34190100
H	3.06018100	-2.25550300	-5.15504600
H	3.46906500	-4.67303800	-5.12023900
H	4.03754200	-6.74886800	-3.87941700
H	4.61256600	-6.62337400	-1.44714400

H	4.69903400	-4.45147300	-0.29557600
H	6.65242400	-2.75083000	-1.84891600
H	8.91302300	-3.57345800	-1.36629000
H	9.75822000	-3.66822400	0.98848200
H	8.31704300	-2.85439400	2.84412200
H	6.22638000	-1.85369400	3.63936900
H	4.03064600	-0.76850400	3.11459800
H	2.85453700	-0.08515500	-3.89553000
O	2.97663100	-0.51913100	0.85062900
O	3.60154600	0.32051000	-1.47723100
N	3.32965000	2.02607700	0.37735100
C	3.06821700	3.35575800	-0.08464600
C	2.73098000	4.33464700	0.87982700
C	3.14861000	3.67627300	-1.44327400
C	2.47233800	5.64066500	0.42470600
C	2.89128900	4.98174600	-1.86470300
H	3.38241800	2.89054000	-2.16082500
C	2.56011400	5.96607400	-0.92786800
H	2.19741500	6.40451100	1.15477900
H	2.93928900	5.22513500	-2.92822500
H	2.35441700	6.98751600	-1.25514700
C	4.53398200	1.92281400	1.16322300
C	4.48981800	2.38112800	2.49623000
C	5.70752800	1.38424300	0.62543100
C	5.62593100	2.17168000	3.30220700
C	6.83009300	1.21334900	1.43442700
H	5.71570400	1.07021600	-0.41707000
C	6.77978500	1.59045100	2.78079300
H	5.59920800	2.49864000	4.34463900
H	7.73301100	0.76105000	1.02006100
H	7.64979600	1.43881500	3.42373600
C	2.59400600	4.01066900	2.30297100
H	1.83715500	4.58563500	2.84387200
C	3.34391800	3.13350800	3.01020300
H	3.16480800	3.07041700	4.08790100
C	-3.25711800	-0.10509700	1.83661800
C	-3.04293600	0.72957000	2.95602900
C	-3.13472900	0.21831600	4.22567100
C	-3.41482100	-1.15859500	4.42980700
C	-3.39552500	-1.73267100	5.73019000
C	-3.60676800	-3.08196900	5.91274300
C	-3.84321900	-3.91147800	4.79076600
C	-3.89277500	-3.37920900	3.51948900
C	-3.69525900	-1.98805400	3.29367700

C	-3.70123700	-1.41297600	1.96905600
C	-3.30396500	-2.42854000	-0.27650400
C	-4.13563800	-2.23639500	0.81431300
C	-5.40813700	-2.90512100	0.80979800
C	-6.43131300	-2.59279200	1.74672400
C	-7.65685500	-3.22195700	1.69677000
C	-7.91985400	-4.21232000	0.71862000
C	-6.95004700	-4.53903000	-0.20385900
C	-5.68436200	-3.89100900	-0.19515200
C	-4.69149500	-4.18491100	-1.16790400
C	-3.53678500	-3.44279000	-1.23201700
H	-2.95520100	0.87208600	5.08150800
H	-3.19200300	-1.07941900	6.58240100
H	-3.57952200	-3.51466300	6.91548900
H	-3.98029600	-4.98625100	4.93066200
H	-4.05938100	-4.03815900	2.66893500
H	-6.24348800	-1.82491700	2.49666700
H	-8.43392000	-2.95121400	2.41539700
H	-8.89256200	-4.70908400	0.69473800
H	-7.14404900	-5.29449700	-0.96983700
H	-4.88112400	-4.97466900	-1.89888900
H	-2.78811000	-3.60105100	-2.00691000
H	-2.81890300	1.78015100	2.80685000
O	-2.16602600	-1.67684700	-0.42506200
O	-3.05592200	0.48605600	0.60423600
N	-3.14516400	0.39937500	-1.88257100
C	-2.74987600	0.81021200	-3.20649100
C	-2.87443600	-0.08517100	-4.29325900
C	-2.28373200	2.10469700	-3.41664100
C	-2.39445600	0.32955800	-5.55098600
C	-1.85628200	2.51143500	-4.67899700
H	-2.23035400	2.77765000	-2.56979500
C	-1.88787800	1.61141600	-5.74536600
H	-2.45835600	-0.36771600	-6.39010400
H	-1.46576900	3.52069900	-4.81203500
H	-1.52931500	1.91227100	-6.73254300
C	-4.56948200	0.21617700	-1.71915100
C	-5.22227100	-0.85629700	-2.36952600
C	-5.28858700	1.07590500	-0.88141400
C	-6.56892300	-1.10815900	-2.03529600
C	-6.62750600	0.82203900	-0.58897300
H	-4.76991400	1.91876400	-0.42840000
C	-7.26221900	-0.29273300	-1.14775700
H	-7.06844400	-1.96464800	-2.49282200

H	-7.16712000	1.48207100	0.09357300
H	-8.29915300	-0.52212700	-0.89414400
C	-3.56182300	-1.36672100	-4.20415800
H	-3.29909800	-2.09205500	-4.98044800
C	-4.58702600	-1.69060300	-3.38227800
H	-5.07675100	-2.65118900	-3.55534400
P	2.56626400	0.64176100	-0.22396300
P	-2.07781400	-0.03469000	-0.63044700
Ir	0.23312500	0.46504800	-0.47083200
C	0.10824500	1.33087300	1.50082000
H	-0.77168900	1.05912000	2.07851300
H	1.03773900	1.17864700	2.05355300
C	0.00212600	2.43625100	0.59835700
H	0.88943100	3.00429700	0.35116000
C	-1.21374900	3.20636300	0.50214300
C	0.48344500	-1.52078500	0.31424100
C	0.56036300	-1.62564600	-0.95379800
C	0.54041800	-2.55663300	-2.10350800
H	1.57257600	-2.78987500	-2.39112000
H	0.11267600	-3.50622400	-1.73312900
C	-0.23492500	-2.05985800	-3.32000100
H	0.14231400	-1.08463600	-3.65649300
H	-0.16007400	-2.78054100	-4.14966500
H	-1.29724800	-1.93159600	-3.07628900
C	0.57670100	-2.18091400	1.59250000
C	1.47977200	-3.25881900	1.71710200
C	-0.20728100	-1.82504200	2.70311500
C	1.58097300	-3.96283200	2.91514700
H	2.10299500	-3.52740300	0.86201500
C	-0.11070900	-2.53991300	3.89716600
H	-0.90676100	-0.99809700	2.62300800
C	0.78386700	-3.60799200	4.00954900
H	2.28727100	-4.79297700	2.99670300
H	-0.74746300	-2.26449400	4.73982700
H	0.85933600	-4.16315400	4.94766300
C	-1.52981700	4.06844900	-0.63865300
C	-0.56890500	4.40911900	-1.60443500
C	-2.83301800	4.59116400	-0.74238900
C	-0.90549400	5.26889800	-2.64826600
H	0.42610900	3.97579400	-1.56117300
C	-3.17021500	5.43581000	-1.79750200
H	-3.56436000	4.33750700	0.02870300
C	-2.20300900	5.78049100	-2.74953000
H	-0.15140800	5.52558100	-3.39540200

H	-4.18512500	5.83066800	-1.87886800
H	-2.46604800	6.44403000	-3.57686400
B	-1.75930700	4.19320800	3.11525800
F	-1.22476000	3.04235400	3.66963900
F	-3.07308200	3.97131700	2.67245200
F	-1.68393900	5.27419900	3.96121100
O	-0.91997600	4.49985400	1.86831900
C	-0.87669900	5.85994800	1.47325100
H	-1.88165200	6.26200500	1.26751500
H	-0.42056100	6.43989000	2.28785300
H	-0.26148600	5.95195100	0.57046500
H	-2.09393700	2.77298100	0.97458000
Cl	0.69538300	1.43250700	-2.73940600

D

Zero-point correction=	1.318160 (Hartree/Particle)
Thermal correction to Energy=	1.403875
Thermal correction to Enthalpy=	1.404819
Thermal correction to Gibbs Free Energy=	1.195834
Sum of electronic and zero-point Energies=	-5446.646051
Sum of electronic and thermal Energies=	-5446.560336
Sum of electronic and thermal Enthalpies=	-5446.559392
Sum of electronic and thermal Free Energies=	-5446.768378

C	3.41445300	-1.76455600	-1.51186300
C	2.75989800	-2.62408700	-2.42422400
C	2.92404000	-3.98178700	-2.32965500
C	3.71781700	-4.54303800	-1.29359000
C	3.81555700	-5.94870500	-1.11959600
C	4.54733200	-6.48631500	-0.08329700
C	5.20122600	-5.62730400	0.83051600
C	5.13811700	-4.25739600	0.67727200
C	4.41213200	-3.66922400	-0.39476900
C	4.31666300	-2.24022100	-0.56929100
C	4.64746600	-0.26553200	0.94270500
C	5.17675300	-1.32481000	0.22556800
C	6.61092900	-1.48344800	0.24324300
C	7.29046700	-2.38221600	-0.62522800
C	8.66569400	-2.49210100	-0.60579800
C	9.43906100	-1.71667900	0.29017100

C	8.81445700	-0.82189300	1.13173600
C	7.40220900	-0.66851000	1.11890600
C	6.76434300	0.31234600	1.92640500
C	5.41493800	0.53000900	1.82150300
H	2.41746000	-4.64819000	-3.03068400
H	3.28090100	-6.59701600	-1.81781300
H	4.61071300	-7.56928100	0.04440200
H	5.75936900	-6.05119500	1.66863800
H	5.64028500	-3.61151000	1.39635200
H	6.71353500	-2.98031400	-1.32892300
H	9.16160100	-3.18119700	-1.29327600
H	10.52649500	-1.81894100	0.30189700
H	9.39931700	-0.19853500	1.81277400
H	7.37111800	0.92660800	2.59467500
H	4.91254900	1.32031400	2.37863700
H	2.12731100	-2.17940500	-3.18822700
O	3.30078000	0.04692100	0.85042600
O	3.17613000	-0.40909700	-1.65219700
N	3.21178500	2.04775700	-0.90990600
C	2.48639600	3.07386900	-1.61975400
C	2.19752300	4.28648400	-0.95998100
C	2.07409500	2.85432700	-2.93179000
C	1.31424900	5.17982700	-1.59541000
C	1.24336700	3.78177400	-3.56253100
H	2.36927700	1.93055700	-3.42805400
C	0.82302700	4.92128700	-2.87206600
H	0.98539300	6.07875500	-1.07333400
H	0.87543200	3.58337100	-4.57136200
H	0.09550800	5.60517200	-3.30748000
C	4.61552000	2.31756600	-0.74121800
C	4.98965000	3.36162100	0.13503400
C	5.58116800	1.56426900	-1.41902100
C	6.36854400	3.56234000	0.35536700
C	6.93596600	1.78788500	-1.18486000
H	5.25445000	0.78303800	-2.10313700
C	7.32842100	2.78694100	-0.28645600
H	6.67626500	4.35613200	1.04061400
H	7.68317200	1.17201000	-1.68883400
H	8.38914200	2.96067200	-0.09165100
C	2.82284500	4.65700200	0.30217400
H	2.30953700	5.43961300	0.86342900
C	4.02626400	4.25076300	0.77899600
H	4.38415800	4.74130300	1.68973600
C	-2.57419300	-2.46684500	1.46231900

C	-1.85806900	-3.14258400	2.48021900
C	-1.85365200	-4.51195500	2.53465400
C	-2.50285800	-5.27047400	1.52552700
C	-2.42186700	-6.68850800	1.50776300
C	-2.96595600	-7.41777300	0.47367400
C	-3.60692200	-6.74401600	-0.59364400
C	-3.73100600	-5.37008800	-0.58543500
C	-3.20828100	-4.58658600	0.48219000
C	-3.33496600	-3.14718000	0.51780400
C	-3.87561400	-1.42149300	-1.24015300
C	-4.26791700	-2.47133800	-0.42662000
C	-5.63734500	-2.91162000	-0.55181600
C	-6.23964100	-3.79640900	0.38451800
C	-7.56128000	-4.17288100	0.26324900
C	-8.35140500	-3.69653300	-0.80977400
C	-7.80349900	-2.82610400	-1.72693300
C	-6.45229600	-2.39927200	-1.61584800
C	-5.90867500	-1.44255600	-2.51695100
C	-4.65205500	-0.93429500	-2.31252700
H	-1.31539600	-5.03162200	3.32958900
H	-1.89095300	-7.18784700	2.32200400
H	-2.88965800	-8.50741600	0.46458200
H	-4.00900400	-7.31651900	-1.43272800
H	-4.22715100	-4.87188000	-1.41700200
H	-5.65018900	-4.16250400	1.22396000
H	-8.00307800	-4.84006500	1.00697200
H	-9.39455200	-4.00779700	-0.89940000
H	-8.40699500	-2.43187000	-2.54829900
H	-6.52774300	-1.06612500	-3.33333800
H	-4.24710100	-0.12740400	-2.92272600
H	-1.34045600	-2.54214900	3.22813300
O	-2.64443000	-0.81079800	-1.05388300
O	-2.52980900	-1.09479500	1.52159200
N	-3.33345800	1.14504100	0.59755200
C	-4.43707400	1.47630400	-0.26740300
C	-5.69779200	0.90699900	0.03251700
C	-4.26253800	2.37770400	-1.31631500
C	-6.77445000	1.24124600	-0.81096700
C	-5.35708400	2.71074900	-2.11673100
H	-3.29082100	2.83630000	-1.49080400
C	-6.60892900	2.13546300	-1.86751900
H	-7.75289400	0.79558300	-0.61563400
H	-5.21972800	3.44278800	-2.91497900
H	-7.46540300	2.39695400	-2.49396900

C	-3.48498500	1.65549000	1.93601900
C	-4.34594600	0.98520000	2.83197200
C	-2.80394200	2.81013200	2.31148000
C	-4.34003400	1.41060200	4.17505300
C	-2.83976400	3.23871900	3.63868300
H	-2.27962600	3.36499100	1.53838800
C	-3.58184100	2.51095800	4.57736900
H	-4.97549700	0.89031500	4.89640600
H	-2.28492500	4.13328200	3.92925500
H	-3.60066600	2.82628200	5.62349000
C	-5.92174800	-0.00540600	1.15594300
H	-6.74125300	-0.71604200	1.01444500
C	-5.31325000	-0.00479600	2.36765400
H	-5.67885800	-0.71388800	3.11680800
P	2.50286800	0.58835900	-0.49488900
P	-2.18319500	-0.03329600	0.29642800
Ir	0.16161100	0.32824200	0.01382900
C	0.54319300	-0.29535300	2.03093500
H	-0.11199300	-1.08994800	2.38299500
H	1.60401200	-0.49188300	2.18200000
C	0.10251100	1.06552200	2.25741600
H	-0.91336900	1.27421100	2.59920200
C	0.94258500	2.12441300	1.97974200
H	2.00333600	1.89285900	1.82941100
O	-2.99803500	4.91492200	-0.15534000
C	0.37111900	-1.72596500	-0.54149400
C	0.03947500	-1.06846100	-1.58443200
C	-0.36323300	-1.02046800	-3.00455200
H	-0.30201700	-2.06100400	-3.37256200
H	-1.42638300	-0.74067200	-3.03561800
C	0.42691800	-0.07242800	-3.90766600
H	1.50785600	-0.26840600	-3.86779000
H	0.09220200	-0.18714200	-4.94952400
H	0.25282500	0.96402800	-3.59684500
C	0.62712900	-3.02316900	0.04036000
C	-0.00894900	-4.13715100	-0.54529200
C	1.52485500	-3.23289500	1.09919500
C	0.25932300	-5.42363000	-0.08916900
H	-0.72270800	-3.97786300	-1.35447900
C	1.77776800	-4.52332100	1.56247200
H	2.05115700	-2.38652200	1.53273700
C	1.15147100	-5.62096300	0.96911800
H	-0.24969200	-6.27402900	-0.54599800
H	2.49115600	-4.67356900	2.37452200

H	1.36107700	-6.63070200	1.32785500
C	0.63256300	3.55661900	2.15524700
C	-0.19323000	4.28445900	1.29126600
C	1.25482800	4.21310000	3.23577200
C	-0.41096900	5.64856400	1.50908300
H	-0.63808000	3.81449200	0.41552700
C	1.01549300	5.56611200	3.46701000
H	1.92167000	3.65451800	3.89788700
C	0.18354500	6.28655300	2.59912200
H	-1.03144000	6.18582200	0.79064400
H	1.48753600	6.06298000	4.31826100
H	0.00949800	7.35200600	2.76847600
C	-3.86839200	5.65393900	0.64490700
H	-4.78302200	5.95138100	0.09999000
H	-4.17138700	5.04786700	1.51732600
H	-3.40433200	6.58512300	1.03611000
B	-2.62729700	5.49860500	-1.44085000
F	-1.60962500	6.48296900	-1.26013300
F	-2.11050000	4.46966600	-2.25514300
F	-3.72898400	6.08726800	-2.07371600
Cl	-0.68795800	2.08768400	-1.39023300

D1

Zero-point correction=	1.588825 (Hartree/Particle)
Thermal correction to Energy=	1.688448
Thermal correction to Enthalpy=	1.689392
Thermal correction to Gibbs Free Energy=	1.449037
Sum of electronic and zero-point Energies=	-5855.326062
Sum of electronic and thermal Energies=	-5855.226439
Sum of electronic and thermal Enthalpies=	-5855.225495
Sum of electronic and thermal Free Energies=	-5855.465850

C	-3.06741200	2.10473800	-1.30195800
C	-2.23325800	3.17107800	-1.71101500
C	-2.38436100	4.41364900	-1.15023600
C	-3.31965700	4.62531800	-0.10451800
C	-3.38514300	5.87172300	0.57596700
C	-4.25490000	6.06048700	1.62724500
C	-5.10003400	5.00010900	2.03400200
C	-5.06982800	3.78493300	1.38229600
C	-4.18210900	3.55168300	0.29368400
C	-4.10324600	2.27980700	-0.38784300

C	-4.73314500	-0.07383100	0.22843400
C	-5.10562800	1.21762400	-0.10602100
C	-6.52000700	1.49380700	-0.17318900
C	-7.03845400	2.69033200	-0.74156800
C	-8.39732800	2.92133400	-0.80686800
C	-9.31485500	1.97228800	-0.29740500
C	-8.84692800	0.79224800	0.23978700
C	-7.45526800	0.51360500	0.29715300
C	-6.97576400	-0.73702700	0.77398300
C	-5.64227700	-1.04155900	0.70520000
H	-1.75226200	5.24147300	-1.46733100
H	-2.71547100	6.67341800	0.25520400
H	-4.29085500	7.01877300	2.15015800
H	-5.78200700	5.14271600	2.87546200
H	-5.72590600	2.98333700	1.71193900
H	-6.34770700	3.42958500	-1.14540600
H	-8.76701400	3.84415300	-1.25994300
H	-10.38800500	2.17066300	-0.34420900
H	-9.54345200	0.03863200	0.61596000
H	-7.68884500	-1.47053800	1.15490400
H	-5.24744500	-2.00870900	1.01166400
H	-1.47138100	2.97228300	-2.46225100
O	-3.41311500	-0.47447700	0.16379900
O	-2.85748600	0.88728200	-1.91718800
N	-3.12553300	-1.63632000	-2.19461000
C	-2.36294900	-2.26888100	-3.22527600
C	-2.28767600	-3.67827800	-3.25132700
C	-1.73891200	-1.49457500	-4.20834100
C	-1.53893200	-4.27330800	-4.28292200
C	-1.01709900	-2.10891500	-5.23318000
H	-1.84723800	-0.40943400	-4.16769500
C	-0.92707200	-3.50388700	-5.27154500
H	-1.45534600	-5.36215800	-4.31090400
H	-0.53288500	-1.50098600	-6.00056400
H	-0.37843500	-3.99615100	-6.07747700
C	-4.54581500	-1.85401700	-2.28189500
C	-5.04770400	-3.13088000	-1.94977700
C	-5.40772600	-0.82250600	-2.66974900
C	-6.44613900	-3.30078600	-1.92732700
C	-6.78739100	-1.01947100	-2.65219600
H	-4.98513600	0.14241100	-2.94456100
C	-7.30623400	-2.25980300	-2.26576700
H	-6.85092200	-4.27708200	-1.64957000
H	-7.45603500	-0.19783000	-2.91525200

H	-8.38710200	-2.41352000	-2.23278600
C	-2.97559900	-4.51784400	-2.27066700
H	-2.49784400	-5.47903100	-2.06105400
C	-4.17337200	-4.27452200	-1.69241200
H	-4.59227800	-5.05898800	-1.05488200
C	3.05382500	-0.22661400	2.18818400
C	2.39672900	0.08837400	3.40162400
C	2.78742600	1.20275100	4.10184400
C	3.80400800	2.06065900	3.59997500
C	4.13890500	3.27267400	4.26208100
C	5.07213000	4.13900800	3.73365700
C	5.71150200	3.81928900	2.51186000
C	5.43263900	2.63347300	1.86291000
C	4.48444900	1.71082400	2.38627300
C	4.14970900	0.48120000	1.71217000
C	4.40002200	-0.31550800	-0.65985100
C	4.96792100	-0.00223700	0.56438700
C	6.39835200	-0.14246100	0.68219000
C	7.06970200	-0.05656000	1.93319400
C	8.43872900	-0.19952000	2.01836300
C	9.21396700	-0.42695900	0.85608400
C	8.59396000	-0.53457600	-0.36967700
C	7.18255400	-0.41387400	-0.48892000
C	6.53134900	-0.58566700	-1.74034900
C	5.16140100	-0.57679000	-1.81818700
H	2.30016800	1.45119900	5.04725800
H	3.62029100	3.51494000	5.19297700
H	5.31105400	5.07350800	4.24632200
H	6.43073900	4.51627400	2.07553600
H	5.93266800	2.40568200	0.92288400
H	6.48583400	0.10575100	2.83815400
H	8.92778100	-0.14363600	2.99353000
H	10.29845500	-0.53059000	0.93619500
H	9.17813800	-0.73092400	-1.27238600
H	7.13342100	-0.77470100	-2.63200700
H	4.63532400	-0.76868100	-2.75256300
H	1.62493500	-0.59376300	3.76406700
O	3.01957700	-0.32836100	-0.80734300
O	2.60294400	-1.34646100	1.52722900
N	2.74962500	-2.95992300	-0.34146200
C	3.03133700	-3.33181600	-1.69339100
C	4.37040200	-3.60031600	-2.07516400
C	2.01033300	-3.32318800	-2.65148600
C	4.63316500	-3.81070000	-3.44320000

C	2.30689600	-3.51859700	-4.00239100
H	0.98119500	-3.16928400	-2.32599700
C	3.62338300	-3.76043100	-4.40031500
H	5.66450000	-4.00525400	-3.74829500
H	1.50185200	-3.48608100	-4.73383000
H	3.86149800	-3.91555400	-5.45528000
C	3.02964400	-3.86277400	0.75546400
C	4.36772200	-4.20973900	1.04623500
C	1.99180500	-4.25258500	1.60185400
C	4.61586000	-4.93784700	2.22655200
C	2.26415100	-4.95727800	2.77721800
H	0.96324900	-3.95327000	1.40155900
C	3.58169100	-5.30363600	3.08529300
H	5.64854000	-5.20600900	2.46502500
H	1.44598700	-5.17375200	3.46591900
H	3.80475500	-5.84319200	4.00869600
C	5.49460100	-3.63209300	-1.14489700
H	6.47186200	-3.50261700	-1.61708700
C	5.49293200	-3.87493000	0.18477700
H	6.47198600	-3.91780700	0.67209000
P	-2.43202200	-0.53137700	-1.13296600
P	2.08433100	-1.43983100	-0.02051900
Ir	-0.16494800	-0.91524600	-0.49920300
C	-0.32328300	-0.66197500	1.74753900
H	0.29262500	-1.52861600	1.98977200
H	0.14687500	0.30347100	1.93814400
C	-1.64821600	-0.82922300	2.25408100
H	-2.03122300	-1.84899400	2.23320200
C	-2.36737900	0.17168500	2.82978800
H	-1.96335200	1.18800600	2.81752000
O	-0.85839500	-3.72810100	2.83053600
C	0.31182000	1.27574000	-0.58183900
C	0.51710100	0.72030400	-1.69063200
C	0.64911200	1.78148100	-3.97273000
H	-0.43885200	1.91822100	-4.06875200
H	1.09164600	2.70605600	-3.57089200
H	1.05820000	1.62425400	-4.98285800
C	0.43243100	2.29131800	0.43339300
C	1.70819500	2.80539200	0.73303900
C	-0.68350600	2.78559300	1.13112500
C	1.85683300	3.81293400	1.68463200
H	2.57953200	2.39570700	0.22564700
C	-0.53140200	3.79605500	2.07833000
H	-1.66807600	2.37527600	0.91966000

C	0.73814200	4.31440300	2.35551400
H	2.85118300	4.19876400	1.90877700
H	-1.41177500	4.18322200	2.59604600
H	0.85823100	5.10310700	3.10152600
C	-3.68357400	0.00116500	3.41796100
C	-4.16122900	-1.26209300	3.83180000
C	-4.53207700	1.12064900	3.52991900
C	-5.47176500	-1.39502800	4.28346300
H	-3.47446100	-2.10967500	3.85435300
C	-5.84877600	0.97645200	3.95985400
H	-4.15350900	2.10302800	3.24193500
C	-6.32569200	-0.28606700	4.32950300
H	-5.82937500	-2.37331700	4.61339500
H	-6.50567500	1.84824600	4.01318400
H	-7.35640600	-0.40113400	4.67384800
C	-1.81093600	-4.73290700	2.68730100
H	-1.59785900	-5.60461000	3.33559800
H	-2.83820200	-4.38588900	2.93461700
H	-1.82515400	-5.07493700	1.63744600
B	-0.52226000	-3.31445100	4.18199100
F	-0.04534500	-4.39496300	4.94101600
F	0.49090600	-2.32387300	4.06771000
F	-1.64850200	-2.75241300	4.82467300
C	4.87478300	4.64092500	-1.26722600
C	4.10468400	4.09790800	-2.49300400
C	2.27051500	5.82338100	-2.05450300
C	3.08451900	6.35515000	-0.85067400
C	4.58870700	6.11916700	-1.00031900
H	4.56910200	4.05850400	-0.38198900
H	5.95663600	4.46726800	-1.39666600
H	2.86960400	7.42656600	-0.69997500
H	2.73517600	5.83300400	0.05504400
H	4.99583200	6.74060800	-1.81567600
H	5.11013200	6.44157300	-0.08399300
N	2.66822400	4.44327100	-2.41290500
H	2.25303000	3.82763800	-1.71503500
C	0.78968000	5.74264300	-1.67053900
H	0.19730100	5.39601900	-2.53126000
H	0.63370700	5.04107400	-0.83663300
H	0.41151700	6.72834500	-1.35826200
C	2.39809300	6.76950400	-3.26038700
H	1.94962800	6.30562400	-4.15105100
H	1.87261100	7.71467700	-3.05251700
H	3.43869900	7.02279900	-3.49778600

C	4.73132300	4.60610700	-3.80249600
H	5.71594800	4.13608500	-3.95145600
H	4.08518600	4.34530300	-4.65336200
H	4.88519000	5.69204900	-3.81350700
C	4.18336100	2.56904200	-2.50193800
H	3.71202900	2.15802300	-3.40735300
H	5.22830600	2.23016000	-2.47159100
H	3.67151400	2.13763200	-1.62973400
Cl	-0.76139600	-3.18852100	-0.32639800
C	0.97456000	0.57303600	-3.08789700
H	0.55228600	-0.34684000	-3.51896400
H	2.06299500	0.40678200	-3.04187700

[D-E]‡

Zero-point correction=	1.584409 (Hartree/Particle)
Thermal correction to Energy=	1.683138
Thermal correction to Enthalpy=	1.684082
Thermal correction to Gibbs Free Energy=	1.445611
Sum of electronic and zero-point Energies=	-5855.296262
Sum of electronic and thermal Energies=	-5855.197533
Sum of electronic and thermal Enthalpies=	-5855.196589
Sum of electronic and thermal Free Energies=	-5855.435060

C	-3.63696900	1.79206400	-0.04113300
C	-3.08814200	3.03004100	0.36547500
C	-3.74662800	3.80784100	1.28409900
C	-4.96915900	3.36601100	1.85683300
C	-5.63486700	4.13562100	2.84880600
C	-6.81017500	3.69544600	3.41666900
C	-7.35114300	2.44946200	3.02474300
C	-6.72865600	1.68016300	2.06594900
C	-5.53465800	2.11695300	1.42980400
C	-4.87276100	1.34338600	0.40575300
C	-4.78690300	-1.10436400	-0.07835400
C	-5.49080200	0.08927000	-0.10184000
C	-6.83949800	0.04733300	-0.59861100
C	-7.56786700	1.22706400	-0.91317200
C	-8.84319800	1.15912900	-1.43172500
C	-9.46751900	-0.09368800	-1.64755100
C	-8.78895700	-1.25651400	-1.35470300
C	-7.46266900	-1.22190900	-0.84405400
C	-6.72975600	-2.41666700	-0.60882800

C	-5.39870900	-2.36055500	-0.27395600
H	-3.32467400	4.76524800	1.59904200
H	-5.18968000	5.08542500	3.15618700
H	-7.31322300	4.29424200	4.17936600
H	-8.25810300	2.07703100	3.50578400
H	-7.14038200	0.70598500	1.81444600
H	-7.09335500	2.19591600	-0.76043800
H	-9.37577700	2.07955500	-1.68235000
H	-10.48195200	-0.13442500	-2.05087700
H	-9.25499900	-2.22986000	-1.52859300
H	-7.22245400	-3.38026900	-0.75854500
H	-4.77901900	-3.25063400	-0.16606200
H	-2.13835400	3.33412600	-0.06995300
O	-3.43200800	-1.10600500	0.17330100
O	-2.89904100	1.09775800	-0.97409100
N	-2.68735900	-0.93992700	-2.44275400
C	-1.74395100	-1.73203300	-3.17635000
C	-2.07022300	-3.04309300	-3.57771500
C	-0.47451700	-1.21040900	-3.44599800
C	-1.09615700	-3.77489700	-4.28597700
C	0.47995500	-1.95735200	-4.13521600
H	-0.24732900	-0.20005900	-3.12708900
C	0.15362800	-3.23798700	-4.58242200
H	-1.33906800	-4.79181500	-4.60411000
H	1.47139800	-1.53858700	-4.31860000
H	0.88381900	-3.82440100	-5.13945500
C	-3.92745600	-0.62083900	-3.10757700
C	-4.86002400	-1.64488500	-3.38289600
C	-4.22504000	0.70616100	-3.44020800
C	-6.12092900	-1.27546100	-3.89074700
C	-5.47309200	1.04410100	-3.96254400
H	-3.48306800	1.47450000	-3.24269800
C	-6.43351600	0.05056300	-4.17039700
H	-6.86272500	-2.05800900	-4.06413900
H	-5.70145800	2.08844600	-4.18580300
H	-7.42628400	0.30987700	-4.54272700
C	-3.35897800	-3.66694000	-3.29231800
H	-3.34090000	-4.75965800	-3.23950000
C	-4.56352900	-3.06215700	-3.19399200
H	-5.43795900	-3.70648700	-3.06945000
C	3.47807100	0.15002400	1.85345700
C	3.10040300	0.55768800	3.15791000
C	3.71967600	1.63704300	3.73041500
C	4.67249600	2.39872800	2.99867200

