Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2020

Supporting Information

Gold-Catalyzed Domino Cyclization to Diverse Polyheterocyclic Frameworks: Mechanism, Origin of cooperative hydrogen bond, and Role of π-stacking interactions

*Yunhe Li, Xiang Zhao**

Institute for Chemical Physics & Department of Chemistry, School of Science, State Key Laboratory of Electrical Insulation and Power Equipment & MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiaotong University, Xi'an710049, China

Table of contents

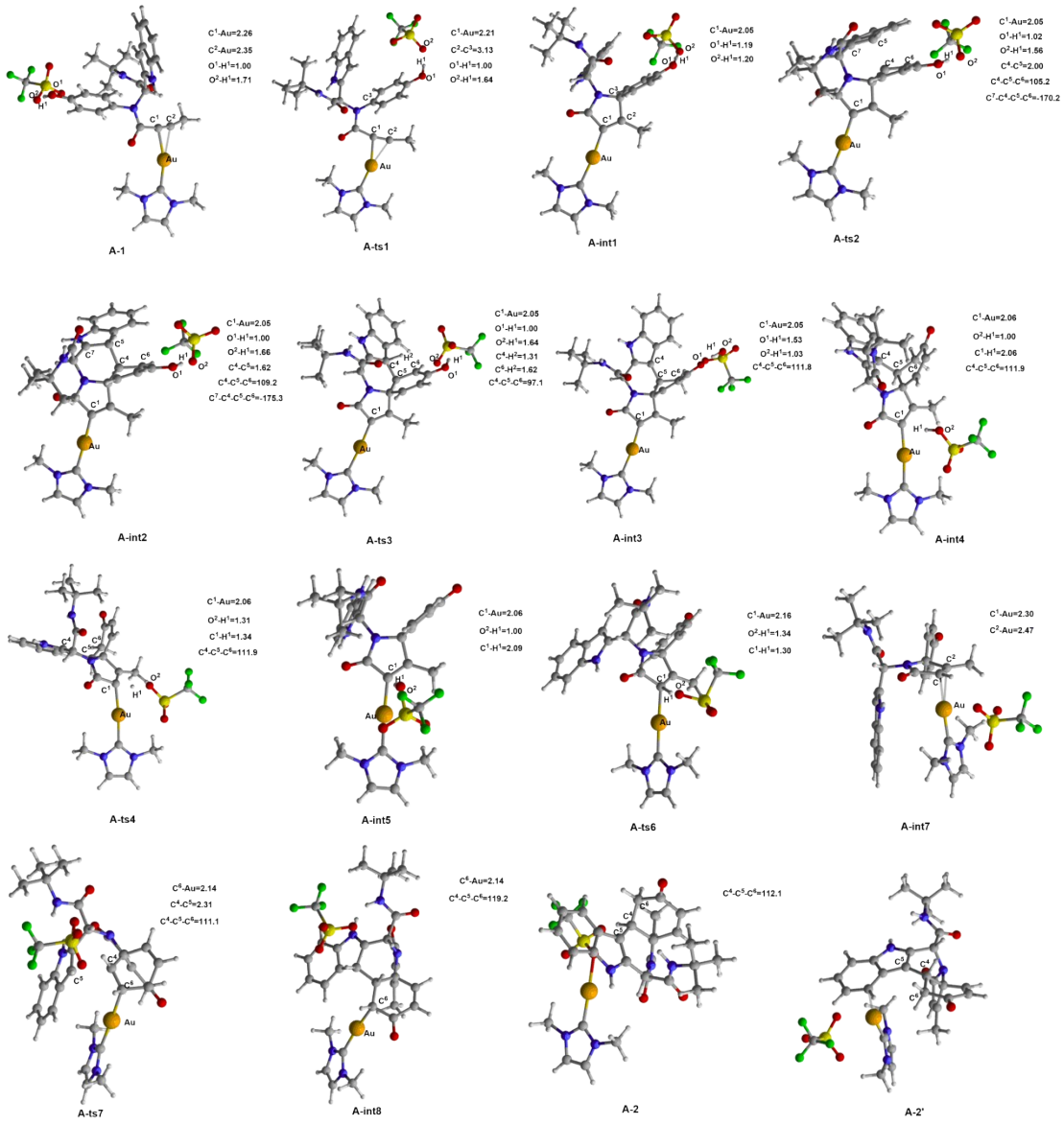

Fig. S1. Optimized geometries for the TSs and intermediates shown in Figure. 1.

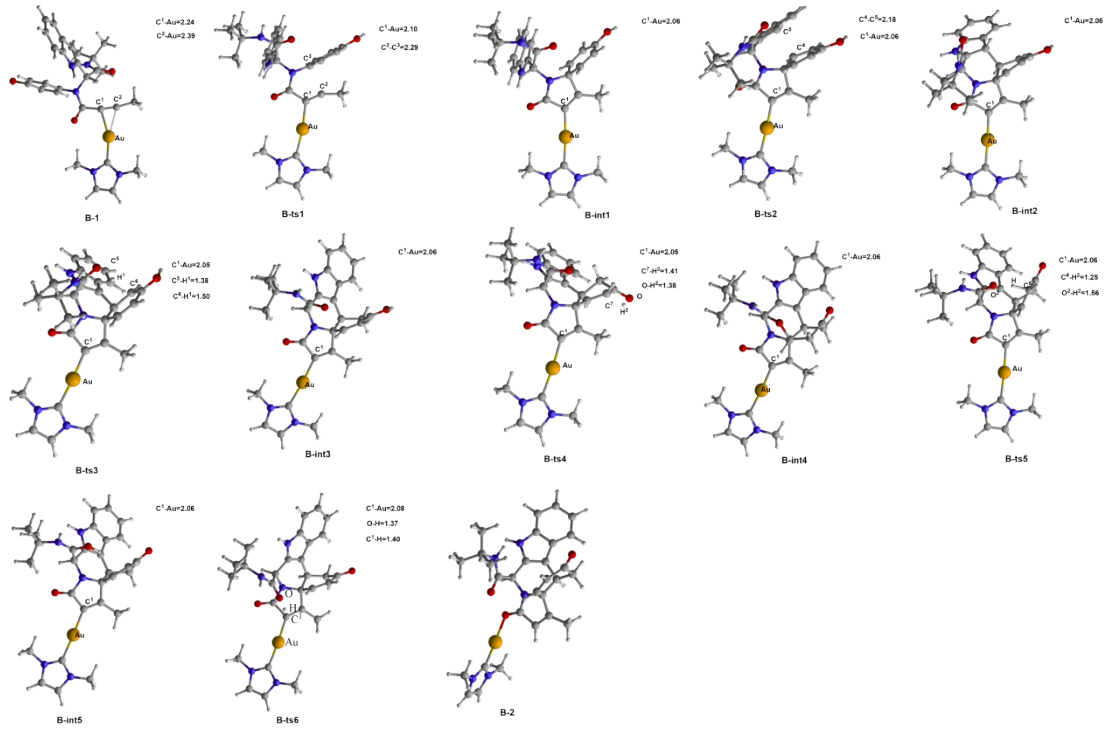

Fig. S2. Optimized geometries of transition states and intermediates shown in Fig. 3.

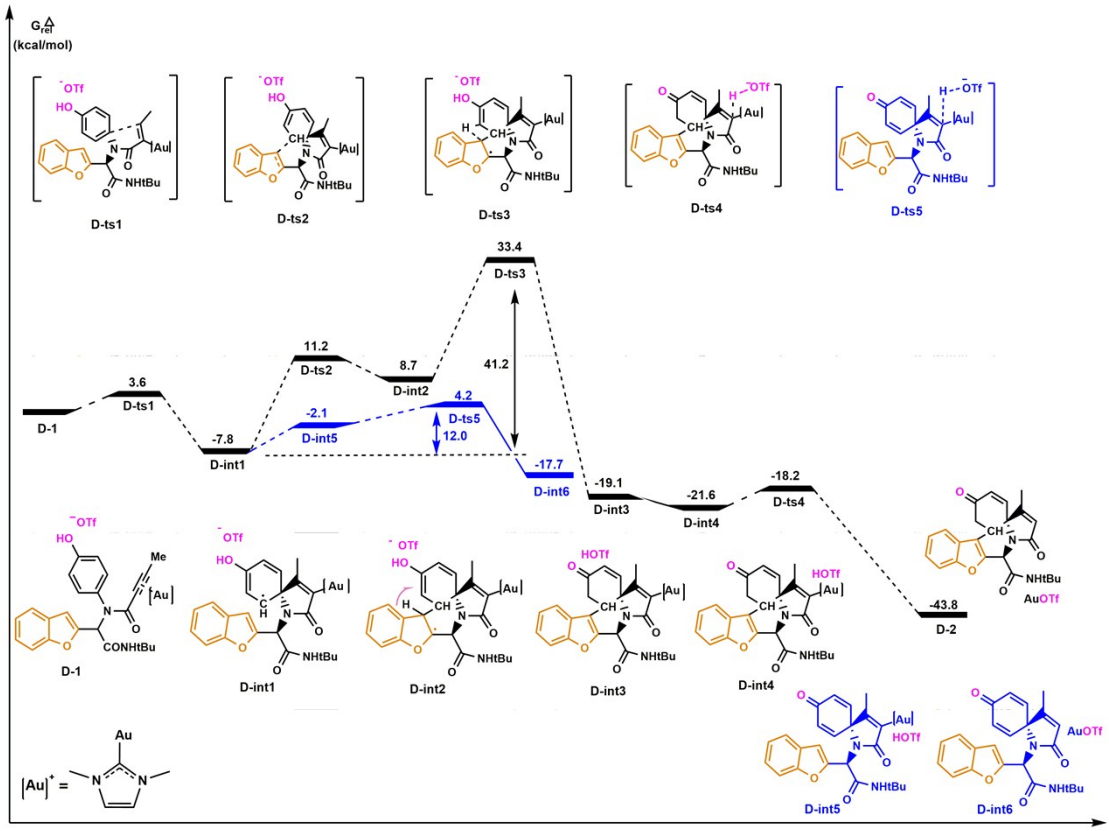

Fig. S3. Calculated energy profiles for the synthesis of (benzo)furans-annulated tricyclic heterocycles.