C	5.20456700	3.60672400	3.52356600
C	6.03746400	4.40788200	2.77127900
C	6.37566100	4.01679100	1.45429200
C	5.90898500	2.82585300	0.93335000
C	5.05529000	1.96936400	1.68471400
C	4.52283600	0.73670300	1.14626900
C	4.35430400	-0.24052600	-1.18854800
C	5.11118700	0.15980300	-0.09585300
C	6.54442300	0.01153000	-0.20883400
C	7.40794700	0.11975000	0.91671400
C	8.77198900	-0.03809900	0.78933500
C	9.35356300	-0.29896700	-0.47443200
C	8.54529900	-0.43323200	-1.58206500
C	7.13315900	-0.30675700	-1.47754700
C	6.28978200	-0.54936700	-2.59488700
C	4.92677500	-0.56944000	-2.43717600
H	3.45175600	1.94786400	4.74253900
H	4.91295700	3.90332300	4.53428400
H	6.42795400	5.34143800	3.18272200
H	7.01870100	4.65664100	0.84501700
H	6.19266600	2.53970900	-0.07812600
H	6.97676700	0.30309100	1.89941300
H	9.40783000	0.03069900	1.67491000
H	10.43630500	-0.41231500	-0.56413100
H	8.97636900	-0.66493600	-2.55948500
H	6.74005500	-0.78741900	-3.56132600
H	4.25458300	-0.84220300	-3.25144000
H	2.34418000	-0.04013400	3.67352900
O	2.97423600	-0.30128200	-1.12559500
O	2.77084600	-0.91411100	1.38525000
N	2.93344900	-2.83409600	-0.13678600
C	3.11346700	-3.64217700	-1.30746100
C	4.43190900	-3.84341600	-1.79078700
C	2.02890700	-4.27269600	-1.92266400
C	4.59407300	-4.61354300	-2.95988700
C	2.22970800	-5.08162800	-3.04189000
H	1.03298100	-4.12554500	-1.50423600
C	3.51158300	-5.23498200	-3.57702100
H	5.60379400	-4.75617300	-3.35365300
H	1.37734700	-5.59065800	-3.49397500
H	3.67076900	-5.85632600	-4.46187600
C	3.44625600	-3.39474200	1.09769900
C	4.84400400	-3.44436400	1.29384300
C	2.55983900	-3.74939400	2.11338500

C	5.31034300	-3.80074600	2.57523000
C	3.04400200	-4.09212700	3.37744000
H	1.48076000	-3.68529200	1.96536800
C	4.42403800	-4.11184200	3.60447900
H	6.38938900	-3.83139300	2.74921400
H	2.33367400	-4.27792100	4.18499800
H	4.80877500	-4.36035600	4.59645100
C	5.62804900	-3.36643800	-1.10294300
H	6.51004300	-3.25028600	-1.73762900
C	5.80458500	-3.19323200	0.22791400
H	6.81496800	-2.93721900	0.56038100
P	-2.32711800	-0.45117500	-0.85613400
P	2.17977700	-1.31831000	-0.07693500
Ir	-0.09237000	-0.85095000	-0.33599500
C	-0.18249900	-0.84272300	1.82856900
H	0.36950700	-1.75952900	2.04339000
H	0.34519400	0.04259200	2.18643300
C	-1.54831500	-0.97425700	2.28752500
H	-2.03755500	-1.90849800	2.01971500
C	-2.19547400	-0.08009700	3.07169700
H	-1.65654200	0.80741500	3.41147400
O	-0.15483100	-3.28735500	3.51548100
C	0.41957000	1.21494300	-0.32080400
C	0.46071800	1.53048500	-1.55891500
C	0.52479000	2.04990900	-2.83769200
H	1.13697700	3.18177600	-2.48196000
H	1.32812800	1.62061500	-3.45922500
C	-0.74856200	2.39075400	-3.60733200
H	-1.22492600	1.49344000	-4.03039500
H	-1.48350700	2.87938900	-2.95205900
H	-0.52099900	3.06659300	-4.44596200
C	0.71648200	2.14946000	0.78800300
C	1.94704600	2.82364500	0.82578000
C	-0.25390700	2.46720300	1.74541600
C	2.18223300	3.83484400	1.75765400
H	2.72965500	2.52246400	0.13441100
C	-0.01675700	3.46961300	2.68743600
H	-1.20128800	1.93658700	1.73711800
C	1.19458900	4.16777900	2.68896900
H	3.14378600	4.34987300	1.76528800
H	-0.79083700	3.70677700	3.42117000
H	1.37709600	4.95359600	3.42524600
C	-3.54749600	-0.22650000	3.59475000
C	-4.37970800	-1.31689500	3.26575200

C	-4.05869900	0.75614000	4.46565600
C	-5.66406900	-1.41767800	3.79263400
H	-4.00674300	-2.09729200	2.60369500
C	-5.33906100	0.64827800	5.00343800
H	-3.42847100	1.60978200	4.72703000
C	-6.14841700	-0.44073400	4.67026200
H	-6.29091900	-2.27149500	3.52381300
H	-5.71145400	1.42246200	5.67765200
H	-7.15465000	-0.52659700	5.08753500
C	-1.21065900	-4.18634200	3.63603900
H	-0.97138400	-5.02818200	4.31801100
H	-2.12641800	-3.70046400	4.02918600
H	-1.44393800	-4.60751700	2.64141200
B	0.23885000	-2.55236800	4.71109300
F	0.83276500	-3.41641300	5.65144600
F	1.20214400	-1.58580100	4.29633500
F	-0.85531300	-1.89540700	5.29068600
C	4.05599700	5.56092300	-2.11879100
C	3.25026800	4.37951800	-2.69874000
C	1.07358800	5.59120600	-1.94573900
C	1.95371200	6.71674000	-1.36563300
C	3.27901000	6.87785900	-2.11182200
H	4.33907100	5.30760100	-1.08187900
H	4.99777100	5.66104700	-2.68226800
H	1.38136400	7.65835600	-1.37002900
H	2.16307900	6.47950900	-0.30780300
H	3.09918100	7.22435000	-3.14284800
H	3.88412800	7.66243700	-1.63104300
N	1.89320000	4.33879500	-2.05747200
H	2.03839000	4.02338100	-1.09335500
C	-0.07326200	5.26996500	-0.97684200
H	-0.72541500	4.48477800	-1.38569600
H	0.29997500	4.93426000	0.00061200
H	-0.68683300	6.16834300	-0.81619700
C	0.46665200	5.99645500	-3.29587400
H	-0.01479300	5.13833800	-3.78383100
H	-0.30299300	6.76343900	-3.12544100
H	1.19901200	6.42040500	-3.99202900
C	3.12994700	4.46813600	-4.22674100
H	4.11117200	4.26295800	-4.67890500
H	2.41850000	3.72126000	-4.60879700
H	2.80835300	5.45492000	-4.57805400
C	3.95413800	3.06284200	-2.34080300
H	3.39850100	2.18414300	-2.69436800

H	4.95276800	3.03503300	-2.79928500
H	4.09603400	2.96134000	-1.25676300
Cl	-0.76844000	-3.17500000	-0.25777000

E

Zero-point correction=	1.590197 (Hartree/Particle)
Thermal correction to Energy=	1.689264
Thermal correction to Enthalpy=	1.690208
Thermal correction to Gibbs Free Energy=	1.450614
Sum of electronic and zero-point Energies=	-5855.313417
Sum of electronic and thermal Energies=	-5855.214350
Sum of electronic and thermal Enthalpies=	-5855.213406
Sum of electronic and thermal Free Energies=	-5855.453000

C	-3.80367600	1.80494400	-0.23516800
C	-3.35137700	3.12621500	0.00040500
C	-4.09045900	3.98585800	0.77249200
C	-5.30568600	3.55402200	1.36732800
C	-6.05819500	4.41811400	2.20736500
C	-7.23044200	3.99332800	2.79309800
C	-7.67775900	2.67011100	2.57676100
C	-6.96683900	1.80784400	1.77045300
C	-5.77532000	2.22143400	1.11382500
C	-5.03022500	1.34953300	0.23445600
C	-4.79386300	-1.13208500	0.09307000
C	-5.56452900	0.00284800	-0.10450200
C	-6.89481200	-0.18871300	-0.61641100
C	-7.68318000	0.88904900	-1.10467600
C	-8.93893700	0.67285700	-1.63002800
C	-9.48314300	-0.63354000	-1.68173400
C	-8.74403600	-1.70128300	-1.22146800
C	-7.43529400	-1.51594900	-0.69808800
C	-6.63876400	-2.62180600	-0.29464500
C	-5.32226200	-2.43954400	0.05228200
H	-3.74513400	5.00760200	0.94856900
H	-5.68314900	5.42982100	2.38271300
H	-7.80197000	4.66571600	3.43701200
H	-8.58209600	2.31522900	3.07586400
H	-7.30772500	0.78198800	1.65732400
H	-7.27039900	1.89693800	-1.08079100
H	-9.51755300	1.51599800	-2.01480200

H	-10.48301800	-0.79160600	-2.09252800
H	-9.14643300	-2.71650300	-1.26916700
H	-7.06918100	-3.62554000	-0.32591000
H	-4.64904100	-3.26530800	0.28310000
H	-2.40910400	3.42829400	-0.45442700
O	-3.44938100	-1.01538900	0.36079000
O	-2.98124200	1.04671400	-1.03475800
N	-2.72988700	-1.14737800	-2.26719700
C	-1.73363300	-1.93840000	-2.92821900
C	-1.95844200	-3.30761600	-3.17405300
C	-0.51558400	-1.34670200	-3.27505700
C	-0.92810400	-4.03806100	-3.79549800
C	0.49887800	-2.09639200	-3.87406900
H	-0.37969600	-0.28333500	-3.10787900
C	0.28104100	-3.44501200	-4.15339400
H	-1.08819700	-5.10162900	-3.98894800
H	1.45011300	-1.62007700	-4.12061600
H	1.06193100	-4.04045800	-4.62592200
C	-3.98029800	-0.97771000	-2.96034000
C	-4.83363200	-2.08848000	-3.14069100
C	-4.36074800	0.28453700	-3.43205700
C	-6.10331300	-1.86357300	-3.70802800
C	-5.61552000	0.47708000	-4.00869000
H	-3.67481200	1.11743300	-3.30629000
C	-6.49830000	-0.59937300	-4.13203200
H	-6.78562400	-2.71012400	-3.81145800
H	-5.91069100	1.47400000	-4.34306500
H	-7.49623600	-0.45129100	-4.54863600
C	-3.20206600	-3.98277900	-2.81478600
H	-3.10961500	-5.05724500	-2.63072900
C	-4.44530800	-3.45297900	-2.79071800
H	-5.27640900	-4.13551600	-2.59283000
C	3.55826200	0.26870900	1.77219800
C	3.25054200	0.80401600	3.04996300
C	3.93476600	1.89884200	3.50580900
C	4.88835700	2.55378700	2.67750900
C	5.47473700	3.78726900	3.06768800
C	6.31459000	4.48127800	2.22148500
C	6.60760600	3.94870400	0.94424700
C	6.08354800	2.73184800	0.55299300
C	5.21428600	1.98690100	1.40023700
C	4.61296100	0.73560400	0.99078400
C	4.33289300	-0.43611500	-1.24072800
C	5.13975800	0.02524100	-0.20891200

C	6.56160500	-0.19381200	-0.34494900
C	7.46152500	-0.02565600	0.74420800
C	8.81365300	-0.25259300	0.59637300
C	9.34680400	-0.64728800	-0.65405400
C	8.50135100	-0.84299400	-1.72422500
C	7.09921800	-0.64701400	-1.59513000
C	6.21341300	-0.95314600	-2.66304400
C	4.85583200	-0.90078700	-2.46849200
H	3.71526100	2.30818800	4.49437500
H	5.22343700	4.18941800	4.05248600
H	6.74909900	5.43445000	2.53137000
H	7.26317900	4.49749300	0.26336900
H	6.33563300	2.33582100	-0.42935200
H	7.06645600	0.25779000	1.71829200
H	9.47728500	-0.13602000	1.45619600
H	10.42079400	-0.81571700	-0.76092500
H	8.89357200	-1.17939100	-2.68752000
H	6.62478100	-1.29798100	-3.61459700
H	4.14852000	-1.21765900	-3.23577900
H	2.48206400	0.29215500	3.63615300
O	2.95753500	-0.41996100	-1.14011300
O	2.76192000	-0.76820100	1.41551300
N	2.87400500	-2.83799400	0.10137900
C	2.97202600	-3.80361300	-0.95479900
C	4.25814000	-4.11046500	-1.46920200
C	1.84364200	-4.48532600	-1.41724000
C	4.34136600	-5.04012500	-2.52531400
C	1.96733800	-5.44796800	-2.41968200
H	0.87445500	-4.25209300	-0.97444400
C	3.21435600	-5.71069400	-2.99307500
H	5.32570100	-5.26697300	-2.94333300
H	1.08010000	-5.98607300	-2.75755600
H	3.31203900	-6.45322900	-3.78908700
C	3.42784400	-3.26158400	1.37264900
C	4.83131800	-3.33800500	1.51293500
C	2.57970500	-3.46809600	2.45977500
C	5.34676400	-3.55471900	2.80711800
C	3.11234100	-3.67814100	3.73327700
H	1.49641300	-3.38719200	2.35314300
C	4.50068500	-3.71353000	3.90270400
H	6.43152300	-3.60266200	2.93652700
H	2.43345100	-3.75146700	4.58508100
H	4.92401200	-3.85788500	4.89968900
C	5.50065200	-3.59117600	-0.90565700

H	6.35420300	-3.59187900	-1.58842900
C	5.74773700	-3.26012000	0.38354000
H	6.78136200	-3.00723400	0.63721800
P	-2.36632000	-0.47144600	-0.75244500
P	2.13768600	-1.31119600	0.00864200
Ir	-0.11650500	-0.82822600	-0.25256000
C	-0.15183900	-0.54345200	1.87654200
H	0.39410900	-1.42002300	2.23082600
H	0.38602900	0.37998400	2.10460200
C	-1.51156100	-0.58742600	2.38477400
H	-2.00892900	-1.54961300	2.27833800
C	-2.14846200	0.43151500	3.00445800
H	-1.60633700	1.36501700	3.17282500
O	-0.09838600	-2.82430700	3.83561900
C	0.37067600	1.16700100	-0.67487300
C	0.34791600	1.57751400	-1.91731900
C	0.20136600	1.99127500	-3.17035700
H	1.41572200	3.54300700	-2.60214700
H	1.03693800	1.86184400	-3.87768300
C	-1.11316700	2.44487700	-3.76646800
H	-1.50802300	1.69024800	-4.46904400
H	-1.86377900	2.59317400	-2.97814000
H	-1.00786200	3.38372100	-4.33782700
C	0.68611600	2.18729700	0.36675300
C	1.97078400	2.74051000	0.49345700
C	-0.32159600	2.66547100	1.21639600
C	2.22759300	3.78608900	1.38819900
H	2.78208400	2.30281200	-0.08105400
C	-0.06798200	3.69524100	2.12268100
H	-1.30800100	2.21376700	1.16914100
C	1.20329000	4.27525700	2.20177400
H	3.23393700	4.19993600	1.46277700
H	-0.87493200	4.04695000	2.77016900
H	1.39982100	5.08287200	2.91017400
C	-3.50170600	0.38914800	3.54725100
C	-4.32575800	-0.75203600	3.45782300
C	-4.02253700	1.52915700	4.19090500
C	-5.60823400	-0.74984700	3.99935300
H	-3.94640300	-1.65208800	2.97502700
C	-5.30211500	1.52834300	4.74190200
H	-3.39983200	2.42466700	4.26333600
C	-6.10145500	0.38642900	4.65076000
H	-6.22707000	-1.64724400	3.92066200
H	-5.68242400	2.42609900	5.23401300

H	-7.10714500	0.38316400	5.07777600
C	-1.17625700	-3.67738500	4.05280500
H	-0.94597600	-4.46675400	4.79820800
H	-2.06788800	-3.13214500	4.42325700
H	-1.44430900	-4.17075600	3.10147200
B	0.33437400	-1.99200900	4.94861900
F	0.92687400	-2.77892600	5.95836600
F	1.31775200	-1.09703100	4.42979600
F	-0.72874400	-1.25334200	5.48138200
C	4.34968900	5.17118800	-2.15717000
C	3.45246800	4.11475400	-2.82221400
C	1.36980500	5.60024500	-2.10828600
C	2.36881000	6.57607900	-1.46730900
C	3.74004700	6.57510600	-2.14873600
H	4.55196100	4.85493700	-1.11970900
H	5.32248400	5.16625400	-2.67259500
H	1.92236100	7.58221500	-1.47972000
H	2.49002400	6.29806900	-0.40654000
H	3.66091400	6.96966200	-3.17468500
H	4.41401400	7.26054500	-1.61281200
N	2.06934400	4.24856900	-2.19010200
H	2.14775900	3.90981600	-1.21193800
C	0.14625600	5.38619300	-1.21029300
H	-0.55177000	4.66380900	-1.65878200
H	0.42550100	5.02615300	-0.21265300
H	-0.38114600	6.34322500	-1.09072700
C	0.89427700	6.05904000	-3.49023500
H	0.37394200	5.24803600	-4.02061800
H	0.17526100	6.87871400	-3.35229600
H	1.69928500	6.43443700	-4.13024300
C	3.36766000	4.27727000	-4.34349800
H	4.31799200	3.93974100	-4.77975500
H	2.56753100	3.65236000	-4.76756000
H	3.20845500	5.31111300	-4.66651300
C	3.94624000	2.69961800	-2.50035900
H	3.23604800	1.92653800	-2.82650800
H	4.90161700	2.52097600	-3.01195300
H	4.12725400	2.56353600	-1.42889300
Cl	-0.87220300	-3.13296400	0.14313000

E1

Zero-point correction= 1.303243 (Hartree/Particle)

Thermal correction to Energy= 1.389398

Thermal correction to Enthalpy=	1.390342
Thermal correction to Gibbs Free Energy=	1.177977
Sum of electronic and zero-point Energies=	-5446.147265
Sum of electronic and thermal Energies=	-5446.061110
Sum of electronic and thermal Enthalpies=	-5446.060166
Sum of electronic and thermal Free Energies=	-5446.272531

C	2.71271500	0.57613600	1.65182900
C	2.00410300	0.05531400	2.75434900
C	1.66033900	0.88786100	3.78921100
C	1.96082400	2.27663900	3.73067300
C	1.49326100	3.17941800	4.72431700
C	1.74835900	4.53160000	4.63611600
C	2.49159000	5.03700700	3.54178400
C	2.97350200	4.18568400	2.56953200
C	2.73051100	2.78554500	2.63104300
C	3.18114300	1.88287900	1.60754800
C	3.86162300	2.09965200	-0.79574900
C	4.14245100	2.29949900	0.55115200
C	5.42456700	2.85697700	0.89635400
C	5.88229000	2.94553800	2.24225000
C	7.11499800	3.48346600	2.54579800
C	7.96507200	3.96556500	1.52137000
C	7.56755300	3.87006100	0.20583600
C	6.30929300	3.30657300	-0.14194600
C	5.91990900	3.15526700	-1.50034700
C	4.73153500	2.54644600	-1.81994700
H	1.09872300	0.49711500	4.64076000
H	0.91070000	2.77687000	5.55714200
H	1.37199400	5.21442500	5.40181100
H	2.67745900	6.11106900	3.46151400
H	3.52533400	4.58668000	1.72007600
H	5.24831800	2.56616500	3.04187400
H	7.44113900	3.52935400	3.58772000
H	8.93740500	4.39493600	1.77499800
H	8.22187100	4.21563600	-0.59916200
H	6.59112000	3.50779800	-2.28738600
H	4.42320800	2.39274700	-2.85440700
H	1.72310100	-0.99475300	2.73040800
O	2.70274000	1.50217600	-1.19221100
O	2.97304900	-0.27635800	0.60606400
N	3.25843800	-1.07887500	-1.71708100
C	4.39794900	-1.73014600	-1.11881100

C	4.31202100	-3.10285000	-0.81350200
C	5.54363200	-0.99435500	-0.79941300
C	5.37325900	-3.68939700	-0.09575200
C	6.59929900	-1.60295900	-0.12278700
H	5.58381400	0.06412000	-1.05439600
C	6.50313200	-2.95207900	0.24271200
H	5.25984400	-4.72557000	0.22735700
H	7.48183300	-1.01615400	0.14377200
H	7.30867200	-3.42487800	0.81031800
C	2.97695000	-1.44103700	-3.07340200
C	2.56055000	-2.75747100	-3.36801400
C	3.07388000	-0.47532200	-4.07822700
C	2.20663400	-3.04345200	-4.70029600
C	2.72650100	-0.78624500	-5.39139400
H	3.38832300	0.53172800	-3.80372300
C	2.28631700	-2.07761300	-5.69930900
H	1.85201400	-4.04931800	-4.93851000
H	2.77904600	-0.01903100	-6.16759300
H	1.99529700	-2.32790200	-6.72279400
C	3.19135400	-3.94124300	-1.22721200
H	2.99911800	-4.80983700	-0.59644000
C	2.45214500	-3.79681100	-2.34980600
H	1.71392100	-4.57358300	-2.55851000
P	2.22356300	-0.06665200	-0.85056900
Ir	-0.04394000	-0.16990900	-0.90803900
C	0.40633600	-2.17774900	-0.05774700
H	0.10787900	-2.81445900	-0.89698200
H	1.44558300	-2.39857500	0.20124100
C	-0.46322900	-2.27850800	1.11372100
H	-1.52523900	-2.10047600	0.95625400
C	-0.25326600	1.79486200	-0.45948600
C	-0.49079000	1.12682000	0.71186400
C	-0.97765800	1.12018100	1.95852000
H	-0.90180400	0.19811600	2.53826400
C	-1.72354800	2.25676800	2.59166600
H	-2.72994400	1.92691300	2.90628100
H	-1.20751100	2.61661400	3.50023800
H	-1.84796600	3.10367800	1.90232000
C	0.35098700	3.07513300	-0.74586200
C	0.46941000	4.07799600	0.23740400
C	0.80053400	3.35138600	-2.05482700
C	1.00538300	5.32439700	-0.08220300
H	0.15687500	3.86080100	1.25815700
C	1.35588400	4.58649700	-2.36702200

H	0.71372200	2.55857400	-2.79815500
C	1.45190000	5.58029000	-1.38209000
H	1.09262200	6.09046300	0.69126700
H	1.71494600	4.78567100	-3.38008300
H	1.88208900	6.55442300	-1.62988700
C	-1.03720600	-2.65398900	3.49715000
C	-0.69992900	-3.42411000	4.63247400
C	-2.28290900	-1.98567400	3.49392600
C	-1.57739800	-3.52644000	5.71153400
H	0.24901800	-3.96726600	4.62143600
C	-3.15349000	-2.08694800	4.57884700
H	-2.55754800	-1.37272500	2.63486000
C	-2.80881900	-2.85849500	5.69460900
H	-1.30124400	-4.13814400	6.57518200
H	-4.10784100	-1.55180400	4.55678000
H	-3.49162600	-2.93582500	6.54509700
C	-0.10211500	-2.59022900	2.38019900
H	0.92535400	-2.90525200	2.56545700
O	2.82078800	-3.49230500	1.82656000
B	2.40674100	-4.88250400	1.97171500
F	1.34971800	-5.12378000	1.07102800
F	3.48483500	-5.74884600	1.66212400
F	1.97470300	-5.13258300	3.29540600
C	3.81456400	-3.03552700	2.68693800
H	4.21708600	-2.08118200	2.30616400
H	3.43495100	-2.86332400	3.71658300
H	4.65977800	-3.74619300	2.76632900
C	-3.12738800	1.55248500	-2.08909400
C	-2.34327000	2.10869200	-3.12432200
C	-2.10947800	3.46071900	-3.13478800
C	-2.55692800	4.28232100	-2.06283200
C	-2.17946100	5.64863400	-1.97647800
C	-2.53670700	6.41814400	-0.89061900
C	-3.29198900	5.84463400	0.15910800
C	-3.69195300	4.52548700	0.09600900
C	-3.34709300	3.70573300	-1.01359400
C	-3.70943800	2.31421500	-1.08661100
C	-4.33142600	0.55230800	0.59715300
C	-4.66045200	1.69405700	-0.12552500
C	-5.98306700	2.24053000	0.05582800
C	-6.48911700	3.29681300	-0.75391300
C	-7.75876000	3.80208400	-0.56426000
C	-8.59912700	3.28098500	0.44802400
C	-8.15133800	2.24152500	1.23462200

C	-6.85417600	1.68966200	1.05497200
C	-6.40868700	0.58431800	1.83015000
C	-5.18465800	0.01628300	1.59263100
H	-1.50619100	3.91159500	-3.92483900
H	-1.56393400	6.06793100	-2.77545500
H	-2.21776100	7.46117200	-0.82649300
H	-3.55195000	6.44701200	1.03305400
H	-4.26159100	4.09048200	0.91672200
H	-5.86112500	3.70348800	-1.54510400
H	-8.11948200	4.60885400	-1.20721300
H	-9.60064300	3.69314900	0.59385200
H	-8.79421700	1.81311500	2.00842200
H	-7.06973900	0.16833900	2.59403700
H	-4.84290000	-0.86358800	2.13572300
H	-1.90955500	1.42444500	-3.85469100
O	-3.13819800	-0.09486200	0.44344100
O	-3.29597700	0.18176700	-2.07495100
N	-3.08174200	-2.19425000	-1.07682400
C	-2.36941700	-3.33636900	-1.58549600
C	-1.99724200	-4.37529600	-0.70149800
C	-2.01494300	-3.38563000	-2.93376100
C	-1.15950700	-5.39349900	-1.19332600
C	-1.22643600	-4.43228300	-3.41250500
H	-2.31191300	-2.56673300	-3.58566500
C	-0.78531300	-5.42684700	-2.53475200
H	-0.78214400	-6.14216100	-0.49487700
H	-0.92119600	-4.44011600	-4.46083300
H	-0.13461500	-6.22795000	-2.89347800
C	-4.43096800	-2.43247300	-0.64362600
C	-4.66129600	-3.24710300	0.49167200
C	-5.49715800	-1.81494700	-1.30830200
C	-5.98943000	-3.35724400	0.95392900
C	-6.80110800	-1.94690600	-0.83159800
H	-5.27754700	-1.19555600	-2.17670700
C	-7.04471000	-2.71666600	0.31000000
H	-6.17863500	-3.96423900	1.84298300
H	-7.62002100	-1.43290300	-1.33948700
H	-8.06079500	-2.81444900	0.70032800
C	-2.44474700	-4.44544100	0.68510800
H	-1.79097200	-5.01577100	1.34964800
C	-3.60310700	-3.96701100	1.19725400
H	-3.81822900	-4.20257700	2.24256300
P	-2.39898600	-0.65197500	-0.93277800
Cl	-0.19110100	-0.84054200	-3.28795300

[B-C]'‡

Zero-point correction=	1.571668 (Hartree/Particle)
Thermal correction to Energy=	1.663167
Thermal correction to Enthalpy=	1.664112
Thermal correction to Gibbs Free Energy=	1.444646
Sum of electronic and zero-point Energies=	-5070.685463
Sum of electronic and thermal Energies=	-5070.593964
Sum of electronic and thermal Enthalpies=	-5070.593020
Sum of electronic and thermal Free Energies=	-5070.812485

C	2.99322900	-0.06705100	2.13413200
C	2.35775700	-0.18290400	3.39076600
C	2.32549300	0.88936000	4.24443600
C	2.88462100	2.13696800	3.85725300
C	2.77460700	3.28092700	4.69114100
C	3.26515600	4.50358800	4.28796000
C	3.87259300	4.62820300	3.01715600
C	4.00671600	3.53191000	2.19125100
C	3.54140600	2.24773000	2.58774400
C	3.66000100	1.08609800	1.74007000
C	3.95779400	0.74317100	-0.73499900
C	4.46488300	1.14682800	0.49023300
C	5.83420000	1.60558000	0.51434500
C	6.54819300	1.80730900	1.72816000
C	7.86442000	2.22126300	1.72296500
C	8.53891600	2.46864200	0.50396200
C	7.88441100	2.26258700	-0.69104500
C	6.53778300	1.81040200	-0.71878800
C	5.89314100	1.50571100	-1.94889900
C	4.63972400	0.95042100	-1.95530800
H	1.84479300	0.80556500	5.22117700
H	2.27700100	3.17426800	5.65811300
H	3.17116200	5.37741500	4.93633900
H	4.23061800	5.60369900	2.68057500
H	4.45803400	3.65444000	1.20825600
H	6.04986800	1.61497800	2.67706000
H	8.39161500	2.35519400	2.67019800
H	9.57738200	2.80654500	0.51377900
H	8.39932000	2.42469000	-1.64123300
H	6.43127400	1.66648700	-2.88535100
H	4.15229300	0.63226600	-2.87673800

H	1.89931200	-1.13755100	3.64233200
O	2.72145300	0.13088000	-0.84058700
O	2.97988200	-1.19104000	1.33116300
N	3.24399800	-2.46997800	-0.86585200
C	2.90781100	-3.85548600	-0.76844000
C	2.89057400	-4.63123000	-1.94915700
C	2.62149200	-4.42986000	0.47602200
C	2.57305800	-5.99662000	-1.82794700
C	2.28599200	-5.78148900	0.56398900
H	2.68076800	-3.80496800	1.36811300
C	2.27122000	-6.56762000	-0.59300300
H	2.55914500	-6.61183300	-2.72957100
H	2.05166500	-6.22339800	1.53473300
H	2.02458700	-7.62956600	-0.53074300
C	4.61428200	-2.23151300	-1.25036700
C	4.96775200	-2.43812100	-2.60043100
C	5.56914100	-1.81564000	-0.31681900
C	6.27487400	-2.09955600	-3.00146000
C	6.86329300	-1.50700400	-0.73270800
H	5.27772600	-1.70353500	0.72550100
C	7.21021000	-1.63213000	-2.08219000
H	6.55636400	-2.23509500	-4.04857300
H	7.59361400	-1.14673800	-0.00609500
H	8.21847900	-1.37477900	-2.41345700
C	3.17126100	-4.05879000	-3.26694800
H	2.65391200	-4.53832400	-4.10257000
C	4.05894500	-3.07736800	-3.55246300
H	4.21798200	-2.83284900	-4.60742700
C	-0.46599400	2.22671900	-2.34553000
C	0.87566000	2.07649900	-2.75751200
C	1.75577300	3.11534100	-2.57945900
C	1.33335400	4.32224200	-1.95999000
C	2.26211000	5.36658400	-1.69629000
C	1.87527200	6.50802900	-1.02864800
C	0.53596700	6.64332200	-0.59070200
C	-0.38981800	5.65182000	-0.83775700
C	-0.03299500	4.46745100	-1.54141700
C	-0.95917300	3.38803700	-1.77203900
C	-2.89663800	2.54822900	-0.42064000
C	-2.37429600	3.47730600	-1.31246600
C	-3.22724200	4.56606400	-1.70799800
C	-2.88337200	5.44514500	-2.77226100
C	-3.71997000	6.47775200	-3.13935700
C	-4.94056900	6.69554200	-2.45467800

C	-5.30898500	5.85672700	-1.42565500
C	-4.47894300	4.76980900	-1.03555800
C	-4.86760100	3.87118600	-0.00637600
C	-4.11097100	2.75790800	0.26723300
H	2.80004200	3.01219100	-2.88008100
H	3.29642400	5.23732200	-2.02438800
H	2.59815100	7.30164200	-0.82754600
H	0.23427000	7.53753900	-0.04072500
H	-1.40525000	5.76516900	-0.46459400
H	-1.94922200	5.28397200	-3.31021000
H	-3.44112000	7.13176300	-3.96857100
H	-5.58997800	7.52227900	-2.75058700
H	-6.25466800	6.00720900	-0.89886400
H	-5.80384300	4.04862500	0.52793800
H	-4.42268600	2.01152500	0.99678500
H	1.18790000	1.12818900	-3.19113300
O	-2.21681500	1.37933800	-0.12319600
O	-1.32146900	1.15554400	-2.53432100
N	-3.27071100	-0.26570700	-1.97352000
C	-4.30088400	-0.77831300	-1.12213200
C	-5.52547100	-0.07653300	-0.98713500
C	-4.06564900	-1.93446500	-0.37119100
C	-6.48583500	-0.59661800	-0.09558100
C	-5.03721300	-2.43055100	0.49912200
H	-3.11298600	-2.44882400	-0.47320700
C	-6.25651000	-1.76284500	0.63075700
H	-7.43437500	-0.06516400	0.01385400
H	-4.83520900	-3.34211700	1.06022100
H	-7.02855700	-2.14840800	1.30070200
C	-3.54664200	-0.07184700	-3.37693100
C	-4.46878700	0.91272700	-3.79238200
C	-2.84561500	-0.81565500	-4.33119700
C	-4.58821900	1.17591000	-5.17143800
C	-2.99528100	-0.55526500	-5.69381900
H	-2.14873800	-1.58654700	-4.00817600
C	-3.85962900	0.45819400	-6.11556400
H	-5.28430900	1.95345400	-5.49493000
H	-2.42381100	-1.13578100	-6.42105800
H	-3.97147500	0.68225200	-7.17852300
C	-5.83570600	1.16401000	-1.69354700
H	-6.60406700	1.77473600	-1.21302900
C	-5.35646900	1.61394300	-2.87364100
H	-5.76923100	2.55490500	-3.24837000
P	2.24225900	-1.29552600	-0.16835400

P	-1.81002200	0.24653500	-1.24764400
Ir	-0.05236000	-1.03025900	-0.52115000
C	-0.21921800	-0.04885800	1.39571100
C	-0.65302800	-1.13248500	1.91245100
C	-1.10685200	-2.26825900	2.56435000
H	-1.78322100	-1.64557900	3.66267800
H	-1.98038600	-2.72592100	2.07273500
C	-0.09616400	-3.29682700	3.06804800
H	0.59511300	-2.86875800	3.80947000
H	-0.61202600	-4.14513300	3.54247600
H	0.51614600	-3.69894700	2.24743600
C	-0.05764300	1.35701700	1.75839100
C	-0.67915400	1.87088700	2.91191900
C	0.71945900	2.22605800	0.98110200
C	-0.53727200	3.20535300	3.27690000
H	-1.28985700	1.20636500	3.51894700
C	0.88198700	3.55994900	1.35835500
H	1.20597500	1.84863200	0.08356100
C	0.25302900	4.05706100	2.49820600
H	-1.03530600	3.58219500	4.17345000
H	1.51300600	4.21399400	0.76127000
H	0.38513700	5.10229300	2.78240300
C	0.38198600	-1.69770300	-2.58335300
H	0.12802900	-0.87428800	-3.25500100
H	1.38459000	-2.10859700	-2.71505200
C	-0.63727300	-2.50923800	-2.06172600
H	-1.67037600	-2.26752700	-2.31758900
C	-0.45660700	-3.99271500	-1.80947800
C	-1.60976500	-4.60124900	-1.03894800
C	-1.43312700	-5.02038400	0.28310500
C	-2.86290100	-4.77391400	-1.64511200
C	-2.48959900	-5.59445400	0.99679800
H	-0.45275900	-4.90873600	0.74629200
C	-3.91419300	-5.36477900	-0.94379800
H	-3.00880600	-4.44771700	-2.67753600
C	-3.73073900	-5.77621900	0.38089900
H	-2.33579700	-5.92053600	2.02856400
H	-4.88388300	-5.49786500	-1.42827300
H	-4.55357700	-6.24199000	0.92843600
O	-0.32388900	-4.53977400	-3.12365600
C	-0.41314000	-5.94517600	-3.24449800
H	-1.45846100	-6.29489300	-3.29543900
H	0.09460400	-6.21961300	-4.18115800
H	0.07737700	-6.46626700	-2.40742700

H	0.46902800	-4.16815600	-1.24242200
C	-4.71117500	-0.20472500	5.36687900
C	-3.93257000	-0.93610500	4.25601400
C	-2.05242100	-1.40740200	6.01739500
C	-2.90892900	-0.65244700	7.05308000
C	-4.40823100	-0.73513600	6.76780500
H	-4.44939500	0.86762100	5.32835000
H	-5.78748900	-0.26985400	5.14198000
H	-2.67401000	-1.04164100	8.05629700
H	-2.60443500	0.40940200	7.05124900
H	-4.76491700	-1.77217300	6.87498900
H	-4.96131800	-0.14713500	7.51612000
N	-2.47406300	-1.00378000	4.63097600
H	-2.11210200	-0.05710500	4.49839800
C	-0.58390800	-0.98250600	6.14595800
H	-0.21797700	-1.19272300	7.16102600
H	0.05369500	-1.52423800	5.43319300
H	-0.46405800	0.09733100	5.96188700
C	-2.15442000	-2.92605300	6.20599400
H	-1.67088100	-3.46047800	5.37766200
H	-1.64071000	-3.20709700	7.13665000
H	-3.18892300	-3.27874700	6.28492500
C	-3.99700400	-0.12270600	2.95577900
H	-3.44320500	-0.59916700	2.13645000
H	-5.04111600	-0.02153600	2.63034700
H	-3.58616100	0.88844700	3.10095100
C	-4.49689700	-2.34214900	4.01594400
H	-5.47923300	-2.25302600	3.53307200
H	-3.84789900	-2.92462700	3.34900300
H	-4.63526600	-2.90888600	4.94380000

C

Zero-point correction=	1.578097 (Hartree/Particle)
Thermal correction to Energy=	1.669909
Thermal correction to Enthalpy=	1.670854
Thermal correction to Gibbs Free Energy=	1.450446
Sum of electronic and zero-point Energies=	-5070.695445
Sum of electronic and thermal Energies=	-5070.603633
Sum of electronic and thermal Enthalpies=	-5070.602689

Sum of electronic and thermal Free Energies= -5070.823097

C	2.89604600	-0.21887700	2.27034200
C	2.34883200	-0.29339700	3.57147000
C	2.35692600	0.80864900	4.38764400
C	2.82720400	2.05785800	3.90213500
C	2.71685200	3.24314800	4.67656200
C	3.08368500	4.46533000	4.15707700
C	3.57103800	4.54632300	2.83084200
C	3.73014100	3.40708400	2.07066900
C	3.38413700	2.12750400	2.58375800
C	3.53455000	0.92506800	1.80352500
C	3.98624000	0.39024900	-0.61511300
C	4.40330400	0.91544900	0.59607700
C	5.76304700	1.40203700	0.67038600
C	6.38668600	1.75688700	1.89933100
C	7.69155800	2.20393500	1.93848700
C	8.44900300	2.32971400	0.75052300
C	7.88695200	1.96969500	-0.45481600
C	6.55354100	1.48378100	-0.52504600
C	6.00605800	1.03376300	-1.75768100
C	4.75761300	0.46999500	-1.79662300
H	1.95019300	0.75196700	5.39929300
H	2.30515600	3.16943400	5.68600600
H	2.98091000	5.37294000	4.75602200
H	3.81693800	5.51837500	2.39959100
H	4.10009800	3.48622400	1.04988200
H	5.82933300	1.65848500	2.82883600
H	8.14497600	2.45807600	2.89925200
H	9.47747100	2.69455600	0.79399800
H	8.46597400	2.03567300	-1.37936000
H	6.61173700	1.09977200	-2.66396400
H	4.33680200	0.05976100	-2.71449200
H	1.92099800	-1.24269200	3.89028800
O	2.74753400	-0.19521500	-0.75326400
O	2.84611100	-1.37185100	1.51765700
N	3.09618300	-2.80197800	-0.57027600
C	2.63512200	-4.14645300	-0.44866100
C	2.65786100	-4.98557400	-1.58690500
C	2.15149900	-4.61873200	0.77771500
C	2.16427500	-6.29782200	-1.44380700
C	1.65726600	-5.91876600	0.88697500
H	2.17241300	-3.95187200	1.64008400

C	1.66640400	-6.76153200	-0.22849500
H	2.17351800	-6.95992800	-2.31220600
H	1.27036300	-6.27683300	1.84324400
H	1.28663800	-7.78206100	-0.14950900
C	4.50270800	-2.66014200	-0.85803200
C	4.95165500	-2.95551800	-2.16306000
C	5.40438000	-2.21929100	0.11722800
C	6.29590500	-2.68261100	-2.48307400
C	6.73524100	-1.97170500	-0.21756500
H	5.04396000	-2.03487900	1.12632800
C	7.17720700	-2.18608400	-1.52661500
H	6.64719400	-2.88839000	-3.49716000
H	7.42058400	-1.58900300	0.54090400
H	8.21423700	-1.97583100	-1.79654200
C	3.13051000	-4.52615500	-2.89304600
H	2.69450500	-5.04172800	-3.75384300
C	4.10065000	-3.61726000	-3.14920500
H	4.37930100	-3.46620200	-4.19680200
C	0.12957000	2.35564100	-1.95926500
C	1.49301200	2.13961700	-2.25404900
C	2.41795100	3.10263200	-1.93480900
C	2.01905600	4.29807400	-1.27968000
C	2.98098800	5.27337000	-0.89727200
C	2.60823200	6.40797200	-0.21224600
C	1.24823300	6.60278200	0.12921200
C	0.28909300	5.68507000	-0.24426600
C	0.63187000	4.51258600	-0.97740300
C	-0.33971200	3.52265100	-1.37447900
C	-2.53627100	2.79443200	-0.38378500
C	-1.79073000	3.72026500	-1.10548500
C	-2.46343800	4.91977000	-1.53469600
C	-1.88832300	5.80490700	-2.48859600
C	-2.55225900	6.94347000	-2.89378000
C	-3.82160000	7.26872200	-2.35654800
C	-4.41299900	6.42744600	-1.43958700
C	-3.76573100	5.23259600	-1.02063700
C	-4.38844100	4.32527200	-0.12344700
C	-3.80660300	3.11197900	0.14866100
H	3.47448900	2.94609600	-2.15825000
H	4.02886000	5.09605300	-1.15221200
H	3.35564000	7.15036000	0.07627200
H	0.95401000	7.48866300	0.69653200
H	-0.74736300	5.85025500	0.04307300
H	-0.91488700	5.56340000	-2.91464900

H	-2.09663000	7.59887200	-3.63939800
H	-4.33207100	8.17882300	-2.67894000
H	-5.39969700	6.65841400	-1.03015000
H	-5.36469200	4.57801600	0.29692800
H	-4.30812500	2.36442100	0.76048000
H	1.78162000	1.20017100	-2.71961900
O	-2.05509600	1.53153900	-0.09612700
O	-0.76213100	1.37148600	-2.31622600
N	-2.88269000	0.16214900	-2.29566800
C	-4.12028600	-0.35683200	-1.80547800
C	-5.25738500	0.48899500	-1.73374100
C	-4.20478300	-1.68451600	-1.37356600
C	-6.44262600	-0.04456200	-1.18490000
C	-5.39779700	-2.19659500	-0.86424400
H	-3.32624200	-2.32144900	-1.43515800
C	-6.52141200	-1.37012500	-0.76369900
H	-7.32190700	0.60102500	-1.11836600
H	-5.43684400	-3.24003900	-0.55030500
H	-7.46201300	-1.76134300	-0.36841700
C	-2.86334600	0.60894500	-3.66788800
C	-3.56168600	1.77577100	-4.04562600
C	-2.10725800	-0.09027000	-4.61376600
C	-3.38143000	2.26850000	-5.35370300
C	-1.96602000	0.39764100	-5.91291400
H	-1.60096200	-1.00920300	-4.32263400
C	-2.58859700	1.59528800	-6.27827300
H	-3.89742700	3.18763500	-5.64151000
H	-1.35581000	-0.15114600	-6.63342800
H	-2.46609000	1.99520300	-7.28713700
C	-5.27070800	1.87184000	-2.20298000
H	-6.04481400	2.49727600	-1.75174800
C	-4.52267200	2.43950000	-3.17598200
H	-4.74353500	3.48094600	-3.42623700
P	2.13261300	-1.51983100	0.00483900
P	-1.55877100	0.41615700	-1.22134000
Ir	-0.11770500	-1.15335400	-0.40784500
C	-0.33753000	-0.57719700	1.61547900
C	-0.65046800	-1.66476600	2.27963200
C	-0.95445300	-2.78770200	2.91454400
H	-2.60121900	-1.60140600	3.67881600
H	-1.96181900	-3.20792100	2.77438800
C	0.00290900	-3.66409000	3.68567400
H	1.01096800	-3.22843000	3.71281400
H	-0.32995700	-3.82091700	4.72673400

H	0.07698700	-4.66342900	3.22407900
C	-0.31408400	0.76512400	2.23927100
C	-0.78774100	0.96361900	3.55164700
C	0.21793200	1.87634500	1.57314000
C	-0.83371700	2.22816800	4.13445500
H	-1.03706900	0.08590500	4.14545600
C	0.19534100	3.14417100	2.15725100
H	0.66440300	1.73744600	0.59047200
C	-0.35838400	3.33480600	3.42326600
H	-1.20315600	2.34985900	5.15703400
H	0.63050800	3.98750100	1.62520500
H	-0.37343200	4.33007400	3.87088400
C	0.52960700	-1.59503400	-2.51767800
H	0.46879100	-0.66446500	-3.08352300
H	1.49116400	-2.11052000	-2.57215000
C	-0.62360100	-2.33071200	-2.21946000
H	-1.58285700	-1.94920400	-2.57349900
C	-0.62246100	-3.84402800	-2.16441000
C	-1.72079000	-4.43301200	-1.29169800
C	-1.52643100	-4.58776300	0.08561900
C	-2.93956200	-4.83627400	-1.85362600
C	-2.52535900	-5.15137900	0.88347700
H	-0.58179600	-4.27436200	0.52860000
C	-3.93940100	-5.40127600	-1.05743900
H	-3.09275300	-4.71004900	-2.92650800
C	-3.73464000	-5.56420800	0.31568700
H	-2.34820700	-5.29752700	1.95188700
H	-4.87835700	-5.72316700	-1.51425800
H	-4.50780800	-6.02292200	0.93699400
O	-0.77952100	-4.22965500	-3.52559800
C	-0.47056400	-5.57237800	-3.81883400
H	-1.02756700	-6.28372700	-3.18254000
H	-0.74742800	-5.74735700	-4.86825500
H	0.60643300	-5.77809400	-3.69907300
H	0.34787800	-4.18996700	-1.77889900
C	-5.64127700	-0.12817100	3.62886600
C	-4.50994900	-0.96289000	3.01216600
C	-3.63010200	-1.35077100	5.50354700
C	-4.82625900	-0.50960600	5.97589200
C	-6.03257600	-0.57441700	5.03790400
H	-5.32175900	0.92867600	3.65877900
H	-6.50009500	-0.17234000	2.94258100
H	-5.09332600	-0.84038600	6.99107900
H	-4.50014200	0.54136800	6.06741600

H	-6.45554500	-1.59125600	5.01911800
H	-6.82988200	0.07765900	5.42469400
N	-3.37072300	-1.00034600	4.03927700
H	-2.94976000	-0.05991500	4.01797500
C	-2.35835300	-0.96455400	6.26647600
H	-2.49869500	-1.18053900	7.33480200
H	-1.48732900	-1.53809100	5.91414200
H	-2.13544300	0.10856000	6.17033400
C	-3.86784100	-2.85630000	5.65327000
H	-3.08815400	-3.43579000	5.13657500
H	-3.82111100	-3.11195900	6.72102200
H	-4.84508100	-3.17955200	5.28031700
C	-3.91931500	-0.26872000	1.78695800
H	-3.14693600	-0.88198800	1.30537400
H	-4.71374100	-0.08977700	1.05203100
H	-3.46086300	0.69572500	2.04706300
C	-4.95882100	-2.37591400	2.64153100
H	-5.63740600	-2.29255100	1.78411800
H	-4.11394900	-2.99946400	2.31485300
H	-5.49479100	-2.89256400	3.44463000

C1'

Zero-point correction=	1.306381 (Hartree/Particle)
Thermal correction to Energy=	1.389753
Thermal correction to Enthalpy=	1.390698
Thermal correction to Gibbs Free Energy=	1.185682
Sum of electronic and zero-point Energies=	-4985.949813
Sum of electronic and thermal Energies=	-4985.866441
Sum of electronic and thermal Enthalpies=	-4985.865496
Sum of electronic and thermal Free Energies=	-4986.070512

C	3.24988300	0.14779500	2.00882300
C	2.99397200	0.46017700	3.36331000
C	3.30953800	1.70088600	3.85497200
C	3.82267700	2.70744000	2.99410300
C	4.03203600	4.03467200	3.45431700
C	4.42644300	5.03173100	2.58950200
C	4.61653800	4.73553600	1.21879400
C	4.45411700	3.44949900	0.74927900
C	4.07499500	2.39054000	1.61960000
C	3.87635700	1.04271600	1.14884700
C	3.52243700	-0.00828000	-1.10863900

C	4.34629900	0.64253300	-0.20376100
C	5.71163800	0.88284100	-0.60965700
C	6.71087800	1.32852400	0.30031500
C	8.01319600	1.53166200	-0.10785000
C	8.39130400	1.30924100	-1.45296700
C	7.45483700	0.85540600	-2.35650400
C	6.11178000	0.61417000	-1.96101400
C	5.16708900	0.06581500	-2.87142700
C	3.90818100	-0.26662500	-2.44507600
H	3.10987600	1.94709600	4.89959700
H	3.83676200	4.25587000	4.50626000
H	4.56655100	6.05286200	2.95153900
H	4.87929800	5.53349300	0.52120200
H	4.58437700	3.24417800	-0.31191400
H	6.44211700	1.49767100	1.34163200
H	8.75970400	1.86381600	0.61741900
H	9.42314200	1.48317700	-1.76669600
H	7.73514700	0.65507100	-3.39391200
H	5.47361100	-0.13343200	-3.90054500
H	3.18304700	-0.74783200	-3.10128800
H	2.52243700	-0.29978000	3.98384000
O	2.24786500	-0.39768000	-0.77409900
O	2.90739700	-1.11956500	1.58608200
N	2.42530300	-2.94746900	-0.12908900
C	1.92541300	-4.16929400	0.40441800
C	1.55444800	-5.20422300	-0.48704500
C	1.79734600	-4.33847700	1.78944500
C	1.10058400	-6.41527900	0.06778300
C	1.30709200	-5.53643700	2.31027800
H	2.09388700	-3.52197600	2.44822000
C	0.97716800	-6.58555700	1.44576900
H	0.82624000	-7.22743100	-0.60847100
H	1.20127600	-5.65611500	3.39052700
H	0.61651800	-7.53507500	1.84765500
C	3.67892400	-3.07285900	-0.82642700
C	3.67909100	-3.66258800	-2.10897400
C	4.87202800	-2.61024600	-0.25927700
C	4.88311900	-3.66864500	-2.83894300
C	6.05642400	-2.64100600	-0.99400900
H	4.84923700	-2.18975000	0.74375000
C	6.05758600	-3.15654600	-2.29406500
H	4.88710600	-4.10208300	-3.84224100
H	6.97286100	-2.23791500	-0.55901400
H	6.97975800	-3.16375400	-2.87935500

C	1.58689300	-5.03552800	-1.94266300
H	0.81829900	-5.58142300	-2.49814600
C	2.49752600	-4.33211500	-2.65363600
H	2.42340800	-4.37132900	-3.74497500
C	-0.65113600	2.04666700	-1.82918500
C	0.50860900	1.55162800	-2.46421400
C	1.58803600	2.37945900	-2.64970500
C	1.56213900	3.71829500	-2.17681300
C	2.70440900	4.55663800	-2.30016900
C	2.70282200	5.83725800	-1.79432600
C	1.55183900	6.32561600	-1.13033900
C	0.42509300	5.54108600	-1.00445200
C	0.38020400	4.22018500	-1.53483900
C	-0.76675000	3.35896400	-1.39242200
C	-2.48918500	3.16967300	0.41361000
C	-2.00186200	3.83151200	-0.70764900
C	-2.69003700	5.02260200	-1.12689500
C	-2.41590700	5.65529600	-2.37153400
C	-3.09201700	6.79364800	-2.75665900
C	-4.07383000	7.36837700	-1.91331000
C	-4.37226100	6.77436900	-0.70612700
C	-3.70674000	5.58971400	-0.28741400
C	-4.03133700	4.94746000	0.93810700
C	-3.45980700	3.74315300	1.26531200
H	2.49276300	2.00634500	-3.13212200
H	3.59119400	4.15422100	-2.79662300
H	3.58789500	6.47037800	-1.89057200
H	1.55903900	7.33040800	-0.70163300
H	-0.43666800	5.92607300	-0.46354000
H	-1.66693000	5.21729100	-3.03132700
H	-2.87179600	7.25324200	-3.72307600
H	-4.59791800	8.27444000	-2.22621500
H	-5.13758300	7.20056600	-0.05209700
H	-4.77607000	5.40286800	1.59532000
H	-3.72872500	3.19608900	2.16866400
H	0.52743800	0.50953400	-2.77549200
O	-1.99901600	1.94289800	0.78918200
O	-1.71011800	1.17876400	-1.64886700
N	-3.70135000	0.29532500	-0.43334800
C	-4.50965100	0.19290900	0.74347400
C	-5.52417900	1.14633700	1.01401600
C	-4.18160500	-0.76884100	1.70697600
C	-6.18077500	1.07507900	2.25905600
C	-4.82988000	-0.79802700	2.94304600

H	-3.38630300	-1.48052300	1.49628000
C	-5.84205600	0.12297400	3.21769800
H	-6.96182000	1.80877800	2.47449200
H	-4.53620800	-1.54394100	3.68188600
H	-6.35912800	0.10743800	4.17985400
C	-4.28609800	0.31993000	-1.74790900
C	-5.15874200	1.36073600	-2.13918500
C	-3.92773800	-0.66049800	-2.67875200
C	-5.58091000	1.41110600	-3.48288400
C	-4.36931300	-0.60239700	-4.00073400
H	-3.26949700	-1.47487000	-2.39284700
C	-5.19223200	0.44846000	-4.41043300
H	-6.23874500	2.22872800	-3.78832800
H	-4.05165300	-1.37804200	-4.70052600
H	-5.53384900	0.51557100	-5.44588900
C	-5.88257200	2.23871200	0.11424800
H	-6.41049900	3.06202000	0.60270900
C	-5.69506100	2.35390500	-1.21767200
H	-6.08585600	3.25928000	-1.69143600
P	1.76371000	-1.45837000	0.39977700
P	-2.02640300	0.57719800	-0.13407300
Ir	-0.48476000	-0.94929700	0.51983400
C	-0.10504900	0.11309100	2.29094300
C	-0.31176200	-0.76079700	3.24692400
C	-0.52478200	-1.69665700	4.15415500
H	-1.56540700	-1.91590400	4.43402800
C	0.53904500	-2.51535400	4.84029500
H	1.54287000	-2.26654900	4.46668500
H	0.53162900	-2.35751400	5.93306100
H	0.37393200	-3.59572400	4.67767000
C	0.14531600	1.54976900	2.51519000
C	-0.24304000	2.16977400	3.71602700
C	0.77902100	2.33083000	1.53715200
C	-0.00854500	3.52792700	3.92915300
H	-0.74553400	1.57097600	4.47922000
C	1.02967800	3.68381000	1.75545600
H	1.07689900	1.86309200	0.59871700
C	0.63203400	4.29146100	2.94795300
H	-0.32886300	3.99381500	4.86512500
H	1.55430100	4.26409600	0.99876600
H	0.83028100	5.35296100	3.11306400
C	-0.50987700	-1.93106500	-1.48227500
H	-0.73782600	-1.19711000	-2.25574000
H	0.36663300	-2.54953600	-1.68174500

C	-1.55641700	-2.44242900	-0.69825000
H	-2.56296800	-2.05810100	-0.85904000
C	-1.57289400	-3.82170700	-0.11501400
C	-2.62712800	-3.98782700	0.94965100
C	-2.24538100	-4.05802200	2.29293900
C	-3.98656400	-4.05179600	0.61060300
C	-3.21166800	-4.20156900	3.29221200
H	-1.18785800	-3.99192900	2.55175900
C	-4.94906000	-4.20370200	1.60880100
H	-4.28723800	-4.00587200	-0.43798600
C	-4.56394700	-4.28304300	2.95098700
H	-2.90456900	-4.25456200	4.33946400
H	-6.00586400	-4.25411000	1.33820200
H	-5.32038800	-4.40005900	3.73053900
O	-1.78998100	-4.84440900	-1.19447800
C	-2.01871800	-6.18298900	-0.70033300
H	-3.09282100	-6.35071400	-0.55645300
H	-1.62273000	-6.86872200	-1.45559600
H	-1.48620000	-6.30488000	0.24624500
H	-0.58813400	-4.07861300	0.28674800
B	-2.42464900	-4.68563500	-2.75208000
F	-1.72527100	-5.65132800	-3.41849300
F	-3.75032600	-4.96502200	-2.57740200
F	-2.17750900	-3.42306100	-3.18364900

[C-E]'‡

Zero-point correction=	1.304112 (Hartree/Particle)
Thermal correction to Energy=	1.387125
Thermal correction to Enthalpy=	1.388069
Thermal correction to Gibbs Free Energy=	1.185345
Sum of electronic and zero-point Energies=	-4985.927158
Sum of electronic and thermal Energies=	-4985.844146
Sum of electronic and thermal Enthalpies=	-4985.843202
Sum of electronic and thermal Free Energies=	-4986.045926

C	-3.34826100	-0.41042600	2.05376000
C	-3.02224800	-0.55413200	3.42091600
C	-3.22248700	-1.75355900	4.05347700
C	-3.70568200	-2.87921800	3.33270200
C	-3.83479500	-4.15092300	3.95054700
C	-4.25558700	-5.25006100	3.23323900
C	-4.54575600	-5.11672400	1.85622200
C	-4.43710400	-3.89203900	1.23160700

C	-4.04189300	-2.72973600	1.94835100
C	-3.93876100	-1.43221300	1.32325800
C	-3.73408400	-0.62710000	-1.05320500
C	-4.47935500	-1.21776000	-0.04411600
C	-5.83852100	-1.58832000	-0.36211600
C	-6.78215500	-1.95139900	0.63937200
C	-8.08482200	-2.27046800	0.31514400
C	-8.51711800	-2.25740700	-1.03210500
C	-7.63527000	-1.89079000	-2.02575700
C	-6.29583700	-1.52982500	-1.71990100
C	-5.41270600	-1.06178300	-2.73062700
C	-4.17000100	-0.58997000	-2.39863300
H	-2.97736100	-1.86494700	5.11209800
H	-3.57790000	-4.24288800	5.00895600
H	-4.34678300	-6.22428800	3.71926900
H	-4.84225100	-5.99391000	1.27634500
H	-4.63869800	-3.81387200	0.16468500
H	-6.47079600	-1.95987900	1.68262000
H	-8.78916100	-2.53216700	1.10827800
H	-9.54797300	-2.52263600	-1.27798400
H	-7.95915100	-1.85092200	-3.06909800
H	-5.75836300	-1.03109100	-3.76628800
H	-3.49480500	-0.16065600	-3.13875700
H	-2.60869300	0.30576000	3.94071700
O	-2.49807600	-0.07163400	-0.81793600
O	-3.12048500	0.83226500	1.49127600
N	-2.92420200	2.49386300	-0.44951500
C	-2.49022700	3.83814400	-0.21581700
C	-2.18134100	4.66245100	-1.32560400
C	-2.37584900	4.32756900	1.08705000
C	-1.73402800	5.97219500	-1.07165500
C	-1.93037500	5.62981500	1.31365800
H	-2.60736400	3.66587100	1.92109500
C	-1.61887000	6.45474400	0.23010200
H	-1.47236400	6.61242600	-1.91726400
H	-1.79365800	5.98557300	2.33485700
H	-1.26557800	7.47330900	0.40310000
C	-4.21908300	2.39323100	-1.06873300
C	-4.34861200	2.74584600	-2.43064200
C	-5.32873900	1.93626700	-0.34839400
C	-5.59564800	2.54554400	-3.05400900
C	-6.55447800	1.75108600	-0.98560800
H	-5.20506800	1.68953800	0.70413400
C	-6.68513800	2.04813600	-2.34593900