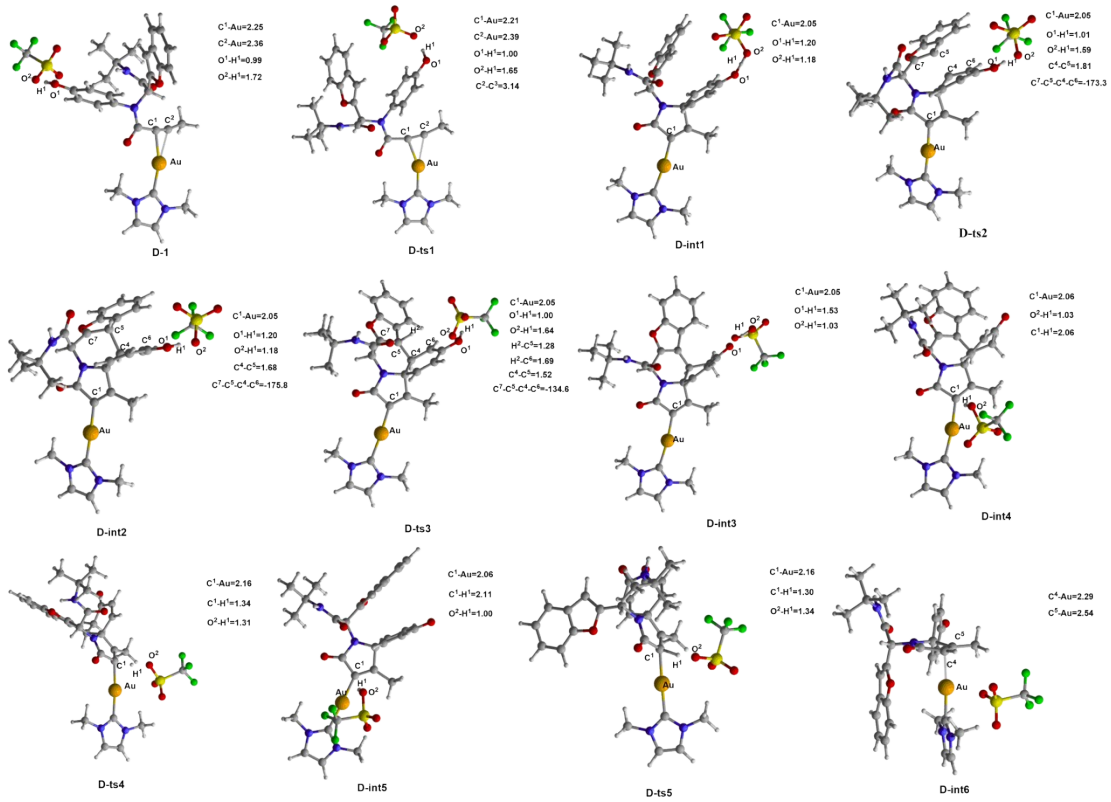

Fig. S4 Optimized geometries of transition states and intermediates shown in Fig. S3.

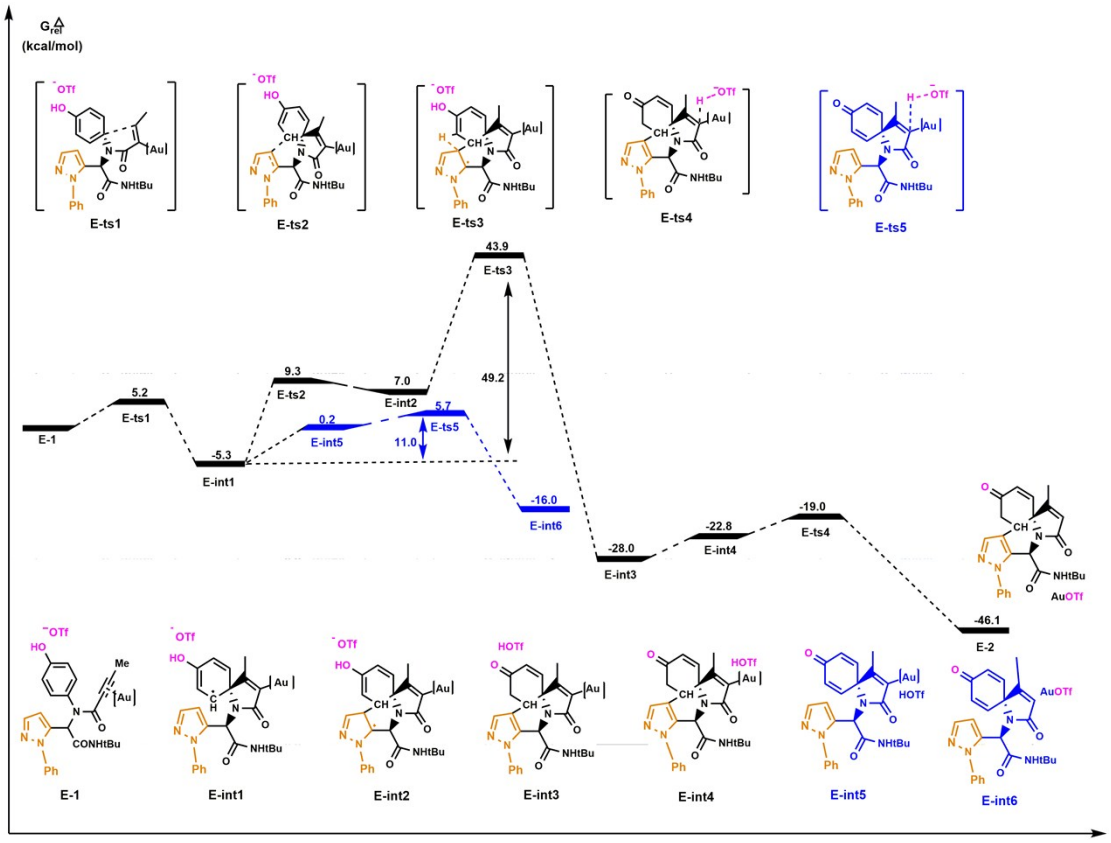

Fig. S5. Calculated energy profiles for the synthesis of pyrazoles-annulated tricyclic heterocycles.