H	-5.69932900	2.79712500	-4.11261200
H	-7.40072600	1.35063700	-0.42426000
H	-7.63985200	1.88820000	-2.85167800
C	-2.32457200	4.20908500	-2.70838900
H	-1.65879500	4.69161000	-3.43117500
C	-3.26055700	3.35882100	-3.19055900
H	-3.29580400	3.21013600	-4.27469700
C	1.74871900	-1.72919700	-2.24573200
C	0.83326400	-1.41834000	-3.27706200
C	0.04993700	-2.40402100	-3.82380900
C	0.12949100	-3.73797600	-3.34179800
C	-0.74545800	-4.74773500	-3.82775400
C	-0.70348400	-6.02733700	-3.31903400
C	0.21757100	-6.34217900	-2.29165600
C	1.08579700	-5.38731300	-1.80757000
C	1.08610800	-4.06053500	-2.32247200
C	1.95068200	-3.02984000	-1.80450600
C	2.92776000	-2.74628100	0.47739300
C	2.96268800	-3.36232500	-0.76459000
C	3.94300400	-4.39377100	-0.96904000
C	4.20607100	-4.94475100	-2.25376800
C	5.15802800	-5.92768800	-2.42558500
C	5.89061100	-6.42235800	-1.31924200
C	5.66417300	-5.90606600	-0.06150600
C	4.70293600	-4.87968100	0.14737800
C	4.48117500	-4.31833100	1.43466200
C	3.63613500	-3.24784100	1.59199300
H	-0.66159800	-2.16736300	-4.61826500
H	-1.46513400	-4.48218400	-4.60630300
H	-1.38655500	-6.79298600	-3.69390300
H	0.23057600	-7.34770700	-1.86494500
H	1.76040100	-5.64209800	-0.99320900
H	3.65052300	-4.56768700	-3.11261000
H	5.35102600	-6.32605100	-3.42446600
H	6.63720100	-7.20609000	-1.46689200
H	6.23022200	-6.27268000	0.79885400
H	5.02803800	-4.72088300	2.29071400
H	3.49076100	-2.75473900	2.55292400
H	0.77627100	-0.38826300	-3.62609200
O	2.13295800	-1.65275000	0.69484400
O	2.46710800	-0.68598100	-1.69501600
N	3.81312800	0.31248800	0.14496300
C	4.29815800	0.35254800	1.48776200
C	5.35804300	-0.50394400	1.87952700

C	3.67262200	1.18391400	2.41930200
C	5.75715000	-0.46961800	3.23157000
C	4.09273800	1.20207500	3.74998200
H	2.84322800	1.80962800	2.09733700
C	5.14402400	0.37398800	4.15579500
H	6.56789500	-1.12946200	3.55143400
H	3.59157000	1.87303200	4.44981800
H	5.48190600	0.38069000	5.19469000
C	4.73900600	0.60308200	-0.91083600
C	5.75540600	-0.31873000	-1.24264900
C	4.62814000	1.79740900	-1.62763400
C	6.52141900	-0.07583100	-2.40010500
C	5.41850800	2.04123200	-2.75113600
H	3.90811100	2.53827000	-1.29221100
C	6.34858400	1.08006000	-3.15834400
H	7.28564900	-0.80448200	-2.68221400
H	5.30214100	2.97558600	-3.30516400
H	6.95864300	1.24456600	-4.04952200
C	6.00793400	-1.45529000	0.98027300
H	6.49603600	-2.28964200	1.48992500
C	6.12454200	-1.42465800	-0.36731400
H	6.68920100	-2.23534600	-0.83687100
P	-2.09522200	1.15560300	0.21463800
P	2.19873300	-0.22336000	-0.11746300
Ir	0.26432300	0.90773200	0.25869400
C	0.05131900	1.75586300	-1.65733000
H	0.31924100	1.07327600	-2.46406700
H	-0.91135800	2.23973600	-1.82610500
C	1.14118200	2.53118700	-1.12602100
H	2.11720700	2.25883000	-1.52239600
C	1.04596500	3.84669700	-0.58509400
H	0.12128400	4.10505700	-0.07243300
O	2.03976800	3.71165800	1.19516600
C	-0.19138900	-0.53203600	1.71046100
C	0.08006500	0.05313200	2.85069400
C	0.44849800	0.71836800	3.92923600
H	1.51336800	0.68043800	4.19234400
C	-0.41547600	1.57623800	4.81279800
H	-1.35664200	1.84866400	4.31730000
H	-0.64729300	1.07497700	5.77006400
H	0.12069300	2.50890200	5.04071000
C	-0.52883000	-1.95372800	1.51453100
C	-0.46340200	-2.85467500	2.59271200
C	-0.88384000	-2.45708000	0.25105300

C	-0.75253300	-4.20686200	2.41638800
H	-0.17403300	-2.47683500	3.57537300
C	-1.18897800	-3.80593400	0.07776600
H	-0.91336900	-1.77551700	-0.59676300
C	-1.12437800	-4.68860500	1.15836700
H	-0.69892000	-4.88833700	3.26865000
H	-1.47663500	-4.17112000	-0.90928300
H	-1.36665500	-5.74450300	1.02088500
C	1.78615700	4.98020700	-1.15186100
C	1.67786300	6.25230400	-0.55403300
C	2.55850700	4.84414800	-2.32104600
C	2.32758700	7.35108400	-1.10943400
H	1.10932200	6.34766600	0.37090400
C	3.20901700	5.94697300	-2.87447700
H	2.62536900	3.87593900	-2.81784600
C	3.09598000	7.20259400	-2.27031000
H	2.24176500	8.32974100	-0.63166600
H	3.79901200	5.82776000	-3.78616800
H	3.60436100	8.06650600	-2.70517900
C	3.33528500	4.27407200	1.23032700
H	3.90225400	3.93549500	0.35204200
H	3.30680900	5.37491400	1.23762200
H	3.85253900	3.92909800	2.13733200
B	1.17363900	4.00584200	2.39566500
F	-0.00638200	3.28911400	2.22137200
F	1.85859200	3.59200700	3.53676200
F	0.91766900	5.38076300	2.44455500

E1

Zero-point correction=	1.246747 (Hartree/Particle)
Thermal correction to Energy=	1.323315
Thermal correction to Enthalpy=	1.324259
Thermal correction to Gibbs Free Energy=	1.133086
Sum of electronic and zero-point Energies=	-4546.403829
Sum of electronic and thermal Energies=	-4546.327262
Sum of electronic and thermal Enthalpies=	-4546.326318
Sum of electronic and thermal Free Energies=	-4546.517491

C	2.34485900	-1.46491400	2.15317100
C	2.01032100	-1.12415500	3.48486200
C	2.70752900	-0.13571400	4.13415400
C	3.70686000	0.60595800	3.44785000

C	4.36525600	1.70483600	4.06081200
C	5.28388800	2.45844900	3.36282400
C	5.57187900	2.14719100	2.01097100
C	4.97489700	1.06818400	1.39674600
C	4.04365300	0.25073200	2.09745800
C	3.42148100	-0.88979800	1.48247300
C	3.16496200	-1.76767100	-0.86456700
C	3.96684800	-1.48045800	0.22837400
C	5.36384900	-1.84206600	0.13816000
C	6.24934600	-1.78326000	1.25056400
C	7.57691100	-2.13864000	1.12883200
C	8.09919500	-2.57189800	-0.11226500
C	7.26452400	-2.67124000	-1.20363700
C	5.88803300	-2.33081200	-1.10633200
C	5.01396500	-2.50798900	-2.21323100
C	3.67206100	-2.25790500	-2.08718600
H	2.47441500	0.11941900	5.16981500
H	4.11380500	1.95368000	5.09429500
H	5.77948700	3.30491600	3.84318000
H	6.27104100	2.76959800	1.44837800
H	5.19369800	0.84568400	0.35321300
H	5.87106300	-1.46783300	2.22103200
H	8.22925200	-2.09146900	2.00364500
H	9.15392300	-2.84191100	-0.19666800
H	7.64541700	-3.02952100	-2.16315300
H	5.41795700	-2.89062100	-3.15289200
H	2.96898100	-2.45480700	-2.89543500
H	1.20074300	-1.67371600	3.96519100
O	1.80244000	-1.54143800	-0.82690000
O	1.60552900	-2.46405800	1.56094000
N	0.49514300	-3.78442400	-0.32994100
C	-0.70935500	-4.49145900	-0.01608600
C	-1.44731600	-5.08443200	-1.06260700
C	-1.15763000	-4.55087900	1.30626600
C	-2.64998300	-5.73359400	-0.72529000
C	-2.36060000	-5.19074900	1.60952600
H	-0.55098800	-4.09420700	2.09066100
C	-3.10226300	-5.79130900	0.58984900
H	-3.24566600	-6.18469200	-1.52169400
H	-2.72081200	-5.21976200	2.63982400
H	-4.05318000	-6.27619800	0.81609400
C	1.58763700	-4.55450500	-0.86902900
C	1.48003000	-5.03133600	-2.19298200
C	2.74245700	-4.78731000	-0.11489500

C	2.60779000	-5.65742600	-2.76006600
C	3.83936000	-5.42570200	-0.69333200
H	2.78479000	-4.43186400	0.91282200
C	3.77583800	-5.84662600	-2.02511000
H	2.54635200	-6.01664000	-3.79022700
H	4.74841900	-5.57691400	-0.10829100
H	4.63640500	-6.33465600	-2.48759900
C	-1.02628200	-5.02050300	-2.46130000
H	-1.83838000	-5.11071000	-3.18960200
C	0.23382200	-4.96532400	-2.95449200
H	0.34498000	-5.01535800	-4.04209700
C	0.03233100	1.86852100	-2.29434000
C	0.55971900	0.74749400	-2.97230800
C	1.91825000	0.62745000	-3.12360200
C	2.79740800	1.60000100	-2.57844100
C	4.20740300	1.42054500	-2.63498000
C	5.06301000	2.35436000	-2.09402900
C	4.53411500	3.51381300	-1.47768200
C	3.17154000	3.71658000	-1.40842800
C	2.25398200	2.76931300	-1.94541000
C	0.82219300	2.91069200	-1.82984600
C	-0.67795700	3.96145800	-0.10857400
C	0.19721900	4.09558000	-1.18020400
C	0.48719200	5.43255600	-1.63502000
C	1.19786500	5.68594600	-2.84147900
C	1.46313200	6.97460600	-3.25538000
C	1.03635200	8.08246200	-2.48469600
C	0.32532200	7.87400100	-1.32298600
C	0.02018300	6.55875200	-0.87814500
C	-0.76086200	6.33592000	0.28857500
C	-1.12750200	5.06456700	0.64955400
H	2.34119500	-0.23590000	-3.63763700
H	4.59731300	0.51490600	-3.10427300
H	6.14378300	2.20358000	-2.13881300
H	5.21152000	4.25691500	-1.05067700
H	2.78702400	4.61450600	-0.92963500
H	1.52504600	4.84531800	-3.45258700
H	2.00170800	7.14161900	-4.19084900
H	1.25902200	9.09754500	-2.82033900
H	-0.02860100	8.72060100	-0.72945800
H	-1.10542600	7.19405100	0.86974600
H	-1.78005700	4.87064800	1.50011500
H	-0.12648200	-0.00705400	-3.35126900
O	-1.11759700	2.72613500	0.33213400

O	-1.33894500	1.90628800	-2.06668400
N	-3.44213100	1.96201100	-0.55225200
C	-4.50820600	1.02140800	-0.73654100
C	-5.33473800	0.71771200	0.36575100
C	-4.73631200	0.45566500	-1.99129900
C	-6.37467000	-0.20973200	0.16836300
C	-5.78531900	-0.44732000	-2.16568400
H	-4.08192800	0.73055300	-2.82022500
C	-6.60435200	-0.77754900	-1.08215600
H	-7.01507200	-0.47740700	1.01112100
H	-5.95834800	-0.89962700	-3.14422700
H	-7.41498200	-1.49688600	-1.20687800
C	-3.84955800	3.32527800	-0.36004300
C	-4.45420600	3.66712500	0.86903500
C	-3.61521100	4.28428000	-1.34807200
C	-4.76363000	5.02442200	1.08815400
C	-3.95207100	5.61737000	-1.11507600
H	-3.13969300	3.97594600	-2.27968600
C	-4.52058300	5.98602500	0.10915500
H	-5.22145600	5.31515000	2.03686800
H	-3.75303800	6.37010600	-1.88016700
H	-4.77762600	7.03025000	0.29970800
C	-5.17804600	1.38145700	1.66066500
H	-5.52951200	0.81072600	2.52639600
C	-4.79403900	2.66363900	1.87900300
H	-4.85925300	3.03637300	2.90621100
P	0.69358400	-2.20301400	0.18001200
P	-1.83332100	1.52129400	-0.52046000
Ir	-0.88406400	-0.51633200	0.15712000
C	-1.70923700	-1.43426200	-1.63433600
H	-2.00084900	-0.67439800	-2.37983900
H	-0.96001800	-2.05582100	-2.15472200
C	-2.90935300	-2.28496300	-1.33786300
H	-3.23183700	-2.92920200	-2.16546200
C	-3.61666300	-2.32234800	-0.19665700
H	-3.28895800	-1.68356800	0.62769800
C	-0.16072400	0.44302100	1.81140900
C	-1.09983300	-0.45153300	2.19578500
C	-1.79092900	-1.14167400	3.11820800
H	-2.45973000	-1.93476500	2.76411100
C	-1.70934300	-0.92764800	4.59576400
H	-2.66782200	-0.54009500	4.98523100
H	-1.53205100	-1.88611100	5.11287200
H	-0.91162300	-0.22633700	4.87354600

C	0.60523400	1.54680400	2.25028800
C	0.34206200	2.15076300	3.50620400
C	1.59643400	2.10219800	1.40887000
C	1.02759000	3.29435300	3.88741300
H	-0.43019900	1.72645200	4.14791500
C	2.29138300	3.23555200	1.80650000
H	1.79464300	1.62638500	0.44983900
C	2.00544100	3.83353500	3.03735600
H	0.80958000	3.77281800	4.84429300
H	3.06629300	3.64602700	1.16366400
H	2.55239500	4.72840600	3.34202000
C	-4.79825000	-3.14110000	0.08535400
C	-5.30484600	-3.17587500	1.39645500
C	-5.45844600	-3.90728000	-0.89268800
C	-6.41007400	-3.95935700	1.72911600
H	-4.81560500	-2.57336700	2.16668800
C	-6.56360200	-4.69106500	-0.56654500
H	-5.10539300	-3.88429300	-1.92491600
C	-7.04515400	-4.72644800	0.74775500
H	-6.78047000	-3.97171400	2.75717000
H	-7.05932000	-5.27811000	-1.34367700
H	-7.91218200	-5.34027300	1.00132600

(*S*,*R*)-**[E-F]**‡

Zero-point correction=	1.302627 (Hartree/Particle)
Thermal correction to Energy=	1.386275
Thermal correction to Enthalpy=	1.387219
Thermal correction to Gibbs Free Energy=	1.181147
Sum of electronic and zero-point Energies=	-4985.919879
Sum of electronic and thermal Energies=	-4985.836231
Sum of electronic and thermal Enthalpies=	-4985.835287
Sum of electronic and thermal Free Energies=	-4986.041359

C	3.90502500	-0.59628700	1.09502700
C	3.88872800	-1.88568800	1.67913300
C	4.39622300	-2.05006800	2.94646100
C	4.89175300	-0.94232900	3.68809100
C	5.33305900	-1.08639000	5.03177500
C	5.78357000	-0.00129200	5.75194200

C	5.80529500	1.28073200	5.15178000
C	5.39913200	1.45169600	3.84480300
C	4.94190700	0.35116800	3.06708200
C	4.50099600	0.50028500	1.70507400
C	3.59983700	2.42068300	0.38882700
C	4.68359400	1.78293500	0.97137200
C	5.98203100	2.37815000	0.80275200
C	7.17961700	1.71785800	1.19551600
C	8.41249500	2.30193400	0.99573000
C	8.51705700	3.58173600	0.39869100
C	7.37884900	4.24154900	-0.01018800
C	6.09304400	3.65949200	0.16336200
C	4.91952200	4.30867600	-0.31133300
C	3.69419200	3.69135200	-0.22279200
H	4.40970000	-3.04346100	3.40216000
H	5.29978200	-2.07994500	5.48620000
H	6.11558700	-0.12477500	6.78530300
H	6.14358600	2.14375900	5.73003600
H	5.41461300	2.44589000	3.39896100
H	7.11540100	0.72759300	1.64441100
H	9.31768300	1.76898000	1.29568900
H	9.49968000	4.03608000	0.25289500
H	7.44683700	5.22158100	-0.48927700
H	5.01034200	5.29338200	-0.77578900
H	2.77976300	4.14899900	-0.60285200
H	3.48485600	-2.72114000	1.09172200
O	2.36716400	1.80553300	0.38456400
O	3.35237600	-0.48709600	-0.16109600
N	2.63590600	0.80623600	-2.14615000
C	3.92295100	0.34041900	-2.59964800
C	4.01239700	-0.95611800	-3.15334800
C	5.06050100	1.12710000	-2.41565200
C	5.29720500	-1.45313100	-3.44844400
C	6.32049600	0.62029500	-2.73411500
H	4.95157400	2.12442100	-1.99433800
C	6.43676500	-0.67900400	-3.24143000
H	5.38656300	-2.46610200	-3.84642200
H	7.20873000	1.23212200	-2.56211400
H	7.42168600	-1.09031400	-3.47428600
C	1.68435300	1.07568700	-3.18497600
C	1.11739000	-0.00300400	-3.90069600
C	1.31518500	2.39427700	-3.46136100
C	0.07921200	0.29249900	-4.80748000
C	0.30692900	2.66587900	-4.38668600

H	1.82552300	3.19612500	-2.92697800
C	-0.32807600	1.60395200	-5.04234100
H	-0.39275100	-0.52981300	-5.34778100
H	0.00934400	3.69770900	-4.58618900
H	-1.13030900	1.80319700	-5.75691400
C	2.83956700	-1.78529200	-3.41677200
H	2.99542500	-2.86662600	-3.39673200
C	1.59278400	-1.37275200	-3.74725300
H	0.87098100	-2.15404300	-3.98803300
P	2.07697400	0.47805500	-0.57786100
Ir	-0.16498900	-0.15050700	-0.32444000
C	0.63053900	-2.09741100	-0.87767800
H	0.17552100	-2.56565500	-1.74386300
H	1.71727100	-2.17386400	-0.87251700
C	-0.06014500	-2.25843600	0.36614900
H	-1.04284500	-2.72081600	0.33336900
C	-0.50932600	1.77552700	0.58171300
C	-0.36593400	0.93819200	1.55094200
C	-0.10672400	0.14491800	2.64599500
H	-0.93826900	-0.45147600	3.03113800
C	1.08801100	0.35246600	3.52370000
H	1.94226900	0.74743300	2.95830300
H	0.84483600	1.07907600	4.32130700
H	1.37690200	-0.58246400	4.02739700
C	-0.66110400	3.20515100	0.41677000
C	-1.15862000	4.00418300	1.46593400
C	-0.22193200	3.82950300	-0.75830800
C	-1.17702100	5.39082300	1.34633800
H	-1.52902200	3.52235900	2.37279200
C	-0.22307200	5.21967900	-0.86858300
H	0.12411700	3.20130300	-1.57400500
C	-0.69637500	6.00602900	0.18453200
H	-1.57777600	5.99831000	2.16028800
H	0.13510500	5.69064500	-1.78799900
H	-0.70977800	7.09471500	0.09699200
C	-0.03715400	-2.81478600	2.82532400
C	0.80366600	-3.16159300	3.90441600
C	-1.42223200	-3.07385500	2.93906800
C	0.28136900	-3.76371000	5.04882900
H	1.87582100	-2.97712200	3.81965400
C	-1.93805300	-3.66766100	4.08500700
H	-2.09228200	-2.78655200	2.12980300
C	-1.08929900	-4.01943600	5.14416300
H	0.94835300	-4.03999400	5.86856600

H	-3.01153300	-3.85929900	4.15749200
H	-1.49842400	-4.49056100	6.04081400
C	0.53618700	-2.18406400	1.65402200
H	1.58765700	-1.91372900	1.71163600
O	3.07778500	-4.01440900	-0.42206400
B	2.08561900	-4.95444300	-0.94937300
F	0.93204300	-4.87846000	-0.13453400
F	1.73192600	-4.57018600	-2.27991700
F	2.57148900	-6.25887300	-0.97573500
C	4.36142500	-4.12249900	-0.96296600
H	4.86364400	-5.06315200	-0.66645600
H	4.35451400	-4.09303700	-2.06992000
H	4.97958000	-3.27447200	-0.61705100
C	-3.51790500	1.80449500	-1.26983900
C	-2.96281800	2.69667600	-2.21205700
C	-3.13428500	4.04845900	-2.04325200
C	-3.78781100	4.55608700	-0.88876200
C	-3.90413700	5.95402700	-0.66328700
C	-4.47428800	6.44287000	0.49081800
C	-4.93723800	5.54269000	1.48044900
C	-4.86263100	4.18031700	1.28100300
C	-4.31232500	3.64146100	0.08466700
C	-4.25258600	2.22596300	-0.16900500
C	-4.37220900	0.14367200	1.24599300
C	-4.99063900	1.25334900	0.68553200
C	-6.40647400	1.40783000	0.92302700
C	-7.19635500	2.36861300	0.23082400
C	-8.55188700	2.48138100	0.46099800
C	-9.19683100	1.64460300	1.40219600
C	-8.46734900	0.68875400	2.07523500
C	-7.07353900	0.53383500	1.84582900
C	-6.33462000	-0.49578400	2.48976000
C	-5.01665200	-0.70277300	2.17719600
H	-2.72699500	4.75203200	-2.77187900
H	-3.50881300	6.63606800	-1.41953200
H	-4.55048300	7.52008400	0.65538900
H	-5.35851800	5.93043100	2.41100100
H	-5.22417000	3.49896200	2.05058900
H	-6.72222800	3.01452800	-0.50631500
H	-9.13318700	3.22104900	-0.09447900
H	-10.26927700	1.74904000	1.58155900
H	-8.95378100	0.01978800	2.78980600
H	-6.84330300	-1.15047500	3.20056300
H	-4.44286000	-1.52427100	2.60588800

H	-2.40629400	2.28043500	-3.05240400
O	-3.06737600	-0.18265700	0.94944100
O	-3.36598000	0.45564600	-1.51247400
N	-3.05967900	-2.01439900	-0.96739900
C	-2.41770600	-2.82576300	-1.96385900
C	-1.98071800	-4.12088600	-1.60526700
C	-2.19814200	-2.32259300	-3.24854500
C	-1.24021900	-4.85408800	-2.54825100
C	-1.50465300	-3.09443600	-4.18416600
H	-2.55827800	-1.32277400	-3.49565200
C	-1.01077600	-4.35195100	-3.82644000
H	-0.82131400	-5.81689000	-2.25660200
H	-1.33246800	-2.70347900	-5.18928900
H	-0.41818900	-4.93451400	-4.53345000
C	-4.36995000	-2.45471100	-0.57328100
C	-4.47097700	-3.62531700	0.21301100
C	-5.51335600	-1.73585300	-0.93950300
C	-5.74670200	-3.98027700	0.69640500
C	-6.76579300	-2.11909000	-0.46232600
H	-5.40065500	-0.85440800	-1.56810000
C	-6.87853000	-3.23699700	0.37091500
H	-5.83893300	-4.87070500	1.32351600
H	-7.64823100	-1.53160500	-0.72278100
H	-7.85499700	-3.53352800	0.76071300
C	-2.24303200	-4.70539100	-0.29155400
H	-1.49820200	-5.43551300	0.03594900
C	-3.32211700	-4.48665300	0.49816200
H	-3.40225600	-5.09168100	1.40661800
P	-2.41567500	-0.51026500	-0.53851100

(*R*,*S*)-**[E-F]**‡

Zero-point correction=	1.302839 (Hartree/Particle)
Thermal correction to Energy=	1.386231
Thermal correction to Enthalpy=	1.387176
Thermal correction to Gibbs Free Energy=	1.183559
Sum of electronic and zero-point Energies=	-4985.923228
Sum of electronic and thermal Energies=	-4985.839836
Sum of electronic and thermal Enthalpies=	-4985.838892
Sum of electronic and thermal Free Energies=	-4986.042508

C	2.29654000	-1.52095400	-2.70626500
C	1.76781400	-1.29885300	-3.99911700
C	2.42445200	-0.47520000	-4.87773100
C	3.62175000	0.18636700	-4.49179400
C	4.27336100	1.09460500	-5.36792900
C	5.41057400	1.76747100	-4.97803800
C	5.92791000	1.56857800	-3.67720200
C	5.31958800	0.69024700	-2.80521100
C	4.16416800	-0.04771600	-3.18499000
C	3.50437000	-0.97096600	-2.29487100
C	3.33816200	-1.15844900	0.20024000
C	4.08228500	-1.29293200	-0.96332600
C	5.43813700	-1.76473300	-0.82502200
C	6.22009800	-2.16922600	-1.94277100
C	7.50761200	-2.63840600	-1.78279500
C	8.08955600	-2.72073600	-0.49531700
C	7.35368600	-2.35395800	0.61097400
C	6.01756600	-1.88807300	0.48188400
C	5.22991000	-1.57910200	1.62458500
C	3.90671500	-1.25241900	1.48837600
H	2.02110700	-0.29817800	-5.87730500
H	3.84430000	1.25749700	-6.35974900
H	5.90131900	2.46468600	-5.66096300
H	6.81172700	2.12371100	-3.35409300
H	5.72122700	0.56789300	-1.80103500
H	5.78386200	-2.11948300	-2.93982900
H	8.08056200	-2.95368100	-2.65798900
H	9.11279300	-3.08600600	-0.38138400
H	7.78174500	-2.43240100	1.61369400
H	5.67481000	-1.65365400	2.61884500
H	3.26294200	-1.07973300	2.34702700
H	0.83221700	-1.79060600	-4.26111200
O	1.98668200	-0.87378500	0.16457200
O	1.58782100	-2.35467900	-1.86935300
N	0.80778400	-3.24080300	0.40425500
C	-0.32368800	-4.11761700	0.42273000
C	-1.02901900	-4.28023500	1.63285400
C	-0.70861000	-4.79651800	-0.74052000
C	-2.19863300	-5.06515200	1.61362100
C	-1.83300900	-5.62201200	-0.71970900
H	-0.11520500	-4.66227200	-1.64680900
C	-2.58521900	-5.73969900	0.45757500
H	-2.80576700	-5.11570000	2.51736300
H	-2.13643400	-6.15258200	-1.62502500

H	-3.48614700	-6.35729900	0.47051700
C	1.95360700	-3.76951700	1.08700800
C	1.91199600	-3.82828800	2.49705800
C	3.07037400	-4.22093800	0.37536900
C	3.07121700	-4.27022600	3.16594000
C	4.19537500	-4.67425700	1.06038200
H	3.05425900	-4.17380800	-0.71287800
C	4.19708700	-4.68581300	2.46060600
H	3.06765900	-4.29842300	4.25837700
H	5.07886500	-4.99291500	0.50421100
H	5.08343400	-5.02430300	3.00212300
C	-0.57939400	-3.67283400	2.88559400
H	-1.37010700	-3.42525100	3.59952500
C	0.71019300	-3.48443800	3.25660600
H	0.88745900	-3.13623000	4.27769100
C	-0.59378500	1.45418100	2.67984600
C	-0.86623300	0.34304800	3.50257300
C	0.15688100	-0.21351000	4.22914600
C	1.48545300	0.27954000	4.11025300
C	2.56493500	-0.32893400	4.80913200
C	3.85448700	0.14134500	4.67926200
C	4.12064100	1.23119800	3.81615900
C	3.09590700	1.84849700	3.13003500
C	1.74733900	1.41700500	3.27167100
C	0.64977000	2.06813600	2.60259200
C	0.38523500	3.60837700	0.61571400
C	0.81619600	3.38096100	1.91644800
C	1.40532600	4.50139500	2.61529900
C	1.68122900	4.46902100	4.01137000
C	2.24578600	5.55003900	4.65599000
C	2.57158200	6.72705500	3.94182600
C	2.29053600	6.80557600	2.59518800
C	1.68985800	5.71691100	1.90636900
C	1.33755000	5.82112200	0.53266200
C	0.67141400	4.79947300	-0.09131400
H	-0.05973300	-1.05448800	4.88877200
H	2.34825200	-1.18433000	5.45371700
H	4.67249200	-0.33574500	5.22410900
H	5.14760200	1.57770100	3.68110600
H	3.31746700	2.67917100	2.46059100
H	1.42621800	3.57822500	4.58272600
H	2.43590400	5.49721200	5.73049700
H	3.02724600	7.57308500	4.46144100
H	2.51239700	7.71672600	2.03341800

H	1.56840000	6.74174100	-0.00811700
H	0.33992100	4.86685000	-1.12746500
H	-1.88041800	-0.04881100	3.56807700
O	-0.29555900	2.66305200	-0.11334900
O	-1.64430700	1.96298000	1.92968100
N	-2.88899200	2.71057400	-0.18929600
C	-4.18755300	2.12700800	-0.29626200
C	-4.87927700	2.22417300	-1.52621800
C	-4.73010900	1.42548900	0.78571100
C	-6.13155300	1.58537100	-1.61910000
C	-5.95955000	0.77528800	0.65524400
H	-4.18656600	1.35528900	1.72815300
C	-6.66520600	0.86706600	-0.54790700
H	-6.68748200	1.65500700	-2.55801700
H	-6.33888600	0.19779300	1.49937300
H	-7.62904900	0.36567400	-0.65824300
C	-2.79834300	4.13704900	-0.26951900
C	-2.99948100	4.74960500	-1.52589000
C	-2.46193600	4.89657300	0.85417500
C	-2.76093500	6.13380600	-1.62856500
C	-2.25251000	6.27063100	0.73158500
H	-2.32844000	4.39074700	1.80998800
C	-2.38833100	6.88667200	-0.51601500
H	-2.89134400	6.62000400	-2.59876100
H	-1.95920400	6.85299300	1.60720300
H	-2.20891200	7.95903900	-0.62075600
C	-4.33242100	2.93979700	-2.67959600
H	-4.71785000	2.61180800	-3.65101100
C	-3.50143500	4.01079800	-2.68359300
H	-3.27636900	4.45941600	-3.65646100
P	0.78699800	-1.80826400	-0.48463400
P	-1.58864100	1.74016900	0.28124200
Ir	-0.95418300	-0.38781000	-0.53409500
C	-2.23192600	-1.21585300	0.99216400
H	-2.91350300	-0.50657500	1.45407800
H	-1.74145200	-1.86307100	1.71371100
C	-2.58890200	-1.81489700	-0.26513700
H	-2.26118400	-2.83839200	-0.43400800
C	-3.58891900	-1.31739800	-1.16939700
H	-3.92357300	-0.29180400	-1.02514700
C	-0.13532400	0.69648300	-2.24842000
C	-1.15270300	0.05909800	-2.69291000
C	-2.22621100	-0.70127500	-3.13396800
H	-3.12477600	-0.15286800	-3.43636100