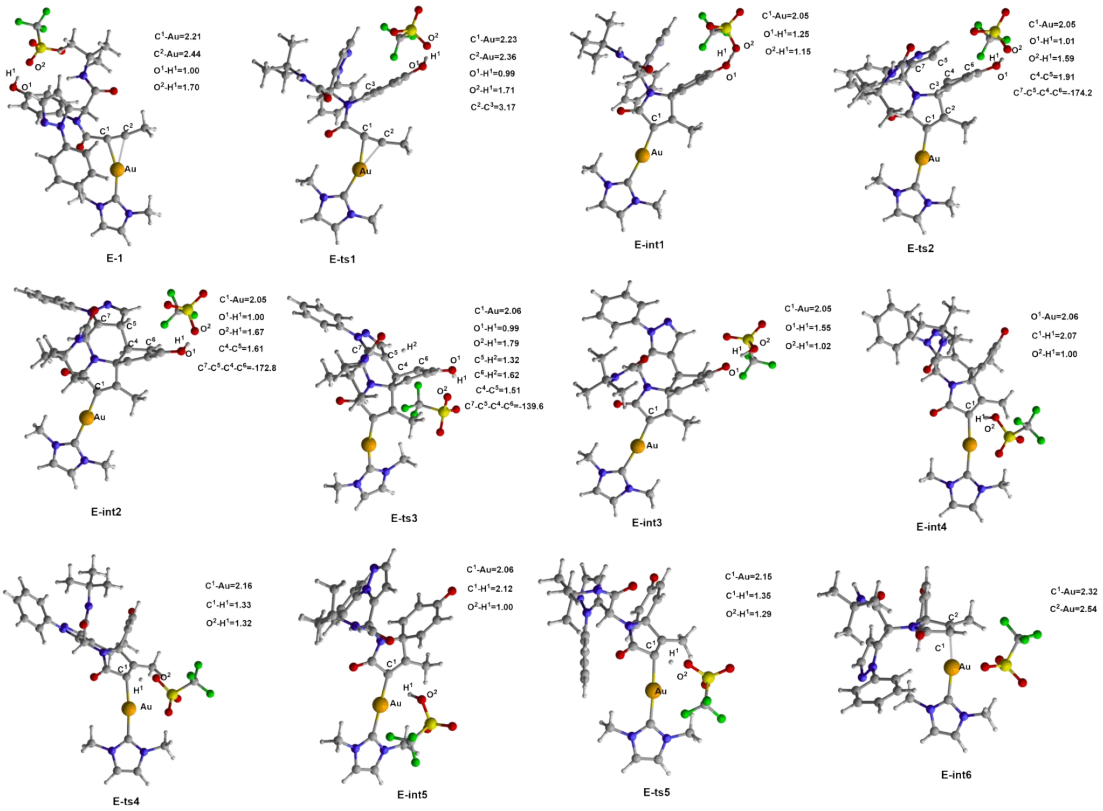

Fig. S6. Optimized geometries of transition states and intermediates shown in Fig. S5.

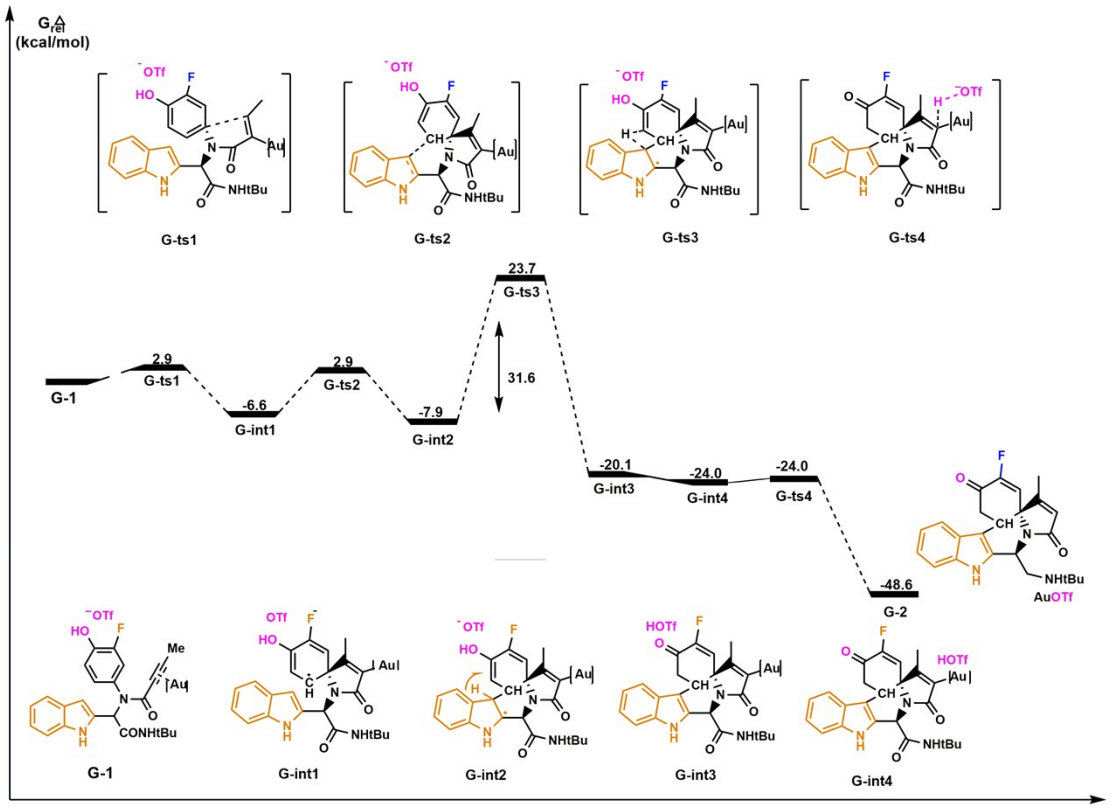

Fig. S7. Calculated energy profiles for the synthesis of indole-annulated tricyclic heterocycles.

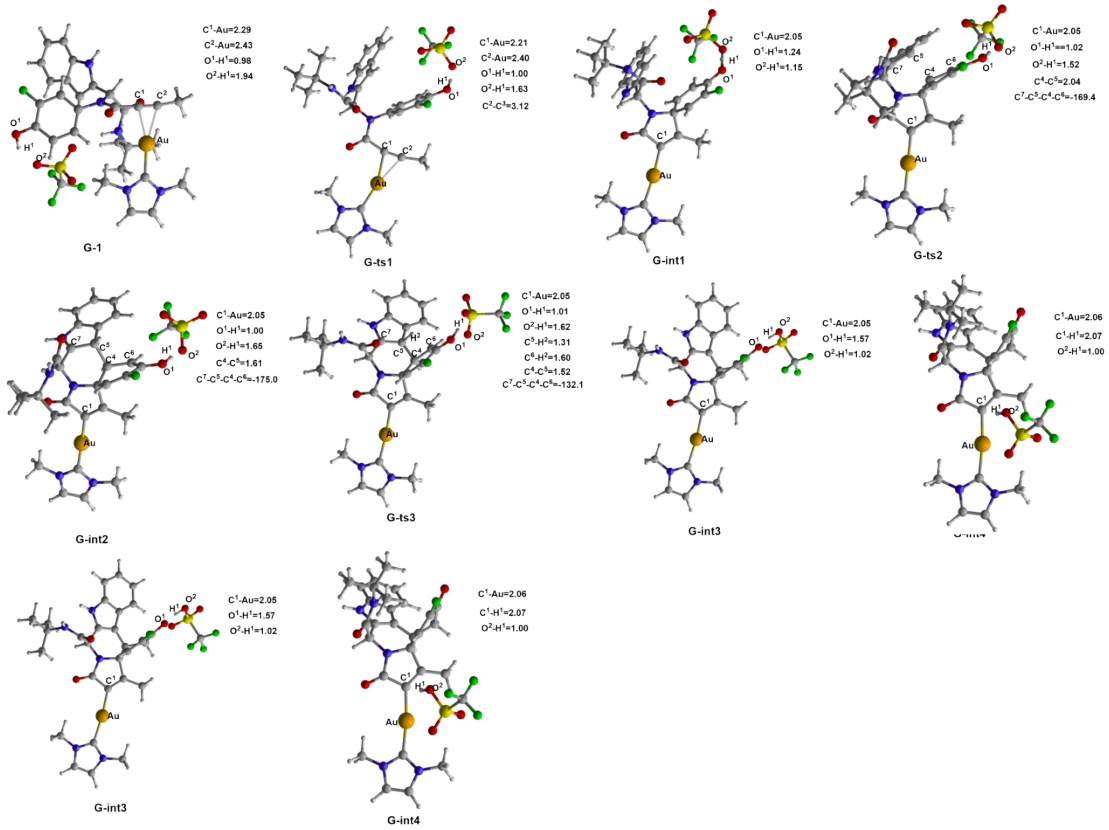

Fig. S8. Optimized geometries of transition states and intermediates shown in Fig. S7.