C	-1.99118100	-2.05461900	-3.74391700
H	-1.64400800	-1.93832500	-4.78645400
H	-2.91181300	-2.65207100	-3.77246400
H	-1.22033900	-2.60778300	-3.18878000
C	0.90276300	1.64317600	-2.57894000
C	0.83495200	2.37144900	-3.78289500
C	1.96836600	1.87885600	-1.69484800
C	1.81594000	3.31068900	-4.09160900
H	0.00123300	2.19447300	-4.46542300
C	2.94371200	2.82242400	-2.00779500
H	2.00729600	1.32527500	-0.75866400
C	2.87430700	3.53808900	-3.20518000
H	1.75924400	3.86704800	-5.03026000
H	3.76569500	2.99779900	-1.31193600
H	3.64730800	4.26872400	-3.45176600
C	-4.49401000	-2.17875900	-1.91623300
C	-4.46282300	-3.58312800	-1.79565200
C	-5.44477100	-1.60617100	-2.78941800
C	-5.34263600	-4.38055000	-2.52501500
H	-3.76034500	-4.05240400	-1.11238900
C	-6.31739000	-2.40461900	-3.52157400
H	-5.48960800	-0.52143000	-2.88180800
C	-6.27024200	-3.79871600	-3.39412200
H	-5.30753500	-5.46607400	-2.40656100
H	-7.04403800	-1.94093600	-4.19283900
H	-6.95884100	-4.42603400	-3.96473400
O	-4.00917900	-2.83373800	2.62655300
B	-4.01988500	-1.85164900	3.69447800
F	-5.03517700	-2.07217700	4.61528200
F	-4.18811700	-0.52445100	3.15216400
F	-2.74945200	-1.90577500	4.32001700
C	-5.14508600	-2.92576000	1.83202900
H	-5.23208600	-2.08589300	1.11029200
H	-6.07745400	-2.94317600	2.42938000
H	-5.10828900	-3.85691900	1.23630600

(*S*,*S*)-**[E-F]**‡

Zero-point correction=	1.302885 (Hartree/Particle)
Thermal correction to Energy=	1.386261
Thermal correction to Enthalpy=	1.387205
Thermal correction to Gibbs Free Energy=	1.183803
Sum of electronic and zero-point Energies=	-4985.926000

Sum of electronic and thermal Energies=	-4985.842625
Sum of electronic and thermal Enthalpies=	-4985.841681
Sum of electronic and thermal Free Energies=	-4986.045082

C	0.70282200	-2.15668100	2.47126700
C	-0.47294400	-2.17256100	3.25491700
C	-0.48634700	-1.56129800	4.48201900
C	0.67368800	-0.90416700	4.97416000
C	0.65155800	-0.21956700	6.21807100
C	1.75942900	0.45871500	6.67706300
C	2.93087000	0.49680300	5.88662200
C	2.98333600	-0.15812100	4.67360700
C	1.87197300	-0.89939000	4.18500700
C	1.88839600	-1.58504900	2.91510000
C	3.12591600	-1.21792000	0.76036000
C	3.12291100	-1.63092700	2.08613500
C	4.37093300	-2.11670700	2.62171700
C	4.44534100	-2.79456400	3.87068500
C	5.64503700	-3.27531000	4.35317100
C	6.84147500	-3.09475000	3.61853800
C	6.80281700	-2.45743500	2.39703100
C	5.57904600	-1.97354100	1.86090800
C	5.52011000	-1.39038100	0.56560600
C	4.31318800	-1.05183700	0.01282500
H	-1.40809700	-1.54190100	5.06644100
H	-0.27395200	-0.23219300	6.79835200
H	1.72847700	0.98280400	7.63502000
H	3.80055500	1.06099000	6.23211500
H	3.88706600	-0.09292800	4.07052000
H	3.53193700	-2.94487000	4.44506400
H	5.67031300	-3.80263400	5.30963700
H	7.78730000	-3.47077100	4.01541800
H	7.71495400	-2.32924900	1.80827700
H	6.44046500	-1.26245400	-0.00789700
H	4.23016200	-0.67005300	-1.00208900
H	-1.36950900	-2.63807400	2.85485500
O	1.95825600	-0.89878500	0.09415400
O	0.65083100	-2.76554600	1.22937800
N	1.32115600	-3.11367300	-1.22349900
C	0.45229200	-3.93731100	-2.00065300
C	0.57751100	-3.92412700	-3.40804300
C	-0.50631000	-4.74308400	-1.37350200
C	-0.34381200	-4.68315700	-4.15708800

C	-1.39092000	-5.50619700	-2.13531700
H	-0.54853600	-4.74968700	-0.28368200
C	-1.31286000	-5.46608700	-3.53283000
H	-0.27720500	-4.66559800	-5.24768400
H	-2.15058900	-6.11507800	-1.64150000
H	-2.00911400	-6.05200200	-4.13705400
C	2.67975400	-3.57231700	-1.19047400
C	3.46506500	-3.41403600	-2.35296800
C	3.21574900	-4.16214400	-0.04038300
C	4.82736600	-3.76809300	-2.28433700
C	4.56029900	-4.52570400	-0.00394000
H	2.57562300	-4.29020800	0.83079800
C	5.37093900	-4.31290700	-1.12496500
H	5.45363800	-3.62502600	-3.16847200
H	4.98224300	-4.94833100	0.90956900
H	6.43014600	-4.57709200	-1.09120500
C	1.64513200	-3.19039300	-4.08658900
H	1.43389100	-2.90054700	-5.12096700
C	2.89912600	-2.96853200	-3.62332700
H	3.61358800	-2.51773700	-4.31789000
C	1.15994200	1.88139800	-2.95249100
C	1.41223000	0.90782100	-3.94625100
C	2.68729200	0.43875900	-4.14093500
C	3.75275600	0.87572600	-3.30853400
C	5.05899200	0.32628800	-3.42678200
C	6.07775800	0.72959900	-2.59040400
C	5.82211700	1.69610200	-1.58832800
C	4.56910000	2.25636900	-1.45609500
C	3.49929800	1.88202100	-2.31682700
C	2.18006100	2.44782900	-2.19829500
C	0.92310700	3.53596200	-0.33002400
C	1.91282700	3.60090100	-1.29904900
C	2.66417800	4.82596500	-1.40644000
C	3.57053800	5.07644000	-2.47443100
C	4.27050000	6.26249200	-2.55457300
C	4.10610100	7.26480800	-1.56915600
C	3.22120900	7.06343200	-0.53192800
C	2.47411400	5.85886100	-0.42798600
C	1.53111600	5.66217200	0.61839600
C	0.75674900	4.53154100	0.65942900
H	2.88955200	-0.29553400	-4.92174100
H	5.23823200	-0.43285900	-4.19225800
H	7.07537500	0.29538000	-2.68805100
H	6.62020700	1.99060300	-0.90344200

H	4.38367300	2.98610100	-0.66921700
H	3.70106200	4.32078900	-3.24823400
H	4.95344500	6.43127500	-3.39054000
H	4.67060400	8.19737800	-1.63986100
H	3.07074700	7.83534200	0.22725400
H	1.40636200	6.44041900	1.37453900
H	0.00400000	4.37032300	1.42837000
H	0.57717500	0.56144100	-4.55328900
O	0.09733600	2.44381900	-0.23464000
O	-0.14780500	2.28180800	-2.76019900
N	-2.23956600	2.83911400	-1.35630300
C	-3.54842300	2.30750700	-1.58973500
C	-4.40402500	2.08779300	-0.48988400
C	-3.94370100	1.98684600	-2.89276600
C	-5.65330200	1.48412600	-0.74029200
C	-5.19888100	1.41964800	-3.12240000
H	-3.25062300	2.18567400	-3.71277600
C	-6.04956100	1.16833900	-2.03949300
H	-6.29573900	1.25673600	0.11151600
H	-5.50550400	1.16049300	-4.13796700
H	-7.02470100	0.70727900	-2.20994100
C	-2.15665200	4.20228200	-0.92892500
C	-2.64612600	4.53411400	0.35461100
C	-1.53669800	5.15713300	-1.74023400
C	-2.46471800	5.86071000	0.79531000
C	-1.37625700	6.46392100	-1.28153500
H	-1.15451900	4.84662100	-2.71317500
C	-1.84400100	6.81313100	-0.00944600
H	-2.82281200	6.13469700	1.79072100
H	-0.87158500	7.20307800	-1.90692700
H	-1.71455000	7.83343300	0.35899900
C	-4.04910100	2.48606100	0.87082300
H	-4.52069600	1.91649200	1.67517600
C	-3.29712000	3.55579300	1.22545400
H	-3.22944600	3.76761500	2.29633500
P	0.67692000	-1.90057200	-0.21849200
P	-0.92315200	1.79479100	-1.34430400
Ir	-0.94793000	-0.49683800	-0.84953400
C	-1.20085900	-0.86847300	-2.96208200
H	-1.60244200	0.00273400	-3.48366200
H	-0.35168200	-1.34487300	-3.45455200
C	-2.10519100	-1.75243100	-2.27904000
H	-1.82110100	-2.80187800	-2.22592400
C	-3.43809600	-1.44190600	-1.85044900

H	-3.74600700	-0.39777800	-1.88164800
C	-1.25049400	0.14234100	1.24489700
C	-2.21783300	-0.62307600	0.92468900
C	-3.22159400	-1.50456500	0.55940800
H	-4.22514700	-1.07085100	0.54707400
C	-3.10180900	-2.96748300	0.83680500
H	-3.48615100	-3.10177400	1.86237200
H	-3.73256400	-3.56485800	0.16571500
H	-2.06287200	-3.31305000	0.78717000
C	-0.71467400	0.98424100	2.28432900
C	-1.57728000	1.41432600	3.31477000
C	0.63244900	1.37973400	2.29088600
C	-1.08464500	2.24096900	4.32224100
H	-2.62105300	1.09719800	3.32110700
C	1.11076000	2.21052300	3.30133700
H	1.28874500	1.03892900	1.49363800
C	0.25548100	2.64431800	4.31771600
H	-1.75610400	2.56653300	5.12027400
H	2.15894500	2.51344400	3.29972600
H	0.63744300	3.28638000	5.11463900
C	-4.51944900	-2.43032200	-1.88054800
C	-4.36225900	-3.66618700	-2.54127000
C	-5.75721400	-2.16377900	-1.25458800
C	-5.39730100	-4.60063700	-2.56951600
H	-3.43003600	-3.88925300	-3.05681200
C	-6.78480900	-3.10186500	-1.27845400
H	-5.89845600	-1.23495300	-0.70403300
C	-6.61170200	-4.32619000	-1.93518600
H	-5.25403700	-5.54806000	-3.09512900
H	-7.72375700	-2.88026400	-0.76662200
H	-7.41961000	-5.06131400	-1.95000500
O	-6.22881000	-0.89787600	3.90563200
B	-5.17679100	-0.37731200	3.11531700
F	-5.61363700	-0.30204900	1.75546900
F	-4.76639400	0.92838900	3.51247900
F	-3.99889900	-1.19488100	3.15760600
C	-6.00628000	-1.01208400	5.27630600
H	-5.17519800	-1.70865800	5.51440400
H	-5.76167500	-0.03837800	5.74763900
H	-6.91710200	-1.40159300	5.76449900

B2'

Zero-point correction=	1.320421 (Hartree/Particle)
Thermal correction to Energy=	1.403692
Thermal correction to Enthalpy=	1.404636
Thermal correction to Gibbs Free Energy=	1.201781
Sum of electronic and zero-point Energies=	-4986.365774
Sum of electronic and thermal Energies=	-4986.282503
Sum of electronic and thermal Enthalpies=	-4986.281559
Sum of electronic and thermal Free Energies=	-4986.484414

C	3.00116900	0.12427100	-2.48082000
C	2.62539200	-0.28018800	-3.78063100
C	3.09562800	-1.46261200	-4.29230600
C	3.92657100	-2.30780100	-3.50778900
C	4.35445500	-3.57192300	-3.99350100
C	5.12789000	-4.40583300	-3.21585100
C	5.48768300	-4.00779700	-1.90773200
C	5.09443400	-2.78233300	-1.41200900
C	4.32305700	-1.88251400	-2.19742600
C	3.90309100	-0.59100300	-1.70615800
C	3.61588300	0.39590500	0.59058700
C	4.44017900	-0.06694900	-0.42122100
C	5.86329500	0.00516100	-0.18891300
C	6.81530900	-0.19600300	-1.22647600
C	8.16929500	-0.08845000	-0.98352800
C	8.64829200	0.21274800	0.31350500
C	7.75296800	0.43191900	1.33782000
C	6.35207600	0.35657800	1.11315700
C	5.42651500	0.67126800	2.14545200
C	4.08181000	0.72223500	1.88199900
H	2.81733400	-1.77887900	-5.29993000
H	4.04920700	-3.87446100	-4.99808800
H	5.45134000	-5.37571300	-3.59979000
H	6.07636100	-4.68021100	-1.27965300
H	5.36739300	-2.50222700	-0.39611300
H	6.46689100	-0.42193300	-2.23319900
H	8.87778700	-0.23448900	-1.80189400
H	9.72285900	0.28354000	0.49498800
H	8.10729200	0.68825000	2.33929800
H	5.80320900	0.91989300	3.13981800
H	3.35166700	1.01079800	2.63714500
H	1.96677000	0.37357200	-4.35144900
O	2.24811000	0.54228600	0.39062300
O	2.46923700	1.32761800	-2.03720800
N	1.95373700	3.11011600	-0.27568100

C	1.12062400	4.21443800	-0.63901400
C	0.65834600	5.09250400	0.36968500
C	0.77142700	4.41589500	-1.97792600
C	-0.17604800	6.15592800	-0.02419300
C	-0.07743900	5.46290600	-2.33949600
H	1.18968900	3.74585400	-2.72968200
C	-0.54669200	6.33990000	-1.35551100
H	-0.53085800	6.84918600	0.74081400
H	-0.35402200	5.60440400	-3.38631200
H	-1.19296700	7.17665400	-1.62993200
C	3.25876200	3.45933100	0.23483900
C	3.34411600	4.03157400	1.52232500
C	4.41221300	3.21445600	-0.51601500
C	4.62531700	4.26416500	2.05859100
C	5.66975400	3.46137000	0.03373200
H	4.31646800	2.79428200	-1.51525300
C	5.77538600	3.97733800	1.32889500
H	4.70546400	4.69055200	3.06134200
H	6.56673800	3.22845800	-0.54275900
H	6.75912700	4.15794800	1.76681400
C	1.00497100	4.92796700	1.78202200
H	0.26462800	5.29926000	2.49497900
C	2.16572500	4.44520500	2.28237100
H	2.28844500	4.47670900	3.36925800
C	-1.71451100	-1.14037900	2.50282800
C	-1.70145800	-0.10576900	3.46127400
C	-0.60261300	0.05402000	4.27256500
C	0.53526500	-0.78188400	4.11030000
C	1.74749500	-0.52861800	4.81061500
C	2.85688400	-1.32154900	4.61477300
C	2.79160000	-2.41492800	3.71734900
C	1.62212400	-2.70485800	3.04766400
C	0.46228900	-1.89814300	3.21094700
C	-0.74784600	-2.13848700	2.46322300
C	-1.37606600	-3.51783600	0.43669800
C	-0.98054400	-3.43074500	1.76371600
C	-0.81959200	-4.67009000	2.49238700
C	-0.61872200	-4.71399100	3.90074200
C	-0.45112400	-5.91210100	4.56375100
C	-0.47263800	-7.13819800	3.85885600
C	-0.69867000	-7.13658700	2.50003100
C	-0.89410800	-5.92012900	1.79160200
C	-1.18541100	-5.92093400	0.40075900
C	-1.45124600	-4.74807900	-0.25673300

H	-0.57465000	0.87318300	4.99342700
H	1.78234800	0.31798400	5.50071000
H	3.78693800	-1.11028900	5.14668200
H	3.67604000	-3.03509300	3.55597100
H	1.57926300	-3.55334400	2.36808300
H	-0.61310000	-3.78698500	4.47109800
H	-0.30852800	-5.91250900	5.64670300
H	-0.32962800	-8.07901900	4.39456900
H	-0.74637500	-8.07602200	1.94372900
H	-1.21507700	-6.87238000	-0.13509100
H	-1.68742200	-4.71906000	-1.31761200
H	-2.54596300	0.57915800	3.51447400
O	-1.62534100	-2.41217700	-0.33629400
O	-2.74475500	-1.11842100	1.56244500
N	-3.87214900	-1.02680400	-0.68545300
C	-4.05135200	-0.82238300	-2.10098300
C	-4.02381700	-1.92760300	-2.98332200
C	-4.26123900	0.46862400	-2.58413400
C	-4.15692300	-1.66776400	-4.36341200
C	-4.43296900	0.69706300	-3.94896700
H	-4.28205300	1.28437900	-1.87187400
C	-4.37039600	-0.37678600	-4.84294500
H	-4.12619300	-2.50890100	-5.06006200
H	-4.59993300	1.71328700	-4.30951500
H	-4.49284200	-0.20894800	-5.91519800
C	-4.92076900	-1.75978000	-0.01672300
C	-5.12657800	-3.12563500	-0.30644800
C	-5.67956800	-1.11117700	0.95955300
C	-6.08180500	-3.82223300	0.46233200
C	-6.63598400	-1.81469000	1.68994200
H	-5.48235500	-0.05857700	1.15661300
C	-6.82886500	-3.17912900	1.44490400
H	-6.24083200	-4.88480100	0.26441100
H	-7.21527100	-1.30542100	2.46284700
H	-7.56494500	-3.74127700	2.02338300
C	-3.94309300	-3.31446600	-2.53076300
H	-3.54779500	-4.02167800	-3.26644600
C	-4.42934500	-3.83052200	-1.37852800
H	-4.38571800	-4.91695000	-1.26281600
P	1.51717600	1.52927700	-0.69525300
P	-2.32376100	-0.96932600	-0.03011900
Ir	-0.66456800	0.62120700	-0.55129100
C	-0.50847300	1.85053300	1.29168600
H	-0.16012200	1.08930400	1.99016800

H	0.11609000	2.73495500	1.22554300
C	-1.84522200	1.91902300	0.92400200
H	-2.57513000	1.27163100	1.40006900
C	-2.39381900	3.22706700	0.40819000
C	0.07566700	-0.92534900	-1.90874200
C	-0.50752900	-0.03955200	-2.59465200
C	-0.96993600	0.57539100	-3.85405900
H	-0.21679000	0.35747900	-4.63091000
H	-1.88024800	0.03068400	-4.15032100
C	-1.26924200	2.06920400	-3.79619700
H	-0.35938100	2.64975300	-3.60483600
H	-1.70264400	2.40746700	-4.74843000
H	-1.98455700	2.28731100	-2.99281000
C	0.72946600	-2.19323100	-1.71047400
C	0.63149100	-3.15712700	-2.73299200
C	1.46067000	-2.49139700	-0.55003900
C	1.26726000	-4.38862100	-2.59890700
H	0.05224400	-2.92638300	-3.62865000
C	2.09386300	-3.72666500	-0.42639400
H	1.52650600	-1.75067000	0.24533500
C	2.00214000	-4.67637500	-1.44523300
H	1.19472800	-5.12733200	-3.40002200
H	2.67726400	-3.94595300	0.46865600
H	2.51064900	-5.63681500	-1.34507900
C	-3.71554200	3.17397500	-0.30845600
C	-4.84287500	2.59157900	0.28993500
C	-3.84659800	3.80360700	-1.55380500
C	-6.07721500	2.62501000	-0.36044200
H	-4.75542700	2.13829300	1.27761700
C	-5.08321800	3.83931700	-2.20319000
H	-2.97314200	4.27536400	-2.01019200
C	-6.20003800	3.24733900	-1.60758100
H	-6.94921000	2.16340900	0.10738400
H	-5.17559600	4.33331800	-3.17291600
H	-7.16757800	3.27119400	-2.11330800
B	-2.65036200	3.63109400	3.19599900
F	-1.38234900	3.29682700	3.55727300
F	-3.51784400	2.56702500	3.13700000
F	-3.15178000	4.72270000	3.81662200
O	-2.51191700	4.15100600	1.58558500
C	-3.12610700	5.42488000	1.28496500
H	-4.21962300	5.33986300	1.32532000
H	-2.77335200	6.13529700	2.03711900
H	-2.80719100	5.73424000	0.28542900

H	-1.64555400	3.71210500	-0.23053000

[B-D]'‡

Zero-point correction=	1.317298 (Hartree/Particle)
Thermal correction to Energy=	1.400503
Thermal correction to Enthalpy=	1.401448
Thermal correction to Gibbs Free Energy=	1.198492
Sum of electronic and zero-point Energies=	-4986.342198
Sum of electronic and thermal Energies=	-4986.258992
Sum of electronic and thermal Enthalpies=	-4986.258048
Sum of electronic and thermal Free Energies=	-4986.461004

C	-3.26777000	-1.18435400	2.12364800
C	-2.83781900	-1.45411900	3.44253600
C	-2.72190000	-2.75054200	3.87701600
C	-2.98879900	-3.83396000	2.99575200
C	-2.77503000	-5.18042700	3.39395400
C	-3.00751200	-6.22138000	2.52098400
C	-3.45440100	-5.94800800	1.20754300
C	-3.68279300	-4.65185700	0.79668000
C	-3.47650100	-3.55505100	1.67707500
C	-3.70310600	-2.18852100	1.27071900
C	-3.85073900	-1.05639700	-0.96049000
C	-4.39541300	-1.90082800	-0.01158900
C	-5.68118000	-2.48478200	-0.30736200
C	-6.44659000	-3.18048100	0.66911200
C	-7.68394900	-3.70762800	0.36195300
C	-8.22085700	-3.57888500	-0.94110200
C	-7.51370700	-2.89609600	-1.90668500
C	-6.24708800	-2.32144300	-1.61554300
C	-5.54722700	-1.55656900	-2.58817000
C	-4.38258900	-0.91093800	-2.25961600
H	-2.40171800	-2.96221800	4.89987300
H	-2.41484700	-5.37464500	4.40726100
H	-2.83869000	-7.25336700	2.83624300
H	-3.60844500	-6.77078400	0.50595200
H	-4.00290600	-4.46032700	-0.22577100
H	-6.05413500	-3.28374800	1.67970600
H	-8.25642300	-4.22618500	1.13421100
H	-9.19723000	-4.00955100	-1.17319900
H	-7.92443800	-2.77163100	-2.91170500
H	-5.97448100	-1.44919800	-3.58728800
H	-3.86097000	-0.26578300	-2.96606800
H	-2.61526700	-0.61125500	4.09368000
O	-2.70096800	-0.33292200	-0.69039100
O	-3.29497300	0.15390600	1.74207100
N	-3.45402400	2.08554800	0.02959800

C	-3.26879800	3.43110900	0.49872100
C	-3.14119600	4.45941000	-0.46022700
C	-3.28348900	3.71816300	1.86572600
C	-3.01507600	5.78217300	0.00859200
C	-3.16186300	5.03552600	2.30178700
H	-3.39119700	2.89839200	2.57772400
C	-3.03862500	6.06962400	1.36918400
H	-2.91960100	6.59132000	-0.71972700
H	-3.15428300	5.25590100	3.37072700
H	-2.93975200	7.10202300	1.70918800
C	-4.73113700	1.87008900	-0.60929000
C	-4.91457500	2.38951100	-1.90823800
C	-5.74936400	1.15683500	0.03063700
C	-6.12207000	2.09615600	-2.57166900
C	-6.94093800	0.89051100	-0.64180400
H	-5.58456400	0.78754400	1.04152900
C	-7.12133200	1.35289600	-1.94999600
H	-6.27457200	2.48004400	-3.58325700
H	-7.72043300	0.30497700	-0.15126900
H	-8.04943500	1.13544400	-2.48264000
C	-3.17541000	4.19880400	-1.90121400
H	-2.61076100	4.90148500	-2.52304100
C	-3.93713700	3.27689800	-2.53827400
H	-3.93843800	3.29095100	-3.63288200
C	2.39698400	-1.26854800	-2.08886800
C	1.65778200	-1.15203100	-3.28783000
C	1.33079200	-2.27764900	-4.00380300
C	1.68368700	-3.56504800	-3.51942500
C	1.27210700	-4.74333200	-4.19984900
C	1.56859000	-5.99067200	-3.69683400
C	2.28390500	-6.10414500	-2.48105400
C	2.71193200	-4.98007900	-1.80778800
C	2.44666200	-3.67611300	-2.30969000
C	2.88111900	-2.48239900	-1.62511200
C	3.45587600	-2.05959300	0.77772800
C	3.79795100	-2.58766500	-0.45602200
C	5.03911900	-3.31246000	-0.54328500
C	5.59985700	-3.71261100	-1.78737000
C	6.79504000	-4.39855300	-1.83982200
C	7.48790700	-4.73387400	-0.65138500
C	6.97711800	-4.35363400	0.57044000
C	5.75806300	-3.62709000	0.65885700
C	5.24534800	-3.19393300	1.91152600
C	4.13430700	-2.38812100	1.96943700
H	0.77768700	-2.19456800	-4.94206100
H	0.70372200	-4.63883700	-5.12736300
H	1.24498000	-6.88992800	-4.22537200
H	2.49249500	-7.09288900	-2.06652400
H	3.24295900	-5.09004000	-0.86436000
H	5.08100100	-3.45674600	-2.71081500

H	7.21328600	-4.68322900	-2.80785000
H	8.42898000	-5.28511200	-0.70746600
H	7.50924900	-4.59543100	1.49378600
H	5.77586200	-3.46850300	2.82607500
H	3.76050200	-1.98160000	2.90900000
H	1.39241800	-0.15491200	-3.63994100
O	2.36419700	-1.21846300	0.89495900
O	2.68006600	-0.08478600	-1.42507000
N	3.63012500	1.08383300	0.55388400
C	3.92956900	1.25453300	1.94598900
C	5.09050900	0.65845500	2.49395300
C	3.03008900	1.94718100	2.75550500
C	5.27081600	0.75768200	3.88835500
C	3.23488700	2.03612700	4.13332000
H	2.17762400	2.43259800	2.29350300
C	4.35883000	1.43032900	4.70150000
H	6.15549000	0.29503000	4.33277000
H	2.51757000	2.58884200	4.74222200
H	4.53312100	1.49061600	5.77798600
C	4.54813300	1.60074200	-0.42227100
C	5.83253100	1.03357300	-0.55672000
C	4.13783400	2.63311600	-1.26692900
C	6.63957400	1.48311100	-1.62193400
C	4.96041900	3.07930900	-2.30056400
H	3.15683600	3.06755100	-1.09904300
C	6.21351900	2.48717000	-2.48747100
H	7.62872800	1.03735100	-1.75041200
H	4.62519000	3.88551000	-2.95577200
H	6.86408900	2.81820700	-3.29971100
C	6.08741800	-0.05731400	1.70191700
H	6.71320300	-0.74318800	2.27783700
C	6.38476900	0.06959300	0.38880000
H	7.22037400	-0.52690800	0.01191800
P	-2.45371400	0.80580000	0.46431000
P	2.23630600	0.22310900	0.13079300
Ir	0.00852300	0.87015300	0.38808300
C	-0.51375900	1.15640500	-1.70964200
H	-0.24914700	0.28624200	-2.31032000
H	-1.54905400	1.48263700	-1.81800200
C	0.48565700	2.15258300	-1.51352800
H	1.47583300	1.93234400	-1.91281100
C	0.17374500	3.52325400	-1.27968000
H	-0.71532200	3.74722000	-0.68716600
O	1.51531800	3.93544200	0.66601800
C	-0.27813000	-1.16618600	1.02305800
C	-0.10956000	-0.42765600	2.04764400
C	0.15701100	-0.19651300	3.48393200
H	-0.21037400	-1.08137100	4.02928200
H	1.25557800	-0.18794100	3.60431800
C	-0.41911300	1.09271200	4.07613700

H	-1.50149200	1.16855200	3.89852200
H	-0.24494800	1.11469200	5.16179100
H	0.04135500	1.98315700	3.63428500
C	-0.37298000	-2.45392600	0.38853200
C	-0.06037600	-3.58970200	1.16421100
C	-0.75964400	-2.62362000	-0.94948500
C	-0.15448600	-4.86280000	0.61150900
H	0.24955300	-3.45835200	2.20165200
C	-0.85812800	-3.90288900	-1.49364800
H	-0.99007700	-1.74838800	-1.54987500
C	-0.55823300	-5.02367800	-0.71782000
H	0.07874700	-5.73599100	1.22358600
H	-1.16494300	-4.02537700	-2.53300500
H	-0.63266300	-6.02252600	-1.15083700
C	0.76135300	4.63242300	-1.97136400
C	0.34997100	5.94178700	-1.61827600
C	1.69986900	4.46291100	-3.01730100
C	0.86187300	7.04233800	-2.29427600
H	-0.33788400	6.06500700	-0.78082200
C	2.20301800	5.56922400	-3.69137500
H	2.01606400	3.46232200	-3.31231600
C	1.78648500	6.85844700	-3.33086800
H	0.54931200	8.04977000	-2.01290100
H	2.91746100	5.43401800	-4.50587300
H	2.18619700	7.72491700	-3.86278700
C	2.51600900	4.92828200	0.62017300
H	3.40817800	4.59377000	1.17616100
H	2.81617200	5.10773600	-0.42503700
H	2.16157300	5.88200400	1.04087700
B	0.48196600	4.15559900	1.67869100
F	-0.36900600	2.99789400	1.57483500
F	1.00273700	4.21339000	2.96033400
F	-0.25546000	5.29632900	1.38335300

D'

Zero-point correction=	1.319018 (Hartree/Particle)
Thermal correction to Energy=	1.402270
Thermal correction to Enthalpy=	1.403214
Thermal correction to Gibbs Free Energy=	1.203663
Sum of electronic and zero-point Energies=	-4986.370200
Sum of electronic and thermal Energies=	-4986.286948
Sum of electronic and thermal Enthalpies=	-4986.286004
Sum of electronic and thermal Free Energies=	-4986.485555

C	-2.99263000	-2.00256500	1.58143900
C	-2.21886700	-2.64736600	2.57229300
C	-2.07237300	-4.01049300	2.54859000
C	-2.66864000	-4.78422500	1.51706700