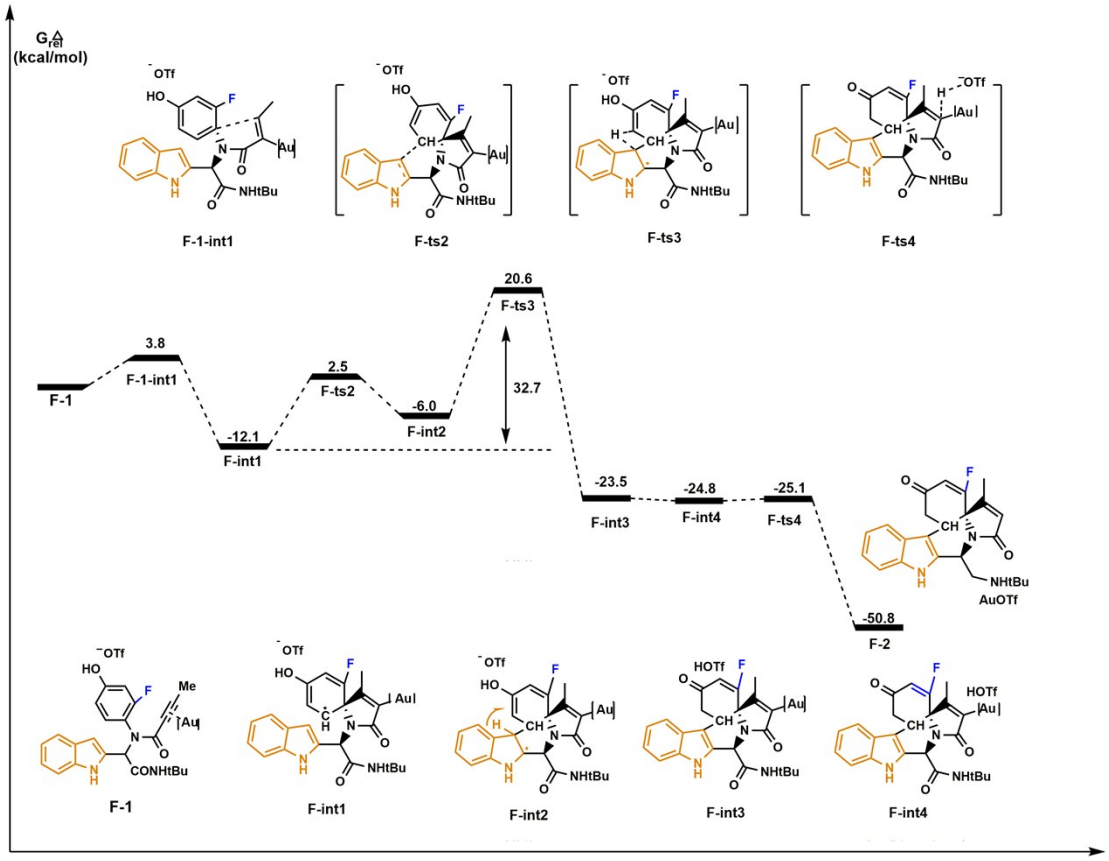

Fig. S9. Calculated energy profiles for the synthesis of indole-annulated tricyclic heterocycles.

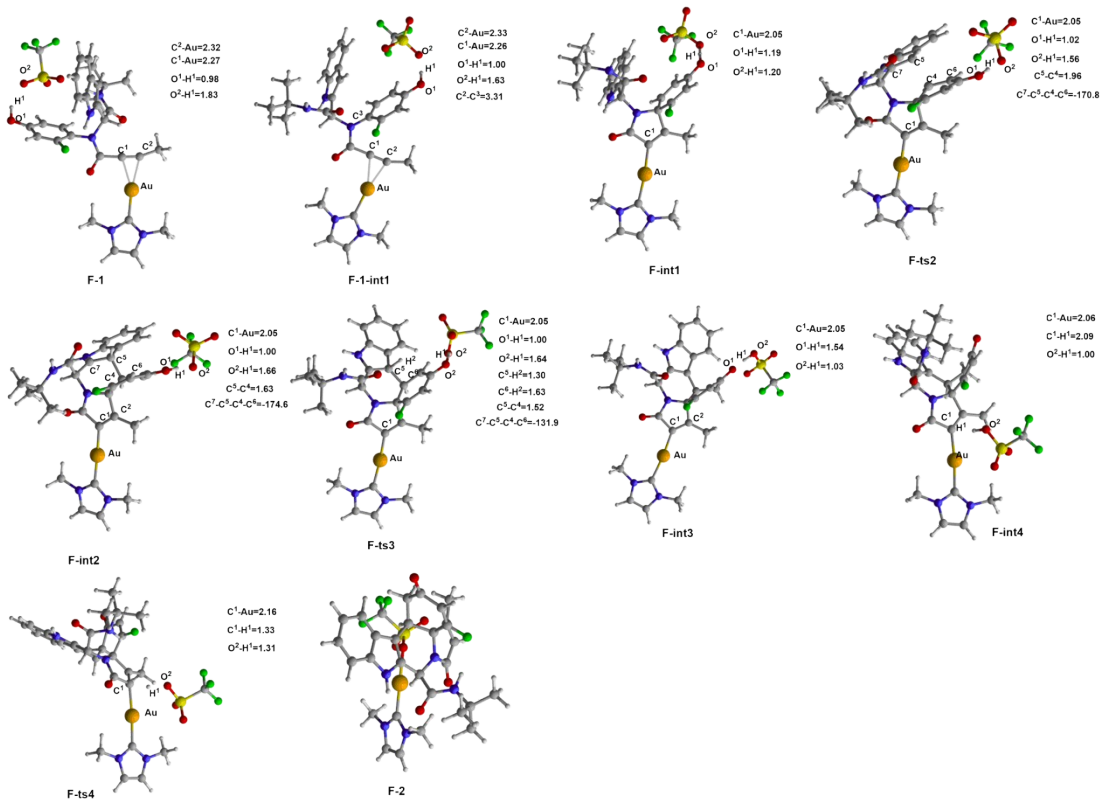

Figure. S10 Optimized geometries of transition states and intermediates shown in Figure. S9.

Table S1. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig. 1.

System	ΔE^{rel}_{gas}	ΔG^{rel}_{gas}	$\Delta E^{\neq}_{gas}$	$\Delta G^{\neq}_{gas}$	ΔE^{rel}_{sol}	ΔG^{rel}_{sol}	$\Delta E^{\neq}_{sol}$	$\Delta G^{\neq}_{sol}$
A-1	0	0			0	0		
A-ts1	6.6	7.7	6.6	7.7	2.8	5.1	2.8	5.1
A-int1	-25.9	-23.5			-5.3	-8.1		
A-ts2	-9.4	-5.8	16.6	17.6	4.0	3.2	9.4	11.2
A-int2	-11.5	-8.4			-5.2	-4.3		
A-ts3	15.7	17.8	27.2	26.1	28.2	25.2	33.4	29.4
A-int3	-39.2	-37.0			-19.0	-20.4		
A-int4	-39.1	-36.7			-20.2	-21.7		
A-ts4	-33.4	-31.2	5.7	5.5	-14.3	-19.9	5.8	1.8

A-2	-60.8	-56.4			-44.7	-42.8		
A-ts8	30.5	34.0	42.0	42.4	45.6	44.3	50.7	48.6
A-int8	-30.7	-27.3			-22.1	-19.2		
A-ts9	-29.4	-25.5	1.3	1.7	-11.8	-13.5	10.3	5.7
A-int9	-48.4	-42.5			-27.1	-25.4		
A-int5	-19.6	-16.9			0.5	0.3		
A-ts5	-13.8	-9.6	5.8	7.2	5.3	2.8	4.8	2.5
A-int6	-33.8	-31.2			-18.8	-19.4		
A-ts6	10.9	16.4	44.7	47.6	23.6	25.8	42.4	45.2
A-int7	-18.7	-13.0			-7.2	-3.2		
A-ts7	57.5	65.1	76.2	78.1	68.5	69.5	75.7	72.7
A-2'	-36.9	--30.5			-23.7	-21.3		

Table S2. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig. 3.

System	ΔE^{rel}_{gas}	ΔG^{rel}_{gas}	$\Delta E^{\neq}_{gas}$	$\Delta G^{\neq}_{gas}$	ΔE^{rel}_{sol}	ΔG^{rel}_{sol}	$\Delta E^{\neq}_{sol}$	$\Delta G^{\neq}_{sol}$
B-1	0	0			0	0		
B-ts1	6.8	6.2	6.8	6.2	12.2	9.4	12.2	9.4
B-int1	-4.1	-2.8			0.8	0.7		
B-ts2	4.7	6.9	8.8	9.6	11.2	10.6	10.4	9.9
B-int2	-3.9	-1.4			-1.3	-0.2		
B-ts3	25.5	27.6	29.4	29.0	33.1	29.8	34.3	30.0
B-int3	-14.2	-12.4			-11.7	-11.8		
B-ts4	41.2	44.6	55.4	57.0	50.4	46.3	62.0	58.1
B-int4	-15.9	-13.5			-14.7	-15.3		
B-ts5	9.5	12.4	25.4	25.9	15.9	12.4	30.6	27.6

B-int5	-12.6	-11.5			-11.6	-12.7		
B-ts6	32.9	35.3	45.5	25.9	40.8	35.9	52.4	48.7
B-2	-42.8	-41.3			-40.9	-41.3		

Table S3. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig S3 and S5.