C	-2.43977900	-6.18226400	1.42072900
C	-2.99141500	-6.92134300	0.39707700
C	-3.78786500	-6.27922300	-0.57915700
C	-4.03703000	-4.92413300	-0.50514900
C	-3.50096900	-4.13416800	0.54859900
C	-3.71955300	-2.70937400	0.63453200
C	-4.34209700	-0.95597800	-1.04597400
C	-4.69231600	-2.04709700	-0.27218300
C	-6.05787400	-2.50461200	-0.35835200
C	-6.60065400	-3.45732500	0.54725200
C	-7.91966200	-3.85245800	0.45898200
C	-8.76518400	-3.32701800	-0.54684200
C	-8.27597600	-2.38907700	-1.42981100
C	-6.92984200	-1.94221500	-1.34831100
C	-6.44724600	-0.91182200	-2.20030000
C	-5.18403000	-0.40351600	-2.03351000
H	-1.47231200	-4.51244000	3.31034700
H	-1.80597500	-6.65924600	2.17186800
H	-2.80759600	-7.99578700	0.33076200
H	-4.20718000	-6.86024500	-1.40365400
H	-4.64158300	-4.44787900	-1.27537800
H	-5.96776200	-3.86809800	1.33258900
H	-8.31560300	-4.57571400	1.17525600
H	-9.80429700	-3.65654200	-0.61177900
H	-8.92331300	-1.95851600	-2.19762200
H	-7.11326800	-0.49354400	-2.95756400
H	-4.81445400	0.43136700	-2.62843700
H	-1.74856200	-2.04112600	3.34125300
O	-3.09250300	-0.35305600	-0.89353000
O	-3.04674100	-0.61088200	1.63846500
N	-3.59020000	1.72651900	0.68652000
C	-3.18662500	2.93045700	1.36688500
C	-3.31119400	4.16389500	0.69514400
C	-2.72936900	2.86977400	2.68407100
C	-2.90160800	5.32405200	1.38041100
C	-2.33583300	4.03157800	3.34392800
H	-2.67736500	1.90242700	3.18128000
C	-2.42305300	5.26253900	2.68599800
H	-2.97588600	6.28571100	0.86892800
H	-1.94476200	3.97415400	4.35974100
H	-2.11972800	6.17782300	3.19835000
C	-5.01842500	1.62580100	0.47114900
C	-5.60419400	2.46744700	-0.49856600
C	-5.79490600	0.71607400	1.19603900
C	-6.97803200	2.30626000	-0.76491500
C	-7.15327000	0.57939100	0.91576000
H	-5.31969700	0.09679300	1.95430800
C	-7.74337400	1.37196800	-0.07429300
H	-7.44331800	2.94220400	-1.52178700
H	-7.74622800	-0.15859700	1.45890200

H	-8.80527500	1.26016400	-0.30265400
C	-3.87427900	4.28394100	-0.64786000
H	-3.52456000	5.14065400	-1.22915400
C	-4.86325600	3.52824300	-1.17948200
H	-5.25216300	3.82625900	-2.15823000
C	2.93260000	-1.73278900	-1.54067200
C	2.32939200	-2.41427100	-2.62605800
C	2.54587200	-3.75427000	-2.81343700
C	3.31554400	-4.49255300	-1.87684500
C	3.44368000	-5.90309300	-1.98395000
C	4.10040100	-6.63007600	-1.01547500
C	4.64916700	-5.96279400	0.10543800
C	4.57063800	-4.58955500	0.21650700
C	3.92355900	-3.80363000	-0.77799400
C	3.81947600	-2.36379600	-0.67648600
C	4.11443000	-0.74544500	1.22904700
C	4.64994800	-1.64776600	0.32830500
C	6.07247700	-1.88603900	0.41912100
C	6.79430600	-2.58321800	-0.58863000
C	8.15800900	-2.76875300	-0.49040700
C	8.87344100	-2.28197600	0.62934400
C	8.20741100	-1.58748600	1.61555100
C	6.80852700	-1.35347600	1.52845800
C	6.13857700	-0.55832200	2.49937800
C	4.81858900	-0.22521000	2.33449900
H	2.09378500	-4.27313000	-3.66100300
H	2.98654000	-6.40363500	-2.84095700
H	4.18584600	-7.71547100	-1.10069300
H	5.14153500	-6.53955700	0.89157500
H	4.99813900	-4.09954400	1.08973700
H	6.26226600	-2.95947400	-1.46126800
H	8.69034500	-3.29422100	-1.28634300
H	9.95069000	-2.44611800	0.70132200
H	8.75017200	-1.18476300	2.47410600
H	6.70379300	-0.16611300	3.34677900
H	4.29547600	0.45171900	3.00871600
H	1.71707900	-1.84008800	-3.32126200
O	2.79636900	-0.31342900	1.08704500
O	2.62086600	-0.39123100	-1.46426400
N	3.27064400	1.87783500	-0.39882400
C	4.58061000	2.06135200	0.18624800
C	5.70010100	1.48437000	-0.45597400
C	4.72583300	2.86569400	1.31755000
C	6.95799100	1.64840700	0.15464800
C	5.99168800	3.04796200	1.87510900
H	3.83664400	3.32605700	1.74212100
C	7.10447300	2.42195800	1.30350000
H	7.82956300	1.17417100	-0.30148100
H	6.10664300	3.67016000	2.76527700
H	8.09364000	2.54585900	1.74990600

C	3.12190700	2.60796100	-1.63517100
C	3.77369500	2.13181800	-2.79777100
C	2.35487800	3.77197100	-1.65262800
C	3.49736200	2.79553900	-4.00976700
C	2.13574500	4.43808300	-2.85892200
H	1.93565200	4.11208900	-0.70651300
C	2.68530900	3.92879400	-4.04114000
H	3.96451200	2.43222200	-4.92838900
H	1.51851800	5.33665700	-2.87889300
H	2.49734100	4.43342400	-4.99149300
C	5.61483600	0.78643500	-1.73867100
H	6.39279500	0.03878500	-1.91637100
C	4.77176200	1.06476900	-2.76135900
H	4.91984600	0.52036500	-3.69871800
P	-2.55646200	0.43111100	0.44881300
P	2.25769000	0.55899600	-0.16262800
Ir	-0.16233000	0.70467800	0.06869800
C	-0.33888200	0.00018400	-1.92407200
H	0.45210600	-0.67577300	-2.23528700
H	-1.34497500	-0.37518000	-2.10142500
C	-0.12551700	1.41737200	-2.15021800
H	0.84287200	1.79566200	-2.48421700
C	-1.12863200	2.31008600	-1.82819900
H	-2.14336900	1.92043400	-1.68876900
O	1.61960700	4.15948800	1.56241600
C	-0.04560300	-1.37147300	0.67549300
C	0.12968800	-0.64980500	1.70473200
C	0.46815500	-0.48401600	3.13219900
H	0.59193900	-1.51130000	3.51898000
H	1.45367600	-0.00123500	3.17973200
C	-0.52104200	0.30645500	3.99158300
H	-1.54268800	-0.09257800	3.92357900
H	-0.20423700	0.26077300	5.04359600
H	-0.53355500	1.36079100	3.69859100
C	-0.03349200	-2.66493800	0.03736400
C	0.84672400	-3.62711500	0.57607300
C	-0.89195100	-3.03178900	-1.01058500
C	0.84193900	-4.93047700	0.09134300
H	1.53404200	-3.33578500	1.37106100
C	-0.87697500	-4.33575100	-1.50304700
H	-1.59628900	-2.30900900	-1.41190800
C	-0.02106500	-5.28847400	-0.94870100
H	1.53469200	-5.66354900	0.50800100
H	-1.55765400	-4.61430300	-2.30860400
H	-0.01956600	-6.31118000	-1.33011500
C	-1.03217000	3.78378600	-1.95209800
C	-0.61632000	4.60722100	-0.90180900
C	-1.43144500	4.35832800	-3.17096000
C	-0.58817800	5.99271000	-1.07532900
H	-0.31564300	4.16455900	0.04387800

C	-1.40236600	5.74297100	-3.33842500
H	-1.76408600	3.71710800	-3.99060900
C	-0.98137300	6.56504200	-2.28731100
H	-0.25891800	6.62707200	-0.25098100
H	-1.70871800	6.18088600	-4.29093100
H	-0.95900300	7.64949400	-2.41547200
C	1.34539400	5.47231300	1.99183600
H	1.71493400	5.65744100	3.01481700
H	1.85263400	6.17073500	1.30819600
H	0.26368200	5.69438500	1.98174200
B	1.11553800	3.05763000	2.27391600
F	-0.03549700	2.43893800	1.42580900
F	2.02731400	2.00817100	2.35828600
F	0.54388900	3.34106100	3.49156500

D1'

Zero-point correction=	1.528873 (Hartree/Particle)
Thermal correction to Energy=	1.618429
Thermal correction to Enthalpy=	1.619373
Thermal correction to Gibbs Free Energy=	1.401981
Sum of electronic and zero-point Energies=	-4955.879136
Sum of electronic and thermal Energies=	-4955.789580
Sum of electronic and thermal Enthalpies=	-4955.788636
Sum of electronic and thermal Free Energies=	-4956.006028

C	2.71690000	-0.28553500	2.45192300
C	1.90043900	-0.22568500	3.60568700
C	1.96440800	0.86157200	4.43823600
C	2.81052100	1.96113500	4.12671800
C	2.83486000	3.12423000	4.94052400
C	3.61916400	4.20814300	4.60967000
C	4.39521300	4.17371000	3.42860800
C	4.39621000	3.05532100	2.62158800
C	3.63207900	1.90318500	2.95369600
C	3.63467800	0.71021900	2.14191200
C	4.21314000	0.17613500	-0.25134400
C	4.60616300	0.55150900	1.02678400
C	6.02113600	0.73612200	1.25169100
C	6.57410800	0.86106900	2.55727000
C	7.93212300	1.01043300	2.75035800
C	8.81745900	1.05385200	1.64751800
C	8.31945600	0.91188300	0.37033000
C	6.92927500	0.72969700	0.14158200
C	6.42706600	0.48422500	-1.16543900
C	5.10440600	0.18042600	-1.35098800
H	1.34190100	0.90914900	5.33474300
H	2.20439400	3.14665100	5.83314300
H	3.62686600	5.09808800	5.24332900

H	4.98822000	5.04578000	3.14300100
H	4.98005900	3.05655100	1.70266700
H	5.91073600	0.82076600	3.41960700
H	8.32651300	1.09126800	3.76605500
H	9.88973500	1.18309000	1.81180200
H	8.99167100	0.91576400	-0.49172900
H	7.11993400	0.48097500	-2.00972200
H	4.70537100	-0.09583900	-2.32608600
H	1.22876000	-1.06108300	3.79685000
O	2.92200300	-0.19173200	-0.54222200
O	2.61709800	-1.41644800	1.67728100
N	2.88510800	-2.82840400	-0.43790600
C	2.23142800	-4.09882100	-0.43363400
C	2.19854200	-4.85991400	-1.62231400
C	1.62023200	-4.57071100	0.73225600
C	1.51643000	-6.09157600	-1.59670700
C	0.95095300	-5.79396600	0.73085900
H	1.67979800	-3.96250800	1.63581900
C	0.90640700	-6.55988900	-0.43699200
H	1.46432100	-6.68207600	-2.51485300
H	0.45157400	-6.14429800	1.63625500
H	0.36646800	-7.50782800	-0.44913000
C	4.30941400	-2.89242500	-0.61011400
C	4.81845000	-3.20863500	-1.88913600
C	5.18106700	-2.63906500	0.45596800
C	6.21310300	-3.15146100	-2.08151400
C	6.55842300	-2.60438100	0.24587600
H	4.76058200	-2.42992800	1.43734500
C	7.07442300	-2.84550500	-1.03182100
H	6.61549300	-3.37161900	-3.07374700
H	7.22641500	-2.36304400	1.07483200
H	8.15204300	-2.79997700	-1.20472500
C	2.83207800	-4.40543500	-2.85897500
H	2.38237800	-4.78877300	-3.78069300
C	3.95860000	-3.66397400	-2.98042100
H	4.34657400	-3.50070000	-3.99113600
C	-0.04291300	1.68387500	-2.97729500
C	1.16585200	1.05007600	-3.34420100
C	2.33435400	1.77063100	-3.33476100
C	2.34521400	3.13622700	-2.94118300
C	3.56351100	3.86589100	-2.86654500
C	3.57967300	5.18230500	-2.45914900
C	2.36886300	5.81674700	-2.09182300
C	1.17331000	5.13146300	-2.13918200
C	1.11362900	3.77943100	-2.57947200
C	-0.10970000	3.02029700	-2.61296200
C	-2.14438500	3.01317400	-1.15553400
C	-1.40432200	3.60527500	-2.17474100
C	-1.93009700	4.80628300	-2.76859400
C	-1.38062900	5.36449000	-3.95718500

C	-1.90991800	6.50622600	-4.52162100
C	-3.01553200	7.15919900	-3.92511100
C	-3.58183600	6.63686900	-2.78215200
C	-3.07092900	5.45207800	-2.18633300
C	-3.67843500	4.87538400	-1.03831200
C	-3.24141800	3.67094000	-0.55152200
H	3.27803800	1.29433600	-3.60587500
H	4.49226600	3.35353000	-3.12976800
H	4.52266300	5.73120400	-2.40487800
H	2.38323200	6.85220300	-1.74369000
H	0.26126700	5.62374800	-1.80898500
H	-0.53397300	4.86749100	-4.43044200
H	-1.47481000	6.90712000	-5.44019200
H	-3.42190300	8.06689000	-4.37733800
H	-4.44574600	7.12111500	-2.31917500
H	-4.53192000	5.37813100	-0.57812500
H	-3.73306400	3.17527300	0.28184500
H	1.14289400	-0.00544900	-3.60864500
O	-1.83515000	1.77726800	-0.64126900
O	-1.20336100	0.93267300	-2.95365900
N	-3.28820000	-0.05548900	-1.81023300
C	-3.69680600	-1.40920600	-2.03112300
C	-4.52083300	-2.03886000	-1.07371300
C	-3.30987000	-2.08141600	-3.19161900
C	-4.87771800	-3.38344600	-1.28861500
C	-3.70409800	-3.40298400	-3.40017700
H	-2.68505000	-1.55632300	-3.91549200
C	-4.48368500	-4.05624600	-2.44186800
H	-5.48813900	-3.89612000	-0.54178900
H	-3.38167900	-3.93205600	-4.29938900
H	-4.76674000	-5.10034000	-2.58238600
C	-4.32534700	0.91586900	-1.96893900
C	-5.35213200	0.96799000	-0.99816200
C	-4.30865300	1.81286700	-3.04291500
C	-6.31526900	1.99065200	-1.11349200
C	-5.28244800	2.80477100	-3.14317700
H	-3.49823600	1.74181900	-3.76768000
C	-6.28403700	2.89684400	-2.17018500
H	-7.10513800	2.05651500	-0.36060600
H	-5.24472700	3.52135400	-3.96589900
H	-7.04106300	3.68155800	-2.23629200
C	-5.08592900	-1.31251000	0.06206500
H	-5.35385800	-1.92513000	0.92746200
C	-5.46025300	-0.00995200	0.08411000
H	-6.01584600	0.33318700	0.96338200
P	2.04008300	-1.44699200	0.08956600
P	-1.67791200	0.33767500	-1.45353600
Ir	-0.10701300	-0.96559200	-0.47220000
C	0.06644400	-2.15164800	-2.24949300
H	-0.37712100	-1.65538100	-3.13280400

H	1.11859600	-2.31727400	-2.54478300
C	-0.59405600	-3.48978000	-2.10933600
H	-0.50469600	-4.15694900	-2.97814900
C	-1.28462400	-3.93036900	-1.04348700
H	-1.36352100	-3.25531600	-0.18640500
C	-0.22199400	0.46259200	1.29256500
C	-0.89705100	-0.57418900	1.51825000
C	-1.82556200	-1.52667900	2.15643300
H	-2.44941700	-0.99104900	2.89233100
H	-2.53183600	-1.88022800	1.38515700
C	-1.14171400	-2.73628200	2.80309800
H	-0.46991900	-2.42741300	3.61841100
H	-1.89521300	-3.41671600	3.23068700
H	-0.54856100	-3.29907600	2.06873500
C	0.30793500	1.79013400	1.44511000
C	-0.09258800	2.59290400	2.53095100
C	1.22872500	2.31416400	0.52060700
C	0.40931100	3.88392500	2.68045400
H	-0.79350500	2.19006200	3.25792400
C	1.74809100	3.59469300	0.69132700
H	1.53441800	1.69762000	-0.32167700
C	1.33613100	4.38811700	1.76421400
H	0.09171200	4.49309500	3.53000700
H	2.48719200	3.97183200	-0.01409800
H	1.75051300	5.38977000	1.89548500
C	-1.96359700	-5.21756900	-0.89166500
C	-2.60824800	-5.50780300	0.32514100
C	-2.01864100	-6.19224000	-1.90667300
C	-3.27713000	-6.71573400	0.52509800
H	-2.57764100	-4.76337800	1.12400800
C	-2.68531100	-7.40000000	-1.71148700
H	-1.53270300	-5.99781100	-2.86407500
C	-3.32079900	-7.67243300	-0.49356100
H	-3.76795100	-6.91264500	1.48191100
H	-2.71274100	-8.13867800	-2.51711500
H	-3.84386200	-8.61962800	-0.34233400
C	-6.30169500	-0.08000700	5.30710300
C	-5.13964600	-0.87611800	4.66781900
C	-4.02313200	1.35016100	4.03521600
C	-5.20893200	2.09479700	4.69254600
C	-5.85798900	1.29095200	5.82037900
H	-7.08239600	0.06882200	4.53915500
H	-6.76268100	-0.67283900	6.11490300
H	-4.87602700	3.08240100	5.05329400
H	-5.97042400	2.28419400	3.91444100
H	-5.15419200	1.17409000	6.66161400
H	-6.72381700	1.83985000	6.22504900
N	-4.37526800	-0.04835500	3.71582800
H	-4.84521600	-0.06270600	2.81437100
C	-3.67552100	2.02167400	2.70072100

H	-3.35842800	3.06335600	2.85544400
H	-2.86671800	1.49304400	2.17614700
H	-4.55510300	2.03268500	2.03750600
C	-2.78410800	1.40266400	4.94805100
H	-1.98049800	0.77665300	4.53503000
H	-2.41658900	2.43710100	5.02888800
H	-2.99393200	1.05180100	5.96634000
C	-4.21423800	-1.45160500	5.75586100
H	-4.74995400	-2.20978700	6.34819400
H	-3.33611200	-1.92407200	5.29164300
H	-3.85439000	-0.68634900	6.45487100
C	-5.70547700	-2.05334900	3.86358800
H	-4.89161700	-2.63553100	3.40404400
H	-6.29063800	-2.72367900	4.51077400
H	-6.37295800	-1.69689300	3.06151200

[D-E]'‡

Zero-point correction=	1.585327 (Hartree/Particle)
Thermal correction to Energy=	1.681064
Thermal correction to Enthalpy=	1.682009
Thermal correction to Gibbs Free Energy=	1.454021
Sum of electronic and zero-point Energies=	-5395.027852
Sum of electronic and thermal Energies=	-5394.932115
Sum of electronic and thermal Enthalpies=	-5394.931171
Sum of electronic and thermal Free Energies=	-5395.159158

C	-3.00032500	-2.19378900	0.17663200
C	-2.18863100	-3.19677200	0.75220300
C	-2.19405300	-4.46858000	0.24321900
C	-2.96217200	-4.77456900	-0.91109400
C	-2.88241100	-6.05123900	-1.52962300
C	-3.58323700	-6.32438200	-2.68367400
C	-4.39039300	-5.31913100	-3.26764300
C	-4.50250700	-4.07587800	-2.68054100
C	-3.80598800	-3.76302100	-1.47951500
C	-3.88872400	-2.46322500	-0.85326500
C	-4.49445900	-0.19960800	-1.72889100
C	-4.88242500	-1.46800200	-1.33404100
C	-6.28007500	-1.79442100	-1.44538900
C	-6.83629400	-2.95699900	-0.84610400
C	-8.18710400	-3.22077900	-0.92870400
C	-9.05154700	-2.34714100	-1.63213000
C	-8.54443100	-1.21198100	-2.22577300
C	-7.16113800	-0.89727500	-2.13657400
C	-6.63903000	0.30135000	-2.69313800
C	-5.33465500	0.66477200	-2.46204900
H	-1.56294500	-5.24157600	0.68486300

H	-2.23824800	-6.80910300	-1.07712700
H	-3.51025500	-7.30690400	-3.15494100
H	-4.92724000	-5.52749800	-4.19578800
H	-5.12144400	-3.31448300	-3.15246800
H	-6.18450100	-3.63274500	-0.29328500
H	-8.59559700	-4.11028200	-0.44391800
H	-10.11808100	-2.57300600	-1.69702600
H	-9.20326200	-0.52477300	-2.76233800
H	-7.30290900	0.95662300	-3.26164900
H	-4.92584300	1.61021500	-2.81688900
H	-1.55421900	-2.92302300	1.58839900
O	-3.21306800	0.25250100	-1.45801500
O	-2.91998300	-0.94432200	0.75995900
N	-3.62769400	1.43273300	0.97494900
C	-3.33744000	2.72829600	1.53854900
C	-3.97789800	3.86764900	1.00340400
C	-2.51070600	2.83948400	2.65685900
C	-3.73018500	5.11265800	1.61035700
C	-2.29051600	4.08019100	3.25192400
H	-2.01772900	1.95848800	3.05535400
C	-2.90885800	5.21878300	2.72879600
H	-4.20306800	6.00356800	1.19283000
H	-1.62938900	4.14256600	4.11724200
H	-2.74017300	6.19557600	3.18663500
C	-4.98836700	0.98442400	1.19866100
C	-6.03645700	1.61099600	0.49113200
C	-5.25214000	-0.07467500	2.07318100
C	-7.32889500	1.06201100	0.60565700
C	-6.54509200	-0.58287800	2.18878300
H	-4.42906900	-0.51738200	2.62957300
C	-7.58286800	-0.02566300	1.43440100
H	-8.14192100	1.51213200	0.03228400
H	-6.73891400	-1.42661800	2.85407400
H	-8.59079300	-0.44042400	1.49389800
C	-4.93625200	3.79632800	-0.09828100
H	-5.00618100	4.69575700	-0.71750000
C	-5.83763800	2.81089500	-0.31844000
H	-6.58032500	2.97381300	-1.10368100
C	2.71104900	-0.62138500	-2.76128800
C	2.04187500	-0.94232200	-3.96766300
C	2.19202000	-2.18176600	-4.53543200
C	2.97573500	-3.17485700	-3.89154300
C	3.04343400	-4.50123000	-4.39685100
C	3.76921400	-5.47296200	-3.74316400
C	4.45487400	-5.14784300	-2.54871700
C	4.42103100	-3.86482100	-2.04443400
C	3.69347400	-2.83269300	-2.69928400
C	3.62661500	-1.48784300	-2.17794900
C	4.09104700	-0.47725300	0.08335300
C	4.54099300	-1.07709300	-1.07949500

C	5.96560700	-1.29411500	-1.19146100
C	6.58534700	-1.66153500	-2.41797800
C	7.95147100	-1.83492000	-2.50385000
C	8.77330700	-1.66439400	-1.36461100
C	8.20759600	-1.29059600	-0.16498500
C	6.80735800	-1.07754700	-0.05099600
C	6.23345100	-0.60472700	1.16146900
C	4.90486300	-0.27311100	1.21766000
H	1.68504400	-2.42533800	-5.47171200
H	2.49639600	-4.73837700	-5.31270200
H	3.81216600	-6.49027900	-4.13817300
H	5.01421600	-5.92192800	-2.01820900
H	4.94374700	-3.63987700	-1.11631200
H	5.97071100	-1.78850300	-3.30791500
H	8.40274800	-2.10219000	-3.46196400
H	9.85219200	-1.81455200	-1.44320300
H	8.83214500	-1.13042400	0.71732600
H	6.87774600	-0.44589000	2.02821900
H	4.45177400	0.18325100	2.09351900
H	1.43095600	-0.17422900	-4.44158000
O	2.77001600	-0.05830500	0.20150400
O	2.45539400	0.63149900	-2.25404600
N	3.05341900	2.47648900	-0.55598100
C	4.38782000	2.52254100	-0.00658900
C	5.49173400	2.26270900	-0.85100000
C	4.56188400	2.89574900	1.32705700
C	6.77490900	2.29694000	-0.27219900
C	5.84868300	2.96244500	1.86210100
H	3.67277100	3.10729800	1.91924800
C	6.95397600	2.64870900	1.06368100
H	7.63930000	2.06156900	-0.89690500
H	5.98744300	3.24758500	2.90732500
H	7.96198100	2.68415900	1.48320500
C	2.81583200	3.55525000	-1.48379000
C	3.40152000	3.50577700	-2.77124700
C	2.02261400	4.62944700	-1.08898300
C	3.01763900	4.49989000	-3.69321900
C	1.68548800	5.62324700	-2.00817900
H	1.66936600	4.63933600	-0.06109700
C	2.16252100	5.53713200	-3.32118900
H	3.43164900	4.46927400	-4.70408600
H	1.03283200	6.44337100	-1.70542000
H	1.88512600	6.29843200	-4.05375700
C	5.36094600	2.00925400	-2.28590200
H	6.15804700	1.40458200	-2.72795200
C	4.44307900	2.54382500	-3.12582000
H	4.55419600	2.33436500	-4.19389300
P	-2.57545000	0.50116500	0.05318700
P	2.09098700	1.10106800	-0.70508000
Ir	-0.29296800	1.05656200	-0.32701300

C	-0.55825400	0.89102900	-2.40804600
H	0.25486900	0.41630700	-2.94713800
H	-1.54321200	0.51413800	-2.68186600
C	-0.43083700	2.32319300	-2.16587300
H	0.48751300	2.86347200	-2.40638900
C	-1.44753200	2.97978100	-1.47883400
H	-2.44809300	2.53913100	-1.54244700
O	1.49538500	3.65787100	2.30667700
C	0.15357600	-0.86476800	0.48076300
C	0.02199000	-0.81745100	1.75602800
C	-0.15384200	-0.81132800	3.12048400
H	0.44590600	-1.88615800	3.47483600
H	0.53916100	-0.11226000	3.61384100
C	-1.55762300	-0.81670200	3.72693900
H	-1.48624400	-0.80402400	4.82336500
H	-2.12738000	0.06936500	3.42110000
H	-2.13568500	-1.70017700	3.42364300
C	0.48902500	-2.06129100	-0.31497900
C	1.38532500	-3.01196300	0.20503700
C	-0.16317700	-2.33731100	-1.52463900
C	1.57294500	-4.23502400	-0.43569200
H	1.95029700	-2.76283500	1.10400400
C	0.02633400	-3.56212200	-2.16347800
H	-0.85969000	-1.61043700	-1.93561100
C	0.87997100	-4.52101300	-1.61589300
H	2.27821800	-4.96163200	-0.02788900
H	-0.50758900	-3.77213400	-3.09191400
H	1.03177200	-5.47481200	-2.12312900
C	-1.41555700	4.38519100	-1.01198000
C	-0.76499300	4.77509900	0.16217300
C	-2.09475100	5.35019100	-1.77694300
C	-0.74909100	6.11952600	0.53812000
H	-0.27615200	4.03222100	0.78889400
C	-2.07835000	6.69214700	-1.39631100
H	-2.62282000	5.04778700	-2.68475600
C	-1.39563200	7.08193200	-0.23879000
H	-0.23191000	6.40959400	1.45388400
H	-2.59503500	7.43615800	-2.00697100
H	-1.38018000	8.13237600	0.06053400
C	1.49493700	4.73387300	3.20940200
H	1.99357400	4.48500800	4.16287100
H	2.03780400	5.57430700	2.74778100
H	0.47155200	5.07634300	3.44792700
B	1.06355200	2.37053800	2.70392500
F	-0.01100100	1.93385100	1.74568100
F	2.06625600	1.39732600	2.57635300
F	0.47646200	2.29808000	3.96118500
C	3.37632800	-3.67773600	5.18993100
C	2.48004000	-2.51440000	4.71545200
C	0.48982800	-4.18561900	4.64394400

C	1.46404000	-5.29317300	5.09782600
C	2.61442800	-4.76096800	5.95036400
H	3.84951100	-4.13418500	4.30201200
H	4.19518900	-3.26600100	5.80098200
H	0.89528200	-6.06666200	5.63797100
H	1.88055200	-5.78176800	4.19845700
H	2.23409700	-4.36692500	6.90660200
H	3.29712400	-5.58382300	6.21302100
N	1.26268600	-3.05933300	4.02227100
H	1.58609200	-3.41096600	3.11804000
C	-0.43481500	-4.73002500	3.54947900
H	-1.22384700	-4.00798300	3.30027600
H	0.12356500	-4.96641400	2.62892700
H	-0.92450500	-5.65249400	3.89313300
C	-0.37546600	-3.70206200	5.81511900
H	-0.95881100	-2.81608300	5.53361900
H	-1.08099100	-4.49884300	6.09263400
H	0.20742800	-3.45800500	6.71001500
C	2.09100500	-1.59851000	5.88505700
H	2.98278500	-1.05045300	6.22168500
H	1.34088900	-0.85512000	5.58219300
H	1.70064400	-2.14748900	6.74951000
C	3.23818900	-1.68827900	3.67107000
H	2.67271900	-0.81025400	3.33236300
H	4.18473200	-1.33094600	4.10094200
H	3.49701400	-2.29753000	2.79033300

P2-(S,S)-**[E-F]**‡

Zero-point correction=	1.302852 (Hartree/Particle)
Thermal correction to Energy=	1.386320
Thermal correction to Enthalpy=	1.387264
Thermal correction to Gibbs Free Energy=	1.183194
Sum of electronic and zero-point Energies=	-4985.925909
Sum of electronic and thermal Energies=	-4985.842441
Sum of electronic and thermal Enthalpies=	-4985.841497
Sum of electronic and thermal Free Energies=	-4986.045567

C	-4.14140800	-0.58061300	-0.50983100
C	-4.39170700	-1.97411000	-0.55707600
C	-5.36436800	-2.50182800	0.25726100
C	-6.07526100	-1.67913900	1.17485600
C	-6.99111200	-2.23436100	2.10940400
C	-7.62951000	-1.43999400	3.03759900
C	-7.37540300	-0.04704400	3.06590200

C	-6.50765500	0.52638500	2.15945700
C	-5.83604700	-0.26343800	1.18474800
C	-4.89877800	0.30328300	0.24937500
C	-3.55287200	2.42168500	0.13330100
C	-4.77703200	1.77579200	0.05748700
C	-5.92609500	2.57316000	-0.29515300
C	-7.19540200	1.99925900	-0.58618900
C	-8.27000900	2.78582200	-0.94676500
C	-8.13863700	4.19206100	-1.03241300
C	-6.91849000	4.77954200	-0.77716700
C	-5.78763100	3.99654000	-0.42067400
C	-4.51364300	4.59667500	-0.22321700
C	-3.41011300	3.82342700	0.03061200
H	-5.57311900	-3.57367800	0.23253200
H	-7.16407300	-3.31303700	2.08773200
H	-8.32556300	-1.88123500	3.75478900
H	-7.86950100	0.57891800	3.81268800
H	-6.31730500	1.59917500	2.19239100
H	-7.31384300	0.91784900	-0.53955200
H	-9.22954200	2.31600900	-1.17496500
H	-8.99854200	4.80449900	-1.31305700
H	-6.79551600	5.86251400	-0.85969700
H	-4.41797800	5.68050400	-0.31724600
H	-2.41116900	4.24693000	0.13719700
H	-3.80077000	-2.58325700	-1.25290200
O	-2.39119200	1.70539900	0.34209000
O	-3.11955700	-0.10038900	-1.30277800
N	-1.24298000	1.42835900	-2.08318500
C	-0.15085100	0.89581800	-2.85465400
C	0.97054000	1.71333400	-3.11879700
C	-0.19346700	-0.42858800	-3.29987200
C	2.06010300	1.13083100	-3.79479500
C	0.89746700	-0.98180600	-3.97215800
H	-1.06736500	-1.05212900	-3.11198300
C	2.02717100	-0.19671400	-4.21626600
H	2.94293400	1.74527400	-3.98798300
H	0.83155900	-2.02440400	-4.28230300
H	2.88521700	-0.62177000	-4.74330500
C	-2.00756900	2.49837000	-2.66606100
C	-1.40133300	3.76850200	-2.79699300
C	-3.34068800	2.30569500	-3.04890300
C	-2.20867100	4.84352100	-3.21987900
C	-4.11519100	3.38500600	-3.47265600
H	-3.77042700	1.30968900	-2.97509700
C	-3.55052900	4.66200000	-3.54216100
H	-1.75539500	5.83454400	-3.30336800
H	-5.16457000	3.22871000	-3.72985600
H	-4.15696600	5.51421000	-3.85710000
C	1.03782500	3.11970300	-2.73998700
H	2.05233500	3.52119600	-2.65636200