System	ΔE^{rel}_{gas}	ΔG^{rel}_{gas}	$\Delta E^{\neq}_{gas}$	$\Delta G^{\neq}_{gas}$	ΔE^{rel}_{sol}	ΔG^{rel}_{sol}	$\Delta E^{\neq}_{sol}$	$\Delta G^{\neq}_{sol}$
D-1	0	0			0	0		
D-ts1	4.3	5.4	4.3	5.4	1.9	3.6	1.9	3.6
D-int1	-24.0	-21.6			-4.9	-7.8		
D-ts2	-1.4	2.9	22.7	24.5	11.8	11.2	16.7	18.9
D-int2	-1.4	1.7			10.0	8.7		
D-ts3	22.4	24.9	23.8	23.2	37.0	33.4	27.0	24.7
D-int3	-38.4	-35.1			-18.6	-19.1		
D-int4	-39.7	-37.2			-19.5	-21.6		
D-ts4	-33.3	-30.3	6.4	6.9	-12.9	-18.2	6.5	3.5
D-2	-64.1	-58.1			-47.1	-43.8		
D-int5	-20.1	-16.8			-2.0	-2.1		
D-ts5	-9.8	-6.3	10.3	10.5	7.4	4.2	9.5	6.3
D-int6	-33.3	-29.1			-18.4	-17.7		
E-1	0	0			0	0		
E-ts1	6.9	6.9	6.9	6.9	4.5	5.2	4.5	5.2
E-int1	-22.4	-20.9			-1.7	-5.3		
E-ts2	-0.9	-0.6	21.5	20.3	13.5	9.3	15.2	14.7
E-int2	-2.5	-1.4			9.2	7.0		
E-ts3	28.5	32.9	31.0	34.3	45.5	43.9	36.3	36.9

E-int3	-45.7	-45.2			-24.5	-28.0		
E-int4	-39.9	-39.1			-18.9	-22.8		
E-ts4	-33.6	-31.7	6.3	7.5	-12.8	-19.0	6.2	3.8
E-2	-61.3	-60.1			-44.0	-46.1		
E-int5	-16.5	-16.2			2.6	0.2		
E-ts5	-11.5	-8.0	5.1	8.2	9.5	5.7	7.0	5.4
E-int6	-29.9	-27.7			-13.3	-8.0		

Table S4. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig. S7 and S9.

System	ΔE^{rel}_{gas}	ΔG^{rel}_{gas}	$\Delta E^{\neq}_{gas}$	$\Delta G^{\neq}_{gas}$	ΔE^{rel}_{sol}	ΔG^{rel}_{sol}	$\Delta E^{\neq}_{sol}$	$\Delta G^{\neq}_{sol}$
F-1	0	0			0	0		
F-1-int1	12.4	12.1	12.4	12.1	3.5	3.8	3.5	3.8
F-int1	-24.4	-22.1			-8.6	-12.1		
F-ts2	-4.8	-0.8	19.6	21.2	2.8	2.5	11.4	14.6
F-int2	-6.8	-4.9			-4.7	-6.0		
F-ts3	18.1	19.6	25.0	24.5	24.8	20.6	29.5	26.6
F-int3	-35.7	-33.8			-21.3	-23.5		
F-int4	-36.8	-34.1			-22.9	-24.8		
F-ts4	-36.9	-33.9	-0.1	0.2	-19.8	-25.1	3.2	-0.3
F-2	-65.4	-61.5			-50.5	-50.8		
G-1	0	0			0	0		
G-ts1	18.6	15.2	18.6	15.2	6.6	2.9	6.6	2.9
G-int1	-11.7	-13.2			1.1	-6.6		
G-ts2	3.3	2.7	15.0	15.9	9.6	2.9	8.5	9.5
G-int2	-0.3	-2.6			-1.4	-7.9		

G-ts3	28.8	25.7	29.1	28.3	33.7	23.7	35.1	31.6
G-int3	-25.7	-27.4			-13.8	-20.1		
G-int4	-28.1	-29.7			-16.7	-24.0		
G-ts4	-27.1	-28.6	1.0	1.2	-13.2	-24.0	3.4	0.0
G-2	-54.0	-54.4			-43.7	-48.6		

The Cartesian coordinates of the stationary points discussed in the text

A-1

Au	-4.5596240	-0.9173015	0.1949800
C	-6.5654250	-3.7707185	-2.1715240
C	-7.6176440	-3.4028225	-1.4018710
H	-6.4886340	-4.4881735	-2.9757720
H	-8.6471540	-3.7304695	-1.3973900
C	-5.8384770	-2.2060245	-0.7423500
N	-7.1515840	-2.4382125	-0.5290260
N	-5.4817990	-3.0251845	-1.7542550
C	5.9659210	-4.5128625	-0.0280270
F	6.3754830	-4.3906565	1.2323020
F	7.0263320	-4.4315535	-0.8243440
F	5.4184500	-5.7159235	-0.1753990
S	4.7536720	-3.1979505	-0.4284200
O	3.6510210	-3.4425615	0.5110830
O	4.4198720	-3.5051375	-1.8465070
O	5.4927440	-1.9464965	-0.2455510
C	-7.9751840	-1.7795315	0.4698830
H	-7.3697550	-1.0284365	0.9820520

H	-8.8255440	-1.2880265	-0.0107820
H	-8.3384700	-2.5082305	1.1999870
C	-4.1377650	-3.1536645	-2.3146070
H	-4.2136510	-3.2433135	-3.4007180
H	-3.5433990	-2.2675195	-2.0711620
H	-3.6480770	-4.0428825	-1.9082330
C	2.7746560	6.6407745	-1.1909390
C	1.6553470	6.7663875	-2.0319620
C	0.6170380	5.8504135	-1.9911910
C	0.7286230	4.7980535	-1.0832200
C	1.8489480	4.6466455	-0.2335610
C	2.8803590	5.5927955	-0.2939080
N	-0.1348620	3.7589065	-0.8102380
C	0.4348920	2.9320115	0.1455530
C	1.6357480	3.4583175	0.5361230
C	-0.3318770	1.7384905	0.6007930
N	-0.6275790	0.8235465	-0.5396340
C	-1.8220560	0.1832815	-0.6321630
C	0.4722010	0.2839375	-1.3039430
O	-2.1648310	-0.5658115	-1.5399810
C	-2.7305370	0.3651195	0.5189780
C	-3.2406380	0.3887265	1.6431440
C	1.1994810	1.0564375	-2.2095210
C	2.3143060	0.5180645	-2.8322810
C	2.7213870	-0.7994145	-2.5692500
C	1.9611620	-1.5824795	-1.6808810
C	0.8603690	-1.0345795	-1.0534360

O	3.8065710	-1.2530585	-3.1823940
H	-1.3046350	2.0885805	0.9703030
C	0.2742190	0.9630005	1.7841920
O	-0.4329650	0.7290645	2.7641510
N	1.5452260	0.5684595	1.6220970
C	2.3333930	-0.2877845	2.5469710
C	1.7324080	-1.6883365	2.5871100
C	3.7369240	-0.3326475	1.9631530
C	2.3560250	0.3500695	3.9310750
C	-3.5812840	0.5991145	3.0391070
H	3.5702720	7.3792875	-1.2524100
H	1.6037510	7.5990935	-2.7295310
H	-0.2496960	5.9483975	-2.6414630
H	3.7515950	5.4968235	0.3501950
H	-0.9515580	3.5217105	-1.3526560
H	2.2925610	3.0476715	1.2930420
H	0.9095150	2.0838925	-2.4177270
H	2.9079970	1.1087895	-3.5246230
H	2.2679810	-2.6018635	-1.4634850
H	0.3008350	-1.6299995	-0.3319860
H	4.0997270	-2.1098265	-2.7747760
H	1.9721680	0.7417945	0.7176780
H	1.8088830	-2.1687825	1.6048500
H	2.3022720	-2.3125295	3.2857640
H	0.6879770	-1.6551695	2.9187800
H	4.3740250	-0.9979555	2.5553040
H	4.1902620	0.6683005	1.9580930

H	3.7466660	-0.7383715	0.9440390
H	3.0076520	-0.2382485	4.5879920
H	1.3551310	0.3931175	4.3698350
H	2.7597850	1.3696825	3.8759830
H	-2.6424890	0.8989255	3.5257370
H	-3.9536430	-0.3155185	3.5090590
H	-4.3309950	1.3883495	3.1537120

Zero-point correction= 0.605583 (Hartree/Particle)

Thermal correction to Energy= 0.652639

Thermal correction to Enthalpy= 0.653583

Thermal correction to Gibbs Free Energy= 0.517094

Sum of electronic and zero-point Energies= -2719.313631

Sum of electronic and thermal Energies= -2719.266575

Sum of electronic and thermal Enthalpies= -2719.265631

Sum of electronic and thermal Free Energies= -2719.402120

A-ts1

H	1.0691106	-4.3112216	-1.0910048
H	2.7817036	-4.5920766	-1.4950978
H	2.2075416	-4.8469256	0.1735782
H	-0.2451254	5.4620804	0.6643222
H	-0.4121524	3.7321934	0.9302662
H	1.0378506	4.3727354	0.0969292
H	-2.7821784	4.3493084	-1.9069758
H	-2.6157434	3.5385274	-0.3410188
H	-2.5889884	5.3149244	-0.4283808
H	-0.8445984	5.5793374	-2.9457278
H	0.7244756	5.6444924	-2.1028248