C	0.02247400	3.99853300	-2.57311800
H	0.29688900	5.03529100	-2.35660000
P	-1.73166200	0.60901500	-0.69688600
Ir	0.05493500	-0.51346100	0.36267800
C	-0.72726000	-2.25553800	-0.63761000
H	0.01022400	-2.83402000	-1.18418800
H	-1.63053800	-2.08768100	-1.22138400
C	-0.82021400	-2.50084800	0.77922900
H	-0.09663200	-3.18817600	1.21404100
C	-1.94893000	-2.16958300	1.59398000
H	-2.65453600	-1.44283600	1.20060800
C	0.27027000	1.31317000	1.48284100
C	-0.29147100	0.49102000	2.29704400
C	-0.89873900	-0.39662300	3.15686000
H	-1.94016400	-0.19505200	3.43362100
C	-0.10383100	-1.30957300	4.04070000
H	-0.67113800	-2.21364400	4.30449600
H	0.13539200	-0.79543500	4.98973200
H	0.84050700	-1.60266700	3.56151300
C	0.69988500	2.68523300	1.37897300
C	0.19466300	3.65130600	2.27555600
C	1.61083200	3.07876600	0.38944800
C	0.61249400	4.97489200	2.18837900
H	-0.52948400	3.34398400	3.03256400
C	2.03135200	4.40640000	0.31237800
H	1.98092200	2.32866600	-0.30620200
C	1.54079300	5.35487900	1.20940800
H	0.22105900	5.71670400	2.88864000
H	2.75256500	4.70082000	-0.45157100
H	1.88200300	6.39054700	1.15194000
C	-2.45748300	-2.95860800	2.69478700
C	-3.62809300	-2.52454400	3.35965100
C	-1.84902400	-4.15941400	3.12100300
C	-4.16548900	-3.25814300	4.41063900
H	-4.11683100	-1.60502700	3.03395100
C	-2.39283300	-4.89205700	4.17450400
H	-0.96134500	-4.52665300	2.60930600
C	-3.54827800	-4.44619600	4.82492500
H	-5.07621100	-2.90800600	4.90097300
H	-1.91581400	-5.82456100	4.48507600
H	-3.97238500	-5.02619400	5.64782500
O	-2.65547700	-2.93796200	-2.92934000
B	-1.80588700	-4.09816700	-3.19984900
F	-2.43397900	-5.02068700	-4.02780700
F	-1.46991800	-4.68240300	-1.96121300
F	-0.59011400	-3.66633900	-3.82521400
C	-3.31381300	-2.35100900	-4.01361400
H	-4.01620700	-1.58482300	-3.63846700
H	-3.88576000	-3.09256600	-4.60001900
H	-2.61127600	-1.84746700	-4.70852800

C	3.42081100	0.66759900	2.28549600
C	2.80238800	1.06855900	3.49289000
C	2.98128600	2.34339200	3.96627500
C	3.76627500	3.28107200	3.24167900
C	3.90015900	4.62378100	3.68429000
C	4.63081800	5.54175800	2.96180700
C	5.24208000	5.14848800	1.74902000
C	5.13206000	3.85079700	1.29446100
C	4.41207700	2.86856000	2.02954600
C	4.26926500	1.50743000	1.57543200
C	4.29627700	0.42574100	-0.68534800
C	4.98056100	1.02781700	0.36134400
C	6.41031500	1.16086500	0.22826100
C	7.24256900	1.54424200	1.31687400
C	8.61072200	1.64370200	1.17013900
C	9.22356100	1.37339900	-0.07659700
C	8.44881100	0.98201800	-1.14727700
C	7.03961300	0.84996400	-1.02255000
C	6.24417800	0.37763300	-2.10233100
C	4.90524100	0.14191700	-1.92907800
H	2.50150000	2.66092800	4.89469300
H	3.39916300	4.91763400	4.60992400
H	4.72469400	6.57202800	3.31252100
H	5.79880900	5.88091900	1.15963700
H	5.59279200	3.57390900	0.34785900
H	6.78724100	1.74776600	2.28539000
H	9.22657900	1.92886300	2.02630100
H	10.30707700	1.46305500	-0.18283400
H	8.90965300	0.74948500	-2.11077200
H	6.72409600	0.15145900	-3.05677300
H	4.28360800	-0.28759000	-2.71082400
H	2.18070000	0.34413800	4.01580100
O	2.95619800	0.10864600	-0.58105300
O	3.18973100	-0.61854300	1.84938500
N	2.93564900	-2.46233000	0.08802200
C	2.26290400	-3.67792600	0.43394200
C	1.70556400	-4.45886500	-0.60044600
C	2.15935100	-4.06740700	1.77463100
C	0.93578400	-5.58091000	-0.23635100
C	1.45011000	-5.22241400	2.10776000
H	2.63367900	-3.44852200	2.53859300
C	0.82045400	-5.96399900	1.09855900
H	0.41353300	-6.13136400	-1.01949500
H	1.36927300	-5.52967800	3.15290000
H	0.22947100	-6.84576000	1.35622400
C	4.20984600	-2.65922300	-0.53824300
C	4.22663600	-3.16147900	-1.85815800
C	5.39619500	-2.36274100	0.14117100
C	5.47939000	-3.28588600	-2.49192600
C	6.62243100	-2.50889600	-0.50370700

H	5.33598500	-1.98418100	1.16120400
C	6.65999400	-2.96531400	-1.82692200
H	5.51288800	-3.65559100	-3.51982300
H	7.54547200	-2.24609800	0.01642000
H	7.61845300	-3.07082300	-2.34046500
C	1.89706400	-4.12811300	-2.01297500
H	1.08966400	-4.42675200	-2.68662500
C	3.00341100	-3.56402900	-2.55410000
H	3.03431100	-3.48628800	-3.64535500
P	2.26660300	-0.96439600	0.47457000

P2-(S,R)-**[E-F]‡**

Zero-point correction=	1.302840 (Hartree/Particle)
Thermal correction to Energy=	1.386232
Thermal correction to Enthalpy=	1.387176
Thermal correction to Gibbs Free Energy=	1.183563
Sum of electronic and zero-point Energies=	-4985.923228
Sum of electronic and thermal Energies=	-4985.839836
Sum of electronic and thermal Enthalpies=	-4985.838892
Sum of electronic and thermal Free Energies=	-4986.042505

C	-2.29658800	-1.52053900	-2.70643400
C	-1.76789400	-1.29820600	-3.99926000
C	-2.42455400	-0.47440000	-4.87771500
C	-3.62185100	0.18708800	-4.49164200
C	-4.27346900	1.09549600	-5.36759500
C	-5.41068300	1.76828000	-4.97756400
C	-5.92801000	1.56912500	-3.67676500
C	-5.31967800	0.69062600	-2.80494900
C	-4.16425300	-0.04725100	-3.18487800
C	-3.50442500	-0.97064900	-2.29493500
C	-3.33817800	-1.15852800	0.20013300
C	-4.08231500	-1.29284900	-0.96343800
C	-5.43815000	-1.76471300	-0.82519100
C	-6.22011900	-2.16903700	-1.94299500
C	-7.50761700	-2.63828100	-1.78307400
C	-8.08953400	-2.72084600	-0.49559900
C	-7.35365500	-2.35423300	0.61074100

C	-6.01755000	-1.88828800	0.48170600
C	-5.22988000	-1.57948700	1.62444200
C	-3.90669700	-1.25274200	1.48826100
H	-2.02122000	-0.29719100	-5.87726100
H	-3.84441300	1.25858700	-6.35938400
H	-5.90143400	2.46563000	-5.66034600
H	-6.81183000	2.12418800	-3.35354100
H	-5.72131400	0.56807100	-1.80079700
H	-5.78390300	-2.11910900	-2.94005200
H	-8.08057600	-2.95342200	-2.65831100
H	-9.11275800	-3.08616500	-0.38170900
H	-7.78169400	-2.43285800	1.61345600
H	-5.67475600	-1.65422000	2.61869900
H	-3.26291400	-1.08019100	2.34692800
H	-0.83229500	-1.78988900	-4.26137000
O	-1.98671000	-0.87379000	0.16447500
O	-1.58782300	-2.35437400	-1.86966600
N	-0.80772700	-3.24079200	0.40384800
C	0.32373000	-4.11762700	0.42206300
C	1.02908800	-4.28053600	1.63212700
C	0.70862800	-4.79623700	-0.74136500
C	2.19869000	-5.06546600	1.61268000
C	1.83301800	-5.62174600	-0.72078100
H	0.11521400	-4.66175600	-1.64761300
C	2.58523600	-5.73974800	0.45646800
H	2.80584400	-5.11624000	2.51639700
H	2.13644100	-6.15207000	-1.62624100
H	3.48615100	-6.35737100	0.46924500
C	-1.95351600	-3.76966100	1.08654100
C	-1.91185500	-3.82864700	2.49658400
C	-3.07028400	-4.22101500	0.37486400
C	-3.07105000	-4.27070600	3.16543300
C	-4.19525100	-4.67447000	1.05984300
H	-3.05419900	-4.17372500	-0.71337600
C	-4.19692700	-4.68622000	2.46006500
H	-3.06745900	-4.29907200	4.25786500
H	-5.07874600	-4.99307500	0.50365000
H	-5.08325200	-5.02481000	3.00155600
C	0.57954500	-3.67339500	2.88501700
H	1.37036900	-3.42607900	3.59890900
C	-0.71000400	-3.48497000	3.25614500
H	-0.88718700	-3.13695700	4.27731500
C	0.59376100	1.45387400	2.67988400
C	0.86630100	0.34268900	3.50250600

C	-0.15677700	-0.21408600	4.22895900
C	-1.48538900	0.27886800	4.11009600
C	-2.56480700	-0.32971500	4.80898000
C	-3.85438600	0.14052000	4.67922500
C	-4.12064300	1.23039700	3.81618300
C	-3.09597800	1.84778100	3.13003300
C	-1.74737300	1.41638600	3.27161300
C	-0.64985500	2.06770000	2.60262100
C	-0.38529200	3.60830000	0.61599500
C	-0.81635700	3.38060900	1.91665100
C	-1.40566700	4.50087300	2.61563500
C	-1.68164100	4.46826100	4.01168600
C	-2.24637400	5.54911000	4.65643600
C	-2.57228900	6.72618700	3.94242800
C	-2.29116500	6.80494800	2.59582100
C	-1.69029900	5.71646600	1.90687800
C	-1.33788800	5.82094200	0.53321800
C	-0.67155900	4.79948200	-0.09085700
H	0.05990400	-1.05512500	4.88848400
H	-2.34804300	-1.18514500	5.45349400
H	-4.67233700	-0.33663300	5.22409900
H	-5.14763100	1.57684400	3.68119100
H	-3.31761800	2.67847300	2.46063700
H	-1.42654000	3.57742100	4.58293000
H	-2.43654000	5.49609900	5.73092400
H	-3.02809700	7.57208000	4.46214100
H	-2.51310500	7.71615400	2.03417400
H	-1.56881700	6.74161400	-0.00743800
H	-0.33999100	4.86706200	-1.12697100
H	1.88056300	-0.04895600	3.56804500
O	0.29571900	2.66323100	-0.11319400
O	1.64428000	1.96286500	1.92984700
N	2.88913200	2.71064800	-0.18895900
C	4.18769300	2.12706000	-0.29582800
C	4.87954900	2.22426500	-1.52570800
C	4.73011600	1.42547000	0.78616400
C	6.13180000	1.58540600	-1.61850300
C	5.95955400	0.77524500	0.65579500
H	4.18646200	1.35521000	1.72853700
C	6.66532800	0.86704600	-0.54728500
H	6.68781300	1.65504500	-2.55737100
H	6.33879100	0.19770400	1.49993600
H	7.62915800	0.36561500	-0.65755200
C	2.79848800	4.13712500	-0.26911700

C	2.99980000	4.74976100	-1.52542200
C	2.46189600	4.89657900	0.85457000
C	2.76125600	6.13396700	-1.62804600
C	2.25246300	6.27064100	0.73203100
H	2.32826600	4.39069500	1.81033400
C	2.38846900	6.88676100	-0.51550900
H	2.89180400	6.62022400	-2.59819400
H	1.95901500	6.85294400	1.60764100
H	2.20905300	7.95913100	-0.62021300
C	4.33286100	2.94000900	-2.67909000
H	4.71841400	2.61210400	-3.65048300
C	3.50191000	4.01103600	-2.68310800
H	3.27699700	4.45974300	-3.65597000
P	-0.78700900	-1.80814600	-0.48485700
P	1.58871800	1.74022700	0.28138300
Ir	0.95415100	-0.38767700	-0.53415700
C	2.23185400	-1.21595100	0.99200200
H	2.91346400	-0.50683100	1.45411600
H	1.74137400	-1.86333400	1.71340400
C	2.58890400	-1.81473500	-0.26541000
H	2.26123400	-2.83821100	-0.43449600
C	3.58892900	-1.31704600	-1.16955800
H	3.92342400	-0.29140900	-1.02523900
C	0.13532900	0.69681600	-2.24833300
C	1.15266500	0.05944000	-2.69294600
C	2.22607000	-0.70101400	-3.13411700
H	3.12460900	-0.15267400	-3.43670500
C	1.99093600	-2.05442000	-3.74388400
H	1.64471900	-1.93826900	-4.78675700
H	2.91133100	-2.65229700	-3.77150900
H	1.21940400	-2.60709000	-3.18922800
C	-0.90276800	1.64353600	-2.57873600
C	-0.83492800	2.37203900	-3.78254800
C	-1.96841100	1.87902000	-1.69463900
C	-1.81593400	3.31130700	-4.09112500
H	-0.00117400	2.19522000	-4.46507500
C	-2.94378000	2.82260900	-2.00745000
H	-2.00735200	1.32527600	-0.75855100
C	-2.87434900	3.53849900	-3.20469900
H	-1.75921300	3.86785100	-5.02966500
H	-3.76579200	2.99783300	-1.31158700
H	-3.64736300	4.26915600	-3.45117900
C	4.49419400	-2.17824800	-1.91636900
C	4.46336800	-3.58261200	-1.79561700

C	5.44479200	-1.60552500	-2.78964300
C	5.34336000	-4.37990200	-2.52491200
H	3.76105100	-4.05197500	-1.11224700
C	6.31758300	-2.40384200	-3.52173500
H	5.48937100	-0.52078300	-2.88215100
C	6.27078700	-3.79793700	-3.39412000
H	5.30854300	-5.46542000	-2.40631900
H	7.04409600	-1.94005700	-4.19307700
H	6.95952400	-4.42514800	-3.96468200
O	4.00913400	-2.83393700	2.62622800
B	4.01967500	-1.85209400	3.69438400
F	5.03485300	-2.07278700	4.61526500
F	4.18791700	-0.52475400	3.15238100
F	2.74915900	-1.90638000	4.31970700
C	5.14516600	-2.92576900	1.83185700
H	6.07746300	-2.94281000	2.42932400
H	5.10871700	-3.85703600	1.23627900
H	5.23200700	-2.08599300	1.10999400

P2-**B-M1**

Zero-point correction=	1.305497 (Hartree/Particle)
Thermal correction to Energy=	1.386304
Thermal correction to Enthalpy=	1.387248
Thermal correction to Gibbs Free Energy=	1.188875
Sum of electronic and zero-point Energies=	-5122.328588
Sum of electronic and thermal Energies=	-5122.247781
Sum of electronic and thermal Enthalpies=	-5122.246837
Sum of electronic and thermal Free Energies=	-5122.445211

C	2.85845300	2.15912100	0.65905000
C	2.00286700	2.90583400	1.49525500
C	1.74871700	4.22484700	1.21361400
C	2.27169700	4.82556300	0.04003800
C	1.92611000	6.15649400	-0.32040100
C	2.36095800	6.70667800	-1.50527200
C	3.15578300	5.93405300	-2.38729500

C	3.52246600	4.64635300	-2.05837500
C	3.11196100	4.05394300	-0.82971700
C	3.46992800	2.70889900	-0.45963800
C	4.07417400	0.66947100	-1.76622600
C	4.42482700	1.91867100	-1.27696600
C	5.74119600	2.41137100	-1.59117700
C	6.28515300	3.57296400	-0.97532500
C	7.55894500	4.01012100	-1.27474800
C	8.35750200	3.31462300	-2.21390200
C	7.86633100	2.17739300	-2.81854800
C	6.56583400	1.69072100	-2.51775100
C	6.07397700	0.48848500	-3.09662600
C	4.86189200	-0.02457000	-2.71299700
H	1.07329600	4.80051200	1.84833000
H	1.28122500	6.72353800	0.35468000
H	2.08100800	7.72741200	-1.77618100
H	3.47604000	6.35945600	-3.34144100
H	4.12441400	4.06346400	-2.75403400
H	5.68469800	4.11427500	-0.24490300
H	7.95575600	4.89915600	-0.77881900
H	9.36201300	3.67444900	-2.44850300
H	8.47778200	1.62030600	-3.53327400
H	6.69535500	-0.04569100	-3.81865400
H	4.47973100	-0.97014200	-3.09552700
H	1.51878300	2.40222500	2.32573300
O	2.90239200	0.05686300	-1.39125300
O	3.10347400	0.83992700	1.00504800
N	3.53585700	-1.63979000	0.53764600
C	3.16670500	-2.78296000	1.31957600
C	2.91912900	-4.01265900	0.67587300
C	3.06167700	-2.66836800	2.70630400
C	2.40419000	-5.06584400	1.45453400
C	2.59635100	-3.73890600	3.47098300
H	3.30799400	-1.71446600	3.16930200
C	2.23746700	-4.93055200	2.83239700
H	2.15449000	-6.00798400	0.96156000
H	2.47418900	-3.62347800	4.54889400
H	1.83692900	-5.76327600	3.41522000
C	4.88782700	-1.67052800	0.05849600
C	5.25790600	-2.66994100	-0.87239500
C	5.81273300	-0.71360800	0.49238500
C	6.58134600	-2.64737200	-1.35930600
C	7.11062300	-0.71031200	-0.01366000
H	5.48150900	0.04583100	1.19959700

C	7.49523800	-1.68586900	-0.94070300
H	6.88146100	-3.40358700	-2.08920200
H	7.81566200	0.06132600	0.30157600
H	8.51002700	-1.68583400	-1.34512500
C	3.28074300	-4.24235600	-0.71861000
H	2.72495500	-5.03276400	-1.22871800
C	4.32938400	-3.68526600	-1.36728500
H	4.56197200	-4.07549600	-2.36324000
P	2.44274000	-0.42277200	0.11400000
Ir	0.10805100	-0.73972500	0.04555400
C	-0.08326500	-2.04945700	1.74535300
H	-0.95050900	-2.70257800	1.66746300
H	0.81348800	-2.58675400	2.03114200
C	-0.28172300	-0.70436500	2.19269800
H	-1.30800900	-0.38945200	2.36064800
C	0.58980100	-0.04341700	3.25002900
H	1.60434000	0.18005700	2.87562500
O	-0.06765000	1.19104000	3.55763300
C	-0.18761400	1.34253100	-0.62186800
C	0.20470200	0.68398700	-1.63232900
C	0.52132500	0.51143600	-3.06176800
H	1.01525000	1.43174100	-3.42124200
H	1.23941900	-0.31329700	-3.16662300
C	-0.71881000	0.20449800	-3.90941600
H	-1.45840400	1.01634400	-3.84507000
H	-0.43409300	0.07534600	-4.96603500
H	-1.19208300	-0.72649300	-3.56843500
C	-0.75566700	2.58214500	-0.14724200
C	-0.78034900	3.67949700	-1.03430000
C	-1.29078000	2.74348600	1.13974100
C	-1.31087700	4.90355500	-0.63613300
H	-0.35833500	3.56252700	-2.03421900
C	-1.81431600	3.97404800	1.53596100
H	-1.25612200	1.91455500	1.84088900
C	-1.82787100	5.05852700	0.65516900
H	-1.30950000	5.74476400	-1.33343600
H	-2.22813800	4.08358800	2.53973100
H	-2.24899100	6.01628500	0.97030900
C	0.74718500	-0.89133600	4.50868400
C	1.92643500	-0.80599900	5.26023000
C	-0.28328100	-1.71681500	4.97750000
C	2.08604400	-1.53680500	6.44024600
H	2.73645000	-0.15996700	4.91061500
C	-0.13143300	-2.45116800	6.15502000

H	-1.20648100	-1.80083300	4.40348000
C	1.05565100	-2.36673500	6.88983500
H	3.01769500	-1.46164300	7.00627800
H	-0.94227900	-3.09770200	6.49973900
H	1.17658000	-2.94586900	7.80844300
C	0.45371900	1.96899700	4.60436000
H	-0.08732600	2.92639200	4.58184400
H	0.31072000	1.49763600	5.59276900
H	1.53394800	2.17659900	4.47760600
Cl	0.86839500	-2.47547800	-1.60444600
C	-3.71057400	0.04022800	1.51337100
C	-3.49200000	0.04903100	2.91207900
C	-3.84495900	1.14180200	3.66241500
C	-4.39822600	2.29194800	3.03878100
C	-4.68106800	3.47115700	3.78052800
C	-5.17066700	4.59931700	3.15862800
C	-5.38793400	4.59071800	1.76018600
C	-5.14161000	3.45561400	1.01787700
C	-4.65865500	2.26610400	1.62889100
C	-4.38424100	1.07135500	0.87086900
C	-4.00060000	0.56795700	-1.56176100
C	-4.85166900	0.94303600	-0.53423900
C	-6.23904700	1.16017100	-0.86932900
C	-7.24937900	1.31941100	0.12040500
C	-8.57205900	1.50027900	-0.22819100
C	-8.96125200	1.54111700	-1.58787300
C	-8.01227100	1.36920400	-2.57231700
C	-6.64595500	1.15841000	-2.24495700
C	-5.67986200	0.90307100	-3.25588700
C	-4.38960000	0.58652400	-2.92098500
H	-3.67445400	1.14737000	4.74113800
H	-4.48689200	3.46868800	4.85620700
H	-5.37678600	5.50267200	3.73736600
H	-5.74168200	5.49567000	1.26106800
H	-5.29111200	3.47300800	-0.06057000
H	-6.97313400	1.28095800	1.17285800
H	-9.32608000	1.60800100	0.55510800
H	-10.01018100	1.69429700	-1.85180100
H	-8.29858200	1.37518900	-3.62723500
H	-5.99101200	0.91216700	-4.30264700
H	-3.64593000	0.32038800	-3.66959800
H	-3.05015000	-0.83583200	3.36789500
O	-2.70184300	0.18976800	-1.31369300
O	-3.29108300	-1.07835500	0.82552600

N	-2.67871900	-2.45330300	-1.22905900
C	-2.06352600	-3.73655700	-1.04679700
C	-1.47148800	-4.37235400	-2.15721000
C	-2.05103500	-4.33950700	0.21178600
C	-0.79177800	-5.58262500	-1.93669800
C	-1.36915200	-5.54076300	0.41058200
H	-2.57094500	-3.84604100	1.03376800
C	-0.72899800	-6.15693900	-0.66876000
H	-0.29761400	-6.06801400	-2.78174100
H	-1.33277500	-5.98847800	1.40595100
H	-0.18676200	-7.09417100	-0.52198500
C	-3.89822800	-2.49271800	-1.98917000
C	-3.81071100	-2.73566500	-3.37808400
C	-5.14014500	-2.28825000	-1.37594400
C	-4.99966900	-2.67626500	-4.13243500
C	-6.30299500	-2.24651400	-2.14243000
H	-5.17362000	-2.12577300	-0.30016600
C	-6.22872600	-2.42972800	-3.52767200
H	-4.94398600	-2.84120400	-5.21144700
H	-7.26277800	-2.04803200	-1.66176500
H	-7.13546000	-2.38194400	-4.13501400
C	-1.53604300	-3.80639600	-3.50204600
H	-0.70626800	-4.07475700	-4.16182800
C	-2.55191800	-3.08814500	-4.03431000
H	-2.48568900	-2.83291300	-5.09659600
P	-2.14990900	-1.06622000	-0.41946500

P2-**[B-D]‡ (R)**

Zero-point correction=	1.320064 (Hartree/Particle)
Thermal correction to Energy=	1.404277
Thermal correction to Enthalpy=	1.405222
Thermal correction to Gibbs Free Energy=	1.201063
Sum of electronic and zero-point Energies=	-5446.667261
Sum of electronic and thermal Energies=	-5446.583047
Sum of electronic and thermal Enthalpies=	-5446.582103
Sum of electronic and thermal Free Energies=	-5446.786262

C	3.97116100	-0.46792600	1.96770700
C	3.57947300	-0.76512600	3.29215300
C	3.96771800	0.06623600	4.31309700

C	4.69933900	1.25479500	4.04308300
C	5.01259000	2.17499400	5.08080500
C	5.64655300	3.36676300	4.80653800
C	5.98319800	3.68991500	3.47028400
C	5.71078300	2.81032600	2.44372900
C	5.08206100	1.55748000	2.69222600
C	4.76623900	0.62309700	1.63843700
C	4.35339400	0.87881800	-0.83124200
C	5.23069400	0.86508600	0.24503000
C	6.62515400	1.09608500	-0.04321800
C	7.64626700	0.87395800	0.92236800
C	8.97620700	1.07652900	0.61607600
C	9.35986200	1.52311600	-0.67074800
C	8.39754600	1.73240700	-1.63510400
C	7.02185200	1.51089300	-1.35782100
C	6.03328700	1.65870200	-2.36945100
C	4.72841400	1.32267400	-2.12006700
H	3.67411200	-0.15226900	5.34229400
H	4.72326000	1.92187800	6.10390400
H	5.87503000	4.06851400	5.61185900
H	6.45818800	4.64822500	3.24774700
H	5.96696500	3.08291800	1.42130400
H	7.36935200	0.52217800	1.91552700
H	9.73986900	0.88558300	1.37361300
H	10.41525100	1.68836300	-0.89890200
H	8.67962900	2.05819900	-2.63959500
H	6.33550200	1.99630400	-3.36307700
H	3.95649800	1.36770200	-2.88776100
H	2.93992700	-1.63256500	3.45065800
O	3.03685600	0.49690500	-0.70189100
O	3.55798900	-1.33680900	0.97771200
N	2.86582400	-2.03857600	-1.36503800
C	2.30325200	-3.35140600	-1.44902000
C	1.73274400	-3.75153800	-2.67858300
C	2.30949900	-4.20289400	-0.33954100
C	1.15183700	-5.03109800	-2.74275800
C	1.72381800	-5.46533400	-0.43297600
H	2.73976000	-3.84971100	0.59823500
C	1.14700300	-5.87970100	-1.63758000
H	0.68936800	-5.35003200	-3.67878200
H	1.70306400	-6.11966800	0.44052200
H	0.67773200	-6.86302700	-1.70897500
C	4.06574200	-1.89266700	-2.15159200
C	3.92335200	-1.76098200	-3.54870700

C	5.33166200	-1.89736800	-1.55599000
C	5.08315300	-1.51304000	-4.30909600
C	6.46786800	-1.67647700	-2.33222700
H	5.40827100	-2.03938700	-0.47957600
C	6.33884800	-1.46452400	-3.70943800
H	4.98598900	-1.38461100	-5.38998000
H	7.45029100	-1.64407600	-1.85780800
H	7.22528900	-1.27085500	-4.31761700
C	1.69400000	-2.86823500	-3.84516000
H	0.83862300	-3.01316900	-4.51205400
C	2.63831800	-1.97150000	-4.21652700
H	2.49809700	-1.45357400	-5.17034300
P	2.42568600	-0.92597100	-0.17015700
Ir	0.15353600	-0.46434100	0.42605800
C	-0.37387600	-0.90006500	-1.61421600
H	-1.24406500	-0.36575500	-1.98731000
H	0.50344500	-0.83044100	-2.26088600
C	-0.62645600	-2.13743000	-0.93875400
H	0.14014500	-2.90184900	-0.92902200
C	-1.95342500	-2.64446600	-0.80372900
C	0.57964800	1.56102100	-0.06391100
C	0.91731000	1.40378500	1.16188200
C	1.56238600	1.98909800	2.35569700
H	2.60465100	1.64859600	2.37273800
H	1.61684900	3.08226000	2.20708800
C	0.91051400	1.65159100	3.69336700
H	0.82677300	0.56232700	3.80578000
H	1.51495900	2.04859300	4.52257500
H	-0.09886800	2.08380100	3.76469300
C	0.63903900	2.39672500	-1.24017900
C	1.68361500	3.34008000	-1.33784100
C	-0.30749200	2.32551500	-2.27510800
C	1.76724800	4.19221100	-2.43613000
H	2.42981400	3.38619600	-0.54279800
C	-0.21797200	3.17969300	-3.37442100
H	-1.12949900	1.61744400	-2.20301300
C	0.81391700	4.11657500	-3.45827300
H	2.58041600	4.91995000	-2.49685600
H	-0.97221800	3.12190000	-4.16106700
H	0.87298400	4.79105200	-4.31533900
C	-2.22389700	-3.93379700	-0.16575000
C	-1.27130700	-4.53583300	0.67402200
C	-3.45976200	-4.57845200	-0.37906900
C	-1.54554500	-5.76487000	1.27653700