H	-0.6803224	6.5276704	-1.4616958
H	-0.1761454	3.4246384	-2.9043468
H	-3.5024714	-4.3158196	-1.5804478
H	-1.2493764	-1.4292546	1.1315362
H	-2.7499864	-3.2399836	0.3125982
H	-0.9977274	-2.9342536	-3.5863398
H	0.4449456	-1.0349756	-2.7869048
H	0.6542296	1.8935754	0.3670662
H	-2.7706334	0.5786294	-1.2285068
H	-0.8206604	1.8770224	2.2887822
H	-5.4230614	0.1970024	0.0751232
H	-2.9830654	1.9244534	4.1129962
H	-5.3975974	1.3454124	4.2290692
H	-6.5911444	0.4772064	2.2480822
C	2.1009756	-4.2259666	-0.7208398
C	-0.0473764	4.4795354	0.2197372
C	-2.2772804	4.3927094	-0.9348508
C	-0.3624234	5.6052024	-1.9597518
C	-0.7628924	4.3895124	-1.1236008
N	-0.3190034	3.2216834	-1.9208448
O	0.6164606	1.3039064	-2.5925678
C	0.1032926	1.9455884	-1.6887418
O	-2.7177384	-4.1701456	-2.1780508
C	-1.1862194	-1.7713436	0.0991022
C	-2.0099254	-2.7897106	-0.3443478
C	-1.9476064	-3.2090136	-1.6865848
C	-1.0203974	-2.6048056	-2.5504858

C	-0.2229704	-1.5612446	-2.1098238
C	-0.3035684	-1.1424526	-0.7813648
C	2.3201556	-2.8213786	-0.4299438
C	2.2658606	-1.6020926	-0.2543428
O	2.6443566	0.6937784	0.1369042
C	1.8367236	-0.1929316	-0.1352378
N	0.5113976	-0.0471506	-0.3192918
C	-0.0300064	1.3296094	-0.2821858
C	-2.5959384	0.9282764	-0.2159618
C	-1.3964464	1.3320114	0.3043882
N	-1.5616524	1.6224384	1.6548182
C	-4.9106304	0.6179384	0.9372502
C	-3.5537034	0.9608404	0.8466262
C	-2.8764354	1.4103124	2.0053432
C	-3.5184244	1.5706294	3.2339112
C	-4.8627214	1.2443164	3.2870162
C	-5.5473044	0.7644254	2.1559362
Au	4.4232526	-1.8620886	0.1619312
C	8.5265916	-1.3210066	1.1595072
C	8.1247926	-0.0337486	1.0352362
H	9.4874006	-1.7474246	1.4092582
H	8.6649346	0.8946784	1.1523992
C	6.3483386	-1.3364736	0.6202822
N	6.7842236	-0.0615696	0.7049882
N	7.4201126	-2.1080556	0.9010882
C	-6.1271754	-2.8292156	1.0711342
F	-6.9731784	-1.8011056	1.1733902

F	-5.0437154	-2.5490826	1.7977732
F	-6.7148184	-3.8986496	1.5959302
S	-5.6808114	-3.1101066	-0.6850708
O	-6.9607084	-3.3648586	-1.3355658
O	-4.7879014	-4.2985876	-0.5545928
O	-4.9676384	-1.8812006	-1.0599658
C	5.9819716	1.1338004	0.4591272
H	4.9207216	0.8704224	0.3885772
H	6.1206496	1.8347254	1.2862842
H	6.2977196	1.6049034	-0.4758028
C	7.4284586	-3.5605546	0.9369392
H	7.7206696	-3.9102696	1.9309432
H	6.4226716	-3.9219456	0.7117662
H	8.1259976	-3.9517646	0.1911522

Zero-point correction= 0.605864 (Hartree/Particle)

Thermal correction to Energy= 0.652766

Thermal correction to Enthalpy= 0.653710

Thermal correction to Gibbs Free Energy= 0.519208

Sum of electronic and zero-point Energies= -2719.303125

Sum of electronic and thermal Energies= -2719.256222

Sum of electronic and thermal Enthalpies= -2719.255278

Sum of electronic and thermal Free Energies= -2719.389781

A-int1

H	0.7481947	-3.5140222	-1.7896258
H	1.4961357	-2.8440862	-3.2366218
H	2.5157877	-3.3191502	-1.8599658
H	-0.7324073	5.4620728	1.0292982

H	-0.6024583	3.7079778	1.0598712
H	0.3193137	4.6571398	-0.1464918
H	-3.9739613	4.3118528	-0.4771838
H	-3.0964643	3.3397668	0.7222452
H	-3.2631643	5.0974448	0.9478052
H	-2.7280973	5.8979318	-2.0029568
H	-0.9634993	6.0724058	-1.8500788
H	-2.0438893	6.6921518	-0.5780768
H	-2.2434513	3.7275918	-2.4533958
H	-3.9544683	-3.1567132	-2.2742458
H	-0.5598373	-1.4010922	0.3097392
H	-2.5133913	-2.6588152	-0.5210978
H	-1.5984453	-1.4334292	-4.5800028
H	0.3200127	-0.0719762	-3.7447978
H	0.3771757	2.4183288	-0.2863338
H	-3.1817643	0.7651368	-0.3151838
H	0.3948737	1.1639588	1.8891822
H	-4.7280143	-0.5137522	1.8732902
H	-0.4355803	0.0569918	4.4119332
H	-2.4027343	-1.0341812	5.4645782
H	-4.5153883	-1.3300472	4.2125382
C	1.5607357	-2.8641942	-2.1408078
C	-0.6324473	4.5754668	0.3924802
C	-3.1143203	4.3045298	0.2041492
C	-1.8888013	5.8782608	-1.2952498
C	-1.8163193	4.5378928	-0.5649098
N	-1.6762943	3.5234408	-1.6359878

O	-1.3525853	1.6500798	-2.8148988
C	-1.1582273	2.2713848	-1.7775658
O	-3.1851653	-2.7250712	-3.0758408
C	-0.8128683	-1.4128032	-0.7502538
C	-1.8562043	-2.1273972	-1.2031648
C	-2.1728173	-2.1270812	-2.6156578
C	-1.3126333	-1.4194322	-3.5322828
C	-0.2932363	-0.6696002	-3.0752118
C	0.1397697	-0.6945012	-1.6519648
C	1.4684837	-1.5001852	-1.5595868
C	2.4036157	-0.8016712	-0.8943268
O	2.2495427	1.3347698	0.2619542
C	1.7992127	0.4873418	-0.5022918
N	0.5545507	0.5988848	-1.1199318
C	-0.3314093	1.6665548	-0.6548018
C	-2.4820783	0.7741548	0.5142382
C	-1.1847743	1.2093268	0.4809652
N	-0.5847553	0.9827328	1.7087192
C	-3.8051463	-0.3809412	2.4319482
C	-2.7062533	0.2360238	1.8208512
C	-1.4972283	0.3774298	2.5464032
C	-1.3679483	-0.0629692	3.8642502
C	-2.4716773	-0.6698982	4.4418172
C	-3.6751573	-0.8332762	3.7326522
Au	4.3241077	-1.2038502	-0.3010758
C	8.2054287	-1.0069262	1.4817052
C	8.3326097	-2.2194362	0.8938102

H	8.8938777	-0.4333332	2.0856632
H	9.1539407	-2.9214972	0.8796302
C	6.2693477	-1.4435722	0.4071172
N	7.1385737	-2.4683232	0.2417392
N	6.9380727	-0.5483052	1.1733492
C	-5.2954843	-3.3811592	1.0018972
F	-5.9245563	-2.6542382	1.9193662
F	-4.0035363	-3.4342002	1.3129932
F	-5.7903923	-4.6068172	1.0125472
S	-5.5256093	-2.6060472	-0.6467158
O	-6.9540193	-2.6411922	-0.8853258
O	-4.7425343	-3.6096902	-1.4918068
O	-4.8370453	-1.3197962	-0.5707108
C	6.8581477	-3.6736702	-0.5160108
H	5.8477247	-3.5940452	-0.9242738
H	7.5722247	-3.7796582	-1.3381498
H	6.9167117	-4.5526042	0.1329372
C	6.4033177	0.7296518	1.6158512
H	7.0111917	1.5488938	1.2206752
H	5.3788627	0.8319358	1.2458092
H	6.3969967	0.7751368	2.7088642

Zero-point correction= 0.606599 (Hartree/Particle)

Thermal correction to Energy= 0.652291

Thermal correction to Enthalpy= 0.653235

Thermal correction to Gibbs Free Energy= 0.522074

Sum of electronic and zero-point Energies= -2719.354932

Sum of electronic and thermal Energies= -2719.309240

Sum of electronic and thermal Enthalpies= -2719.308296

Sum of electronic and thermal Free Energies= -2719.439457

A-ts2

H	-0.5147945	-2.2321666	-2.1635532
H	0.0430225	-1.0536756	-3.3443852
H	1.2163895	-2.1441446	-2.5655052
H	3.0723355	3.8131204	-1.7840462
H	1.8622175	2.5538094	-1.4706462
H	1.5308035	3.8348384	-2.6622062
H	1.5892955	4.8135684	1.5388008
H	2.1778685	3.2096354	1.0045308
H	3.1214985	4.6527774	0.6651398
H	1.1832505	6.6345014	-0.2182432
H	1.0815495	6.1929784	-1.9417262
H	2.6490665	6.1911994	-1.1199642
H	-0.6115475	5.0338054	-1.0018512
H	-4.4398515	-1.2769916	-2.8337082
H	-1.2989775	-0.9466996	0.5162478
H	-3.3531295	-1.5625616	-0.7605422
H	-2.4133985	1.4478004	-3.6837212
H	-0.3278115	2.0754094	-2.4647782
H	0.3694485	2.5856674	1.5829418
H	-3.2336565	1.4864214	0.3133048
H	-0.2625035	0.9455994	3.1986978
H	-5.0338975	-0.7337826	1.3412078
H	-1.5500435	-0.8746786	4.9632788
H	-3.5919955	-2.2983666	5.0963568

H	-5.2983115	-2.2274606	3.3103728
C	0.3108595	-1.5503006	-2.4034292
C	1.9966555	3.6181164	-1.6922062
C	2.0970255	4.2677984	0.7333778
C	1.5843105	5.9685934	-0.9916772
C	1.3962115	4.5030184	-0.6014212
N	-0.0735245	4.3229034	-0.5171782
O	-2.1475555	3.6784444	0.0450108
C	-0.9447435	3.4769094	0.1043868
O	-3.8449645	-0.5323796	-3.1846262
C	-1.6663165	-0.2740856	-0.2654972
C	-2.6799205	-0.7874586	-1.1165642
C	-2.9192935	-0.1816956	-2.3369532
C	-2.0885355	0.9301774	-2.7848762
C	-0.9741665	1.2678604	-2.1259942
C	-0.5183115	0.4903514	-0.9331922
C	0.5487405	-0.5732196	-1.3108492
C	1.6193335	-0.4988396	-0.4936852
O	1.9944705	0.9306944	1.4555578
C	1.3776795	0.6084364	0.4473378
N	0.2480115	1.3012544	0.0014178
C	-0.4019405	2.2679414	0.8697988
C	-2.6212255	0.9332944	1.0172458
C	-1.4546455	1.4999324	1.5831458
N	-1.1617325	0.8722524	2.7370838
C	-4.2806405	-0.7655146	2.1277168
C	-3.1369595	0.0246004	2.0404718

C	-2.1785905	-0.0315546	3.0676388
C	-2.3052225	-0.8501456	4.1813498
C	-3.4488115	-1.6371586	4.2451428
C	-4.4185725	-1.5937396	3.2362438
Au	3.3086765	-1.6481246	-0.3181622
C	6.9993955	-3.4709926	0.8584448
C	6.6994355	-4.2906766	-0.1760182
H	7.8372925	-3.4636196	1.5407788
H	7.2210565	-5.1456486	-0.5817102
C	5.0468895	-2.7604726	-0.0237202
N	5.5023955	-3.8398186	-0.7022922
N	5.9779265	-2.5425906	0.9361348
C	-5.9785095	-3.2570706	0.0586728
F	-6.6757155	-2.9666556	1.1583668
F	-4.6833335	-3.2816276	0.3955128
F	-6.3222315	-4.4671976	-0.3536972
S	-6.2899005	-1.9952956	-1.2383062
O	-7.6995735	-2.1554546	-1.5564702
O	-5.3333205	-2.4355006	-2.2980742
O	-5.8695185	-0.7388626	-0.6005592
C	4.8259125	-4.4525256	-1.8312252
H	3.9043755	-3.8971596	-2.0224782
H	5.4615535	-4.4142506	-2.7208442
H	4.5778735	-5.4937116	-1.6048802
C	5.9196275	-1.4762186	1.9218648
H	6.7714245	-0.8007726	1.7986398
H	4.9917535	-0.9154626	1.7777878

H	5.9320635	-1.8973786	2.9314558

Zero-point correction= 0.609040 (Hartree/Particle)

Thermal correction to Energy= 0.653901

Thermal correction to Enthalpy= 0.654845

Thermal correction to Gibbs Free Energy= 0.526155

Sum of electronic and zero-point Energies= -2719.328549

Sum of electronic and thermal Energies= -2719.283688

Sum of electronic and thermal Enthalpies= -2719.282743

Sum of electronic and thermal Free Energies= -2719.411433

A-int2

H	-0.4795616	-2.4597267	-1.7280215
H	0.0084474	-1.4127587	-3.0493445
H	1.2349184	-2.4008867	-2.2096805
H	3.2259794	3.3611613	-2.1831665
H	1.9544274	2.2489393	-1.6458575
H	1.6418744	3.3833973	-2.9813755
H	2.0183784	4.9234533	1.0298035
H	2.4034664	3.2027143	0.7218205
H	3.4777944	4.4646433	0.1362535
H	1.6524114	6.5026723	-0.9310745
H	1.4154664	5.8433823	-2.5712765
H	3.0230014	5.8207433	-1.8303345
H	-0.2979046	5.0509613	-1.2824525
H	-4.1453586	-1.7081917	-2.7514785
H	-1.2842946	-0.7930927	0.7063565
H	-3.2273386	-1.6724387	-0.5742795
H	-2.2790976	1.0782173	-3.7293725

H	-0.2524656	1.8794123	-2.5316895
H	0.5338344	2.6512123	1.5141555
H	-2.9057236	1.6706733	-0.1460275
H	-0.9523286	1.9422963	3.3934285
H	-5.0125026	-0.4376657	0.7289075
H	-2.8356976	0.7329893	5.1111125
H	-4.9472156	-0.5982587	5.0362345
H	-5.9941936	-1.1742757	2.8706305
C	0.3275054	-1.8021767	-2.0748245
C	2.1467444	3.2614783	-2.0146985
C	2.4229724	4.2124873	0.2980435
C	1.9535304	5.7074323	-1.6239945
C	1.6791444	4.3276073	-1.0282615
N	0.2045294	4.2866753	-0.8421275
O	-1.8150706	3.9882073	0.1066275
C	-0.6532246	3.6196323	-0.0313855
O	-3.6150606	-0.9640867	-3.1519155
C	-1.6621216	-0.1480027	-0.1022845
C	-2.6089326	-0.8775897	-0.9818215
C	-2.7790386	-0.4561287	-2.2607785
C	-1.9691886	0.6515793	-2.7778435
C	-0.8811916	1.0873343	-2.1301115
C	-0.4341506	0.4136793	-0.8610375
C	0.5893094	-0.7089937	-1.1040815
C	1.6728744	-0.5831157	-0.3062165
O	2.1402244	1.0635423	1.4403775
C	1.4869714	0.6277323	0.5015435

N	0.3528014	1.2941123	0.0068975
C	-0.2205076	2.3813913	0.7576905
C	-2.4462676	1.0597023	0.6382235
C	-1.4359346	1.8074713	1.3980245
N	-1.5984466	1.6112713	2.6845405
C	-4.5253756	-0.1843957	1.6726315
C	-3.3462186	0.5425353	1.7122415
C	-2.7716166	0.8540813	2.9477335
C	-3.3051136	0.4733073	4.1655865
C	-4.4845306	-0.2670137	4.1101795
C	-5.0795816	-0.5872267	2.8886065
Au	3.3135394	-1.7823937	-0.0321645
C	6.9239624	-3.7193977	1.2251425
C	6.5522054	-4.5960697	0.2632785
H	7.7765794	-3.7103937	1.8889685
H	7.0131974	-5.5093237	-0.0847515
C	4.9961974	-2.9612707	0.3268085
N	5.3719034	-4.1152137	-0.2740395
N	5.9609144	-2.7276157	1.2490745
C	-5.7472516	-3.4883137	0.3905365
F	-6.6771996	-3.1778977	1.2961065
F	-4.5611106	-3.1157227	0.8935985
F	-5.7323056	-4.8039947	0.2370045
S	-6.0867036	-2.6273577	-1.1962785
O	-7.3421536	-3.2103697	-1.6461295
O	-4.8814786	-2.9907577	-1.9905345
O	-6.1064646	-1.2101147	-0.8027765

C	4.6346354	-4.7711717	-1.3390875
H	3.7462044	-4.1746067	-1.5609375
H	5.2531644	-4.8452767	-2.2384405
H	4.3257044	-5.7726087	-1.0252645
C	5.9863544	-1.5884987	2.1504905
H	6.8826384	-0.9864917	1.9734085
H	5.0990244	-0.9766897	1.9654925
H	5.9770934	-1.9305547	3.1896605

Zero-point correction= 0.610390 (Hartree/Particle)