H	-0.34445700	-4.01479600	0.90643000
C	-3.71357200	-5.81836800	0.19777400
H	-4.19628000	-4.09425900	-1.02090000
C	-2.75540100	-6.41713300	1.02765600
H	-0.80712000	-6.21135600	1.94648600
H	-4.66580600	-6.31991600	0.01014500
H	-2.96034400	-7.38705600	1.48794800
B	-3.47818700	-2.22775600	-3.27634600
F	-3.12342600	-0.89342600	-3.10345900
F	-4.60498700	-2.52533000	-2.46760800
F	-3.72271000	-2.55025400	-4.59285000
O	-2.32452700	-3.05696300	-2.77387500
C	-2.26554100	-4.39493900	-3.20200500
H	-3.24529000	-4.89802200	-3.14579600
H	-1.91439600	-4.43614400	-4.24681700
H	-1.55684300	-4.94144500	-2.56406700
H	-2.78041700	-1.94076800	-0.86597100
Cl	0.52388800	-2.02073200	2.33712000
C	-2.00417400	3.03363700	0.75877100
C	-1.00872000	3.94791700	1.17366100
C	-0.75315000	5.07177000	0.43169200
C	-1.46242800	5.31499900	-0.77630900
C	-1.13540900	6.40996700	-1.61851500
C	-1.80633600	6.61839900	-2.80421900
C	-2.82889100	5.72405900	-3.19686500
C	-3.17731400	4.65779900	-2.39347500
C	-2.51838200	4.42398700	-1.15576300
C	-2.84375800	3.29803400	-0.31414700
C	-4.00299500	1.10450600	-0.70977300
C	-4.05544300	2.48179600	-0.58674700
C	-5.35273000	3.10641000	-0.67914300
C	-5.57059800	4.47225700	-0.34521000
C	-6.83007600	5.03252200	-0.41060600
C	-7.94145100	4.26072600	-0.82453700
C	-7.76805600	2.92983400	-1.13848400
C	-6.48872700	2.31775000	-1.05721500
C	-6.32022900	0.92812000	-1.30415700
C	-5.10684200	0.32043300	-1.11022200
H	0.02262000	5.77455300	0.74325500
H	-0.32616800	7.07756000	-1.31264400
H	-1.54059800	7.46020400	-3.44779300
H	-3.34331100	5.87229300	-4.14924700
H	-3.95520100	3.96809300	-2.71851400
H	-4.72907000	5.08048200	-0.01663300

H	-6.96933100	6.08107900	-0.13687000
H	-8.93220600	4.71746200	-0.88257600
H	-8.61932100	2.31436500	-1.44055100
H	-7.18147900	0.33456700	-1.61769400
H	-4.97227500	-0.74601700	-1.27708300
H	-0.45538900	3.72387400	2.08231700
O	-2.81582300	0.42842000	-0.46312500
O	-2.15253900	1.88872300	1.52107000
N	-3.04875400	-0.44840300	2.03303500
C	-2.56079800	-1.11179400	3.20987200
C	-2.85852300	-2.47696700	3.39780400
C	-1.81195900	-0.40556200	4.14977700
C	-2.26480400	-3.13005000	4.49420100
C	-1.25725600	-1.06598200	5.24436900
H	-1.64855200	0.65856800	3.99288400
C	-1.46863800	-2.43877600	5.40342100
H	-2.45205100	-4.19801400	4.62970200
H	-0.64311100	-0.51304000	5.95841400
H	-1.01806500	-2.96942600	6.24530600
C	-4.47305600	-0.21465300	2.04525000
C	-5.33003100	-1.32463200	1.87797600
C	-4.99997400	1.07121000	2.21559600
C	-6.71437500	-1.07908400	1.77541100
C	-6.37364000	1.28521700	2.12474300
H	-4.31989100	1.90371700	2.37871300
C	-7.23210400	0.20671500	1.88663900
H	-7.38400800	-1.92780800	1.61645700
H	-6.76956300	2.29866100	2.21193700
H	-8.30726300	0.37352600	1.79128000
C	-3.78459400	-3.20316800	2.54018900
H	-3.65185800	-4.28668200	2.52169600
C	-4.85040900	-2.70197900	1.87270400
H	-5.49906200	-3.42088900	1.36461000
P	-2.00438600	0.32185900	0.95473200

P2-**D**

Zero-point correction= 1.319585 (Hartree/Particle)

Thermal correction to Energy= 1.405028

Thermal correction to Enthalpy=	1.405972
Thermal correction to Gibbs Free Energy=	1.199182
Sum of electronic and zero-point Energies=	-5446.659154
Sum of electronic and thermal Energies=	-5446.573711
Sum of electronic and thermal Enthalpies=	-5446.572767
Sum of electronic and thermal Free Energies=	-5446.779557

C	3.08226500	2.23144200	1.33762800
C	2.39000000	3.02980800	2.27765500
C	2.19631600	4.36559300	2.03830400
C	2.65193200	4.95780000	0.83018500
C	2.36300600	6.31195900	0.51750700
C	2.77149900	6.86675500	-0.67563300
C	3.47532300	6.07373900	-1.61089900
C	3.78043000	4.75799700	-1.32972700
C	3.39638600	4.16041300	-0.09801200
C	3.68464800	2.78033600	0.21364800
C	4.23823800	0.77658000	-1.18626600
C	4.60352000	1.99986700	-0.65371600
C	5.92794000	2.48318700	-0.95827600
C	6.50457700	3.59904700	-0.29063700
C	7.78529500	4.02154900	-0.58211500
C	8.55696400	3.35936000	-1.56625700
C	8.03480200	2.26442200	-2.22032400
C	6.72877200	1.78977400	-1.92490100
C	6.21674400	0.61550600	-2.54171100
C	5.00513100	0.09991200	-2.15971800
H	1.65519000	4.98079000	2.76016700
H	1.79229600	6.90168200	1.23875700
H	2.53740800	7.90775600	-0.90920400
H	3.77278400	6.50271200	-2.57053800
H	4.30737000	4.15909900	-2.07090000
H	5.92766900	4.11672000	0.47446800
H	8.20791400	4.87382000	-0.04502500
H	9.56580400	3.70983100	-1.79549300
H	8.62587100	1.73017100	-2.96845200
H	6.82241800	0.10115300	-3.29061100
H	4.61369500	-0.82958500	-2.57208600
H	2.00948200	2.55790900	3.17895000
O	3.05197300	0.16995300	-0.81266500
O	3.19474800	0.87715900	1.62550000
N	3.71650800	-1.57829600	1.04158300
C	3.44048900	-2.65956600	1.94714500

C	3.48156900	-3.98143200	1.45987200
C	3.18250100	-2.39631300	3.29315700
C	3.17280700	-5.01991900	2.36009300
C	2.88543300	-3.43925800	4.16658400
H	3.20001600	-1.36369700	3.63749800
C	2.87176200	-4.75558000	3.69281300
H	3.17343300	-6.04742800	1.99109800
H	2.65233100	-3.22437900	5.21140000
H	2.63192600	-5.57893300	4.36925400
C	5.09887500	-1.51195700	0.63340700
C	5.57995300	-2.50031200	-0.25252500
C	5.93802100	-0.49149200	1.09381900
C	6.90793700	-2.38501800	-0.70828300
C	7.24876300	-0.40142600	0.62955200
H	5.53931800	0.24673500	1.78736300
C	7.73170400	-1.34912800	-0.27939500
H	7.28856900	-3.13379600	-1.40719600
H	7.88596600	0.42026100	0.96167700
H	8.75478400	-1.27457300	-0.65427900
C	3.86070000	-4.30297200	0.08475200
H	3.43097600	-5.22176400	-0.32192200
C	4.77171400	-3.64552600	-0.66983200
H	5.02929200	-4.08090900	-1.64041100
P	2.60557400	-0.36615300	0.67786100
Ir	0.19090100	-0.68660400	0.55252500
C	0.29040600	-0.34071900	-1.59654900
H	-0.49024100	0.29186400	-2.00678200
H	1.30634100	-0.05974700	-1.85895700
C	-0.01347500	-1.74247200	-1.55894400
H	-0.99990700	-2.08510500	-1.86619300
C	0.87033300	-2.66029300	-1.01986400
H	1.91698700	-2.37240600	-0.87821300
O	-1.36935900	-0.54087000	-4.02533500
C	0.08854400	1.44630700	0.85418700
C	0.04545400	0.87013000	1.99083600
C	-0.12041500	0.85954400	3.45813100
H	-0.33160300	1.89945900	3.75899700
H	-1.02321500	0.26735900	3.67585400
C	1.03172700	0.27873000	4.28338100
H	1.99544600	0.75135800	4.05083700
H	0.82454500	0.42384900	5.35461600
H	1.11340400	-0.79575100	4.08735800
C	-0.01665300	2.64614300	0.05662500
C	-0.75070100	3.72300000	0.59199100

C	0.60192300	2.80125200	-1.19352100
C	-0.88042700	4.91378900	-0.11597100
H	-1.22218300	3.61017900	1.56577100
C	0.47219600	3.99767300	-1.89830400
H	1.20388600	1.99514100	-1.60100100
C	-0.27122200	5.05358400	-1.36690500
H	-1.46854600	5.72964800	0.30872600
H	0.96495000	4.10642600	-2.86593100
H	-0.37016400	5.98758700	-1.92385500
C	0.63082900	-4.12342300	-0.97813600
C	0.69934600	-4.87449200	0.20238200
C	0.47581900	-4.78424700	-2.21053200
C	0.66473300	-6.26846500	0.14902800
H	0.76790400	-4.35738800	1.15615100
C	0.46748200	-6.17985700	-2.25637900
H	0.35662200	-4.19875400	-3.12347300
C	0.57403300	-6.92688300	-1.08027900
H	0.71296700	-6.84279200	1.07778100
H	0.36165000	-6.68268700	-3.22060700
H	0.56427800	-8.01910600	-1.12038100
C	-1.49313700	0.65519700	-4.73083000
H	-2.54921000	0.91607900	-4.95395700
H	-1.07725500	1.48068800	-4.12250700
H	-0.95434600	0.62971800	-5.69606500
B	-1.78265900	-1.77645000	-4.67636400
F	-1.53188600	-1.76322700	-6.04227100
F	-1.08000500	-2.84234900	-4.04983200
F	-3.17603000	-1.99604200	-4.45154200
Cl	-0.04875000	-2.32598900	2.36802000
C	-3.28692100	1.60139200	1.73968400
C	-3.06899400	2.19755800	3.00693900
C	-3.33254100	3.52862400	3.21145400
C	-3.77179700	4.34552600	2.13505300
C	-3.91691200	5.75212200	2.27840700
C	-4.29372500	6.53720500	1.21008200
C	-4.53411900	5.93807000	-0.04971200
C	-4.42055600	4.57370600	-0.21269500
C	-4.05066300	3.73000700	0.87163500
C	-3.90472700	2.30314300	0.70836200
C	-3.66897800	0.79966600	-1.27709900
C	-4.44568900	1.64984100	-0.51141100
C	-5.82026000	1.83130000	-0.90712200
C	-6.77387900	2.50653800	-0.09471800
C	-8.08969400	2.62880400	-0.48947700

C	-8.52713600	2.08713600	-1.72212200
C	-7.63753800	1.40243700	-2.52043100
C	-6.27892200	1.23840700	-2.13298700
C	-5.38137100	0.46097400	-2.91633500
C	-4.09776500	0.22024500	-2.48737100
H	-3.17667900	3.97697400	4.19544100
H	-3.71046800	6.20106000	3.25339600
H	-4.39596700	7.61830400	1.32882800
H	-4.80401200	6.56261900	-0.90426900
H	-4.59177000	4.13108600	-1.19273800
H	-6.46225300	2.91538700	0.86490900
H	-8.80205100	3.14345400	0.15969000
H	-9.56988500	2.19879700	-2.02788400
H	-7.96467200	0.95550900	-3.46239000
H	-5.72418600	0.01659400	-3.85322800
H	-3.40526600	-0.39535000	-3.06233300
H	-2.71478500	1.55865600	3.81219200
O	-2.40104100	0.46371500	-0.82847500
O	-2.92321500	0.27348600	1.66376600
N	-3.26669700	-1.82734900	0.40093700
C	-4.51334600	-1.78566200	1.13286800
C	-4.57031900	-2.39527600	2.40440400
C	-5.62920100	-1.14603500	0.59251800
C	-5.73874400	-2.20030500	3.16874200
C	-6.78675000	-0.99142500	1.35416000
H	-5.57961500	-0.76679700	-0.42339900
C	-6.82732700	-1.49615500	2.65941800
H	-5.78998400	-2.63947100	4.16836500
H	-7.64320500	-0.46315000	0.93046700
H	-7.72182000	-1.36073900	3.27210300
C	-3.00241100	-3.11241200	-0.18477300
C	-2.74380600	-4.20247700	0.67432100
C	-3.08250000	-3.27835100	-1.56879900
C	-2.53454500	-5.46096300	0.07782400
C	-2.88099700	-4.53671100	-2.13122400
H	-3.29875200	-2.43661900	-2.22409600
C	-2.61614800	-5.63004700	-1.30113800
H	-2.31852100	-6.31667600	0.72034000
H	-2.90901200	-4.63346500	-3.21659400
H	-2.45340300	-6.61822700	-1.73370300
C	-3.51478300	-3.27665100	2.89221700
H	-3.44335800	-3.38544400	3.97861300
C	-2.73657300	-4.08134500	2.13037100
H	-2.08375200	-4.78761000	2.65124000

P	-2.18037600	-0.54959100	0.44617500

P2-**[B-D]‡ (S)**

Zero-point correction=	1.319349 (Hartree/Particle)
Thermal correction to Energy=	1.404063
Thermal correction to Enthalpy=	1.405007
Thermal correction to Gibbs Free Energy=	1.198776
Sum of electronic and zero-point Energies=	-5446.654619
Sum of electronic and thermal Energies=	-5446.569905
Sum of electronic and thermal Enthalpies=	-5446.568961
Sum of electronic and thermal Free Energies=	-5446.775192

C	3.17881100	0.91453800	1.51969300
C	2.70805500	1.03496700	2.84990400
C	2.75721900	2.25180500	3.48253400
C	3.24597800	3.40091400	2.80399000
C	3.19296700	4.68811300	3.40475000
C	3.60753500	5.80903500	2.71826300
C	4.08856400	5.68072800	1.39378900
C	4.16941700	4.44293000	0.79118100
C	3.76734800	3.26214800	1.47480700
C	3.79836300	1.96028700	0.85332700
C	3.73469200	1.25129500	-1.54820800
C	4.43554600	1.78474900	-0.47696800
C	5.78980900	2.20832800	-0.71540600
C	6.67869200	2.53072600	0.34679200
C	7.98526100	2.89281500	0.09640400
C	8.46991000	2.97117500	-1.23202100
C	7.63448700	2.66631300	-2.28456200
C	6.28946900	2.26570800	-2.05881700
C	5.43193700	1.90256300	-3.13206800
C	4.19010700	1.37369400	-2.88057800
H	2.37908500	2.34611600	4.50271900
H	2.80018200	4.77095800	4.42127900
H	3.55346800	6.79449500	3.18661100
H	4.38804100	6.57165500	0.83708900
H	4.51869700	4.36943000	-0.23707000
H	6.32038600	2.46373400	1.37366900
H	8.65403500	3.11696000	0.93072900
H	9.50510300	3.26673600	-1.41766100
H	7.99876200	2.71294400	-3.31419900
H	5.79283100	2.00236300	-4.15858300

H	3.53300300	1.02839200	-3.67727500
H	2.28433400	0.16731500	3.35348300
O	2.52034000	0.63659000	-1.36812200
O	3.04691900	-0.32444500	0.93109000
N	3.25058500	-1.94806200	-0.92790800
C	2.84582200	-3.14354500	-1.61940000
C	3.06326700	-3.24724300	-3.01136000
C	2.27316400	-4.19826700	-0.91084400
C	2.58754300	-4.39603600	-3.67248500
C	1.85371200	-5.34699100	-1.58008400
H	2.13162200	-4.09769800	0.16243600
C	1.99045900	-5.43589300	-2.96668800
H	2.72260200	-4.47251600	-4.75423100
H	1.38658700	-6.15307800	-1.01626400
H	1.63755700	-6.32286100	-3.49804500
C	4.68117300	-1.76926900	-0.83103100
C	5.42664800	-1.46865500	-1.99310300
C	5.31169700	-1.84362800	0.41573200
C	6.78454400	-1.12422800	-1.83381800
C	6.66261800	-1.52539300	0.54290000
H	4.71579500	-2.10955600	1.28712500
C	7.39537800	-1.13879800	-0.58485100
H	7.35909400	-0.84232900	-2.71868800
H	7.13718800	-1.55554200	1.52606000
H	8.44372200	-0.84927900	-0.48835100
C	3.82788000	-2.26870300	-3.77598900
H	3.61878800	-2.25014900	-4.85011300
C	4.86174600	-1.51325100	-3.33713700
H	5.41370200	-0.94125500	-4.08660300
P	2.20735500	-0.70184200	-0.45155700
Ir	-0.13367400	-0.83083400	-0.22325500
C	-0.08929600	-0.18095700	1.80734700
H	0.57404100	0.64301100	2.04339300
H	-1.09480300	-0.03683200	2.18239100
C	0.42901600	-1.50908300	1.88965300
H	1.50907800	-1.62476700	1.97108900
C	-0.30725300	-2.65784000	2.31763800
C	-0.12302300	1.08911500	-1.21563400
C	-0.31488900	0.18692200	-2.09430000
C	-0.58511800	-0.27886800	-3.46568000
H	-1.46710200	-0.93955200	-3.43899300
H	-0.85203700	0.59891300	-4.08085900
C	0.59190000	-1.03930200	-4.08350400
H	0.36827600	-1.32366600	-5.12382400

H	1.50687800	-0.42843100	-4.07956100
H	0.78290300	-1.95527100	-3.50992400
C	0.05922000	2.49163700	-0.93886600
C	-0.16406600	3.40580800	-1.99187000
C	0.49560100	2.98669500	0.29903000
C	0.06091400	4.76644300	-1.80806200
H	-0.51382700	3.02936900	-2.95515500
C	0.72167900	4.35106600	0.47694000
H	0.66283100	2.29936900	1.12177300
C	0.51110900	5.24480900	-0.57251900
H	-0.12100300	5.46164600	-2.63134300
H	1.06427300	4.71728000	1.44516500
H	0.68267100	6.31250000	-0.42377900
C	0.35318200	-3.97535400	2.20325700
C	1.61628600	-4.18808300	2.78409200
C	-0.27128700	-5.02054600	1.51175000
C	2.23519600	-5.43215500	2.68398600
H	2.08610800	-3.38113300	3.34872900
C	0.35023300	-6.26764600	1.41701000
H	-1.22853200	-4.84857300	1.02845100
C	1.60066700	-6.47789400	2.00158500
H	3.21208400	-5.59290000	3.14551200
H	-0.14850400	-7.07684800	0.87837200
H	2.08490800	-7.45442100	1.92660300
B	-0.76888900	-1.17734600	4.80576300
F	-1.93047000	-0.73651700	4.14251400
F	0.30328000	-0.32883100	4.56781900
F	-1.00575800	-1.34531900	6.15053800
O	-0.41149400	-2.54710600	4.21850800
C	-1.10074100	-3.63456900	4.81520500
H	-0.92916400	-4.53914900	4.21621500
H	-0.71349000	-3.79669300	5.83095700
H	-2.18216300	-3.43453000	4.87542100
H	-1.38372500	-2.65028100	2.16566100
Cl	-0.60812100	-3.01588700	-1.31998100
C	-2.88921000	1.75257800	1.29717200
C	-2.27253900	2.11063600	2.51957200
C	-1.99229300	3.43044100	2.77507000
C	-2.26762800	4.43331000	1.80779200
C	-1.93019500	5.79405600	2.03884800
C	-2.17181900	6.75701000	1.08440300
C	-2.74346900	6.38640300	-0.15538700
C	-3.09355600	5.07663200	-0.40400500
C	-2.89722100	4.06284400	0.57368300

C	-3.29981400	2.69375400	0.36234800
C	-3.90615900	1.28984800	-1.64826500
C	-4.18648500	2.33331900	-0.77731400
C	-5.41984400	3.05369900	-0.99856200
C	-5.95537500	3.95994600	-0.04027900
C	-7.14559900	4.62028500	-0.26487300
C	-7.86677500	4.42142500	-1.46582300
C	-7.39012700	3.53374300	-2.40583200
C	-6.18021600	2.81970900	-2.19257700
C	-5.72680000	1.84861000	-3.12612900
C	-4.62986700	1.07801300	-2.84460900
H	-1.53729200	3.71760100	3.72575100
H	-1.46016700	6.05793900	2.98960000
H	-1.90505000	7.79963200	1.27234100
H	-2.89748100	7.14235300	-0.92889300
H	-3.51603100	4.80548400	-1.37033900
H	-5.42243900	4.11968800	0.89542900
H	-7.53648600	5.29946600	0.49637000
H	-8.80275000	4.95816800	-1.63674500
H	-7.94616200	3.34967100	-3.32881000
H	-6.29495500	1.68679000	-4.04473700
H	-4.29880500	0.27638400	-3.50395100
H	-2.06703500	1.32888800	3.25068100
O	-2.87236100	0.41148300	-1.43467700
O	-3.16695100	0.40906200	1.09924000
N	-3.68430400	-1.71759200	-0.19854500
C	-3.61861700	-2.99505200	0.44137500
C	-3.63137300	-4.14760900	-0.37282900
C	-3.65623400	-3.09623900	1.83633300
C	-3.63827100	-5.40306900	0.26154200
C	-3.69355400	-4.35492800	2.44120900
H	-3.65697300	-2.18483200	2.43879800
C	-3.68390100	-5.50841300	1.65122300
H	-3.63157500	-6.30491300	-0.35543800
H	-3.72703900	-4.43276100	3.52855400
H	-3.70578400	-6.49374600	2.12183000
C	-4.97635900	-1.46060400	-0.78220900
C	-5.31247900	-2.14123200	-1.97223300
C	-5.86876300	-0.55980900	-0.19052200
C	-6.54044300	-1.82416100	-2.58585500
C	-7.08432500	-0.27399400	-0.80948600
H	-5.57974700	-0.06511800	0.73568900
C	-7.41398000	-0.90190200	-2.01591000
H	-6.80798100	-2.32846800	-3.51787600

H	-7.76268100	0.45505100	-0.36247400
H	-8.35916600	-0.66945800	-2.51175700
C	-3.70652600	-4.06347000	-1.83297600
H	-3.19417300	-4.85832900	-2.38181000
C	-4.45241000	-3.18224200	-2.53698900
H	-4.51372200	-3.32003900	-3.62116700
P	-2.51242300	-0.51105400	-0.13128400

P2-**B-M3**

Zero-point correction=	1.304972 (Hartree/Particle)
Thermal correction to Energy=	1.385776
Thermal correction to Enthalpy=	1.386720
Thermal correction to Gibbs Free Energy=	1.187994
Sum of electronic and zero-point Energies=	-5122.322039
Sum of electronic and thermal Energies=	-5122.241235
Sum of electronic and thermal Enthalpies=	-5122.240291
Sum of electronic and thermal Free Energies=	-5122.439017

C	2.74959400	2.28510700	0.14876500
C	1.91601800	3.22492300	0.79027500
C	1.56233600	4.38615600	0.15274500
C	1.96723000	4.62299800	-1.18600800
C	1.49916800	5.75467500	-1.90744500
C	1.83528900	5.94177800	-3.23019700
C	2.65242900	4.98988400	-3.88692500
C	3.13310200	3.88851500	-3.21007100
C	2.82045400	3.67170800	-1.83788800
C	3.28305600	2.51535000	-1.11195500
C	3.97609300	0.22796100	-1.82119300
C	4.26030400	1.58037200	-1.72077600
C	5.52563000	2.03869500	-2.23254700
C	6.01025400	3.35485300	-1.99513200
C	7.23785000	3.76119400	-2.47635700
C	8.04495000	2.87622900	-3.23044600
C	7.61039600	1.58978700	-3.46841400
C	6.36002200	1.13507000	-2.97049900
C	5.92651100	-0.20459700	-3.16865500
C	4.76938500	-0.65635600	-2.58782600
H	0.89671300	5.09695300	0.64577300
H	0.84535300	6.46196300	-1.39156600
H	1.46222600	6.81050400	-3.77776400

H	2.89790700	5.12336500	-4.94324700
H	3.74801100	3.15982600	-3.73643400
H	5.40227100	4.04443400	-1.41023300
H	7.59121100	4.77424700	-2.26977000
H	9.01206000	3.21142000	-3.61247500
H	8.23020500	0.89043000	-4.03571100
H	6.55039600	-0.88240000	-3.75570500
H	4.42971100	-1.68706600	-2.68042200
H	1.53205700	2.99156000	1.77688500
O	2.85520700	-0.30986400	-1.23697700
O	3.05305100	1.12411200	0.84402900
N	3.65827200	-1.34647600	1.08133100
C	3.37074800	-2.42991300	1.98096700
C	3.25606400	-3.74338500	1.47986400
C	3.24402800	-2.18456900	3.34848300
C	2.81947100	-4.75006100	2.35960600
C	2.86865200	-3.20711500	4.21984000
H	3.41699600	-1.17301700	3.71259900
C	2.61701700	-4.48503800	3.71274200
H	2.66823100	-5.75886000	1.96879900
H	2.74412400	-2.99935800	5.28275300
H	2.28232800	-5.28298400	4.37950400
C	5.02617300	-1.30250200	0.64181100
C	5.54445800	-2.38221700	-0.11299800
C	5.82042400	-0.18737000	0.93254100
C	6.87955300	-2.28742000	-0.55519400
C	7.12999300	-0.11216800	0.46261100
H	5.37791000	0.63137700	1.49790500
C	7.66332800	-1.17309000	-0.27760800
H	7.28965100	-3.10651200	-1.15137300
H	7.72998600	0.77752600	0.66424500
H	8.68807300	-1.11906900	-0.65178100
C	3.70401500	-4.10191400	0.13931100
H	3.24866100	-4.99581600	-0.29323700
C	4.74488900	-3.53838700	-0.51453300
H	5.07622200	-4.02642900	-1.43688100
P	2.46662200	-0.37407600	0.36555700
Ir	0.15600900	-0.82177400	0.40875100
C	-0.02941400	-2.00513500	2.23694300
H	-0.87623700	-2.68165600	2.15849800
H	0.88915000	-2.50248400	2.53280300
C	-0.24326900	-0.65176900	2.60083500
H	-1.27327400	-0.31709100	2.72247100
C	0.71095000	-0.01815300	3.60508300

C	-0.30047500	1.15159300	-0.35051100
C	0.12285100	0.46457300	-1.34271400
C	0.36816800	0.42318100	-2.80244200
H	-0.25221000	1.21366700	-3.26313700
H	1.41519100	0.71913500	-2.98374100
C	0.09413600	-0.92344200	-3.47272600
H	-0.93919100	-1.25126000	-3.28916100
H	0.24948600	-0.84966000	-4.56095900
H	0.75101700	-1.69967600	-3.06095500
C	-0.97396400	2.37656500	0.00759100
C	-1.29118900	3.29860000	-1.01376700
C	-1.30636400	2.70429000	1.32846000
C	-1.88846600	4.51778200	-0.70825600
H	-1.03517300	3.05838600	-2.04645300
C	-1.88811500	3.93404100	1.63484800
H	-1.08189500	1.99291000	2.11540000
C	-2.17888300	4.84900000	0.62117700
H	-2.11984500	5.22137500	-1.51199700
H	-2.12014500	4.17105000	2.67306600
H	-2.64715400	5.80539600	0.86228700
C	0.38109400	1.39319700	4.04430300
C	1.35189700	2.39804100	4.00887800
C	-0.86675400	1.68249300	4.61552000
C	1.06847500	3.68651800	4.47380400
H	2.34061200	2.16512000	3.60772900
C	-1.15385600	2.96302600	5.08576000
H	-1.61045100	0.88998600	4.69706000
C	-0.18928700	3.97431500	5.00553800
H	1.83369500	4.46444100	4.41972800
H	-2.13447200	3.17761800	5.51762700
H	-0.41646500	4.97999000	5.36695000
Cl	1.03806800	-2.86201800	-0.75619500
H	1.73768500	-0.01556800	3.20239200
O	0.66306900	-0.88596000	4.74928200
C	1.45184100	-0.49631100	5.84399200
H	2.50724400	-0.31532900	5.55899600
H	1.07884700	0.41971500	6.33664700
H	1.42273700	-1.32093400	6.57139300
C	-3.78702900	0.09820300	1.39321900
C	-3.69712500	0.37991500	2.77647600
C	-4.17180700	1.56880100	3.27179800
C	-4.69316000	2.55613200	2.39505100
C	-5.10389300	3.82868200	2.87615900
C	-5.55991700	4.79933800	2.01189000

C	-5.60744600	4.53428000	0.62258200
C	-5.23228300	3.30366800	0.12844800
C	-4.78671300	2.26729600	0.99383600
C	-4.41357000	0.96352500	0.50467000
C	-3.80059800	0.01335500	-1.74368200
C	-4.74505600	0.55802200	-0.88690300
C	-6.09369500	0.68285400	-1.38823900
C	-7.19821300	0.98809800	-0.54410000
C	-8.48082800	1.07590300	-1.04498200
C	-8.73370300	0.87318800	-2.42217600
C	-7.69087900	0.55474500	-3.26500900
C	-6.36286200	0.43328300	-2.77515100
C	-5.30040800	0.02836300	-3.62868200
C	-4.05070300	-0.20487600	-3.11839400
H	-4.12773400	1.77889900	4.34256500
H	-5.03493100	4.02652100	3.94902700
H	-5.86709000	5.77647900	2.39177900
H	-5.93165500	5.31679200	-0.06723800
H	-5.25467700	3.12274400	-0.94496800
H	-7.02778100	1.13765600	0.52078900
H	-9.30928800	1.29948700	-0.36869800
H	-9.75205900	0.95509300	-2.80893400
H	-7.87120700	0.37176000	-4.32749400
H	-5.50525100	-0.14449600	-4.68736700
H	-3.23290100	-0.57921900	-3.73312800
H	-3.27457800	-0.38701600	3.42592700
O	-2.53673900	-0.30621100	-1.31507000
O	-3.31018400	-1.12628700	0.97891800
N	-2.50757400	-2.86348900	-0.69715200
C	-1.92771500	-4.08322100	-0.21549500
C	-1.21847600	-4.90136200	-1.11856900
C	-2.07064700	-4.45103600	1.12344900
C	-0.58068600	-6.04429100	-0.60682800
C	-1.43281500	-5.59313800	1.61083400
H	-2.67381400	-3.82043600	1.77858600
C	-0.67517800	-6.38357100	0.74159900
H	0.00372600	-6.66800600	-1.28760500
H	-1.52126300	-5.85823400	2.66653400
H	-0.16396000	-7.27365500	1.11599500
C	-3.63550700	-3.06061900	-1.56669800
C	-3.39384800	-3.54828900	-2.87014100
C	-4.93695500	-2.77105700	-1.13987900
C	-4.49186700	-3.64815300	-3.74817800
C	-6.00782600	-2.89102600	-2.02331600

H	-5.08902300	-2.41715900	-0.12160000
C	-5.78010800	-3.32009900	-3.33565500
H	-4.31736700	-4.00433800	-4.76663700
H	-7.01482400	-2.62729100	-1.69470100
H	-6.61393200	-3.40041800	-4.03682700
C	-1.12570800	-4.58712500	-2.54224100
H	-0.22829800	-4.95799200	-3.04502300
C	-2.07024200	-3.99202100	-3.30670800
H	-1.88174200	-3.93024000	-4.38306500
P	-2.06159500	-1.33564200	-0.13120800