Thermal correction to Energy= 0.655528

Thermal correction to Enthalpy= 0.656472

Thermal correction to Gibbs Free Energy= 0.526873

Sum of electronic and zero-point Energies= -2719.331945

Sum of electronic and thermal Energies= -2719.286807

Sum of electronic and thermal Enthalpies= -2719.285863

Sum of electronic and thermal Free Energies= -2719.415462

A-ts3

H	-0.3372281	-3.4298377	-0.7626592
H	0.2277299	-3.1261307	-2.3996522
H	1.3718049	-3.7141607	-1.1674052
H	3.1043159	4.9263643	-0.1343572
H	2.4689539	3.2819823	-0.3071882
H	2.6634069	4.3144723	-1.7397072
H	-0.4306811	5.3960803	1.0572338
H	0.5801659	3.9683883	1.4450828
H	1.2678669	5.5829373	1.5132398
H	-0.0352261	6.7669963	-0.9802852

H	1.2766519	6.3437603	-2.1106242
H	1.6620429	6.9499313	-0.4924112
H	-0.2904171	4.6509323	-2.1858172
H	-4.5873941	-1.9935767	-2.2232032
H	-1.0698361	-1.5574297	0.6300238
H	-3.4215161	-1.8041197	-0.2648612
H	-1.8993641	-0.8230317	-4.1614722
H	0.2322149	-0.0295317	-3.1807692
H	0.7166709	2.3233783	0.3852748
H	-2.8194451	0.2542073	-0.5563662
H	-1.7256881	3.5551833	1.1355228
H	-4.0209781	-1.3085777	1.7855598
H	-3.9412821	3.5960333	2.8748158
H	-5.6559201	2.0804613	3.8615378
H	-5.6853821	-0.3314517	3.2890948
C	0.5171119	-3.0529247	-1.3428932
C	2.3794679	4.3099183	-0.6805482
C	0.5684179	4.9492123	0.9557658
C	0.9651689	6.3231263	-1.0587952
C	0.9802239	4.8969033	-0.5144572
N	-0.0184311	4.1627193	-1.3373662
O	-0.7372151	2.3893153	-2.5379812
C	-0.2364541	2.8234533	-1.5178972
O	-3.8604151	-1.7534997	-2.8706372
C	-1.3972451	-0.8598557	-0.1535282
C	-2.6546331	-1.3285227	-0.8742612
C	-2.7720581	-1.3707637	-2.2458372

C	-1.7044161	-0.8766187	-3.0938582
C	-0.5583531	-0.4433947	-2.5585852
C	-0.1967881	-0.5646257	-1.1009672
C	0.8624349	-1.6567577	-0.9697942
C	2.0289909	-1.1777627	-0.4944202
O	2.6189529	1.0754063	0.2448558
C	1.8449599	0.2666453	-0.2526292
N	0.5628639	0.6100583	-0.6768222
C	-0.0001791	1.8813023	-0.3210022
C	-1.9772041	0.4211723	0.4223318
C	-1.2988891	1.6623523	0.3698278
N	-1.9567601	2.5697163	1.1042878
C	-3.9734561	-0.2456707	2.0217908
C	-3.0077101	0.5934913	1.4732018
C	-3.0157511	1.9616393	1.7942538
C	-3.9493941	2.5324073	2.6486398
C	-4.9000301	1.6779223	3.1921278
C	-4.9116271	0.3130333	2.8813178
Au	3.8109209	-2.0684877	-0.0193172
C	7.7726179	-2.9940297	1.3180328
C	7.4147349	-4.2324587	0.9054358
H	8.6890359	-2.6278667	1.7582938
H	7.9540599	-5.1688217	0.9116568
C	5.6644249	-2.8584827	0.5212288
N	6.1231409	-4.1287947	0.4216788
N	6.6904619	-2.1683167	1.0752358
C	-6.8879221	-4.2334147	-0.0749722

F	-7.0457021	-4.8944007	1.0664358
F	-6.2430061	-5.0187337	-0.9329622
F	-8.0856841	-3.9549827	-0.5746852
S	-5.9370421	-2.6944467	0.2153258
O	-6.7597621	-1.9178527	1.1393598
O	-5.8244271	-2.1193197	-1.1509922
O	-4.6535631	-3.1846937	0.7510598
C	5.3621559	-5.2404827	-0.1183362
H	4.3797469	-4.8688387	-0.4201102
H	5.8719059	-5.6616347	-0.9900402
H	5.2355009	-6.0181317	0.6407838
C	6.6638759	-0.7472517	1.3790368
H	5.6876189	-0.3451677	1.0929088
H	6.8179419	-0.5887457	2.4505388
H	7.4459179	-0.2273057	0.8176798

Zero-point correction= 0.605185 (Hartree/Particle)

Thermal correction to Energy= 0.650429

Thermal correction to Enthalpy= 0.651373

Thermal correction to Gibbs Free Energy= 0.519990

Sum of electronic and zero-point Energies= -2719.288611

Sum of electronic and thermal Energies= -2719.243367

Sum of electronic and thermal Enthalpies= -2719.242423

Sum of electronic and thermal Free Energies= -2719.373805

A-int3

H	-0.2039609	-3.6161369	0.0532592
H	-0.3338059	-3.2760279	-1.6793958
H	1.2272241	-3.7539999	-0.9729008

H	3.1239271	4.9057901	0.7606412
H	2.5640031	3.2665951	0.3500982
H	3.0483491	4.3818711	-0.9335908
H	-0.5659769	5.3539511	1.2083502
H	0.3302041	3.9181451	1.7459292
H	1.0179191	5.5235151	1.9789332
H	0.1882991	6.7363501	-0.7119768
H	1.7131601	6.3619231	-1.5558488
H	1.7459881	6.9454761	0.1154172
H	0.3712151	4.5856051	-2.0082658
H	-5.3687699	-2.3067249	-1.1354238
H	-1.1156959	-1.0378029	1.3411392
H	-2.0976679	-2.7189509	-0.1386478
H	-2.3776509	-0.7783239	-3.4728308
H	-0.1107519	-0.0923769	-2.7412958
H	0.6427571	2.2760931	0.7551312
H	-1.9088879	3.8572251	0.0894572
H	-4.7441399	-0.5906349	1.2969852
H	-4.5734239	4.3916041	0.8026752
H	-6.6943119	3.2235241	1.3844232
H	-6.7419749	0.7608331	1.6258362
C	0.3188361	-3.1661449	-0.8030418
C	2.5434161	4.3179971	0.0383062
C	0.4328351	4.9061901	1.2870092
C	1.1938911	6.3148961	-0.5899228
C	1.1287211	4.8804481	-0.0713698
N	0.3384681	4.1375961	-1.0960338

O	0.1198111	2.3302941	-2.4375098
C	0.2291211	2.7780451	-1.3109598
O	-4.1740339	-1.6919019	-1.8773008
C	-1.5197179	-0.6925799	0.3758572
C	-2.5462749	-1.7165559	-0.1115318
C	-3.0264029	-1.4303209	-1.5041698
C	-2.0545519	-0.8842179	-2.4400338
C	-0.8291279	-0.5079209	-2.0370318
C	-0.3356519	-0.6056479	-0.6181048
C	0.6874521	-1.7463689	-0.5425218
C	1.9208981	-1.2870909	-0.2518538
O	2.6922001	0.9746711	0.2586822
C	1.8199821	0.1758471	-0.0645348
N	0.5100891	0.5357041	-0.3008698
C	0.0500251	1.8768891	-0.0805998
C	-2.1231919	0.6827491	0.5142822
C	-1.3988709	1.8178561	0.2702622
N	-2.1906329	2.9344951	0.3894312
C	-4.6757529	0.4856461	1.1610592
C	-3.4691359	1.1173071	0.8117272
C	-3.4704579	2.5321621	0.7016122
C	-4.6102399	3.3083821	0.8996282
C	-5.7838119	2.6507211	1.2248082
C	-5.8104369	1.2539561	1.3584372
Au	3.7570821	-2.1550479	0.0057442
C	7.9168031	-2.7572549	0.7834882
C	7.5946291	-4.0465779	0.5263942

H	8.8589451	-2.2985739	1.0476472
H	8.1969291	-4.9437429	0.5200372
C	5.7096661	-2.8214149	0.3138662
N	6.2411151	-4.0647519	0.2415442
N	6.7527091	-2.0236269	0.6488382
C	-5.1277149	-5.0326869	-0.1013898
F	-4.8613969	-5.8229729	0.9227632
F	-3.9856209	-4.6054549	-0.6336968
F	-5.8095219	-5.6984169	-1.0121568
S	-6.0885619	-3.5843789	0.4924882
O	-7.3870839	-4.0700809	0.8843332
O	-6.2280529	-2.7807419	-0.8373098
O	-5.2062009	-2.9122339	1.4301692
C	5.4914251	-5.2612629	-0.0913908
H	4.4505891	-4.9753959	-0.2615878
H	5.8926371	-5.7210669	-0.9996408
H	5.5381471	-5.9805369	0.7318492
C	6.6680471	-0.5843449	0.8422832
H	7.3208631	-0.0712199	0.1299262
H	5.6348131	-0.2633939	0.6778932
H	6.9666721	-0.3250849	1.8623372
H	-3.4003969	-1.8003599	0.5637612

Zero-point correction= 0.610500 (Hartree/Particle)

Thermal correction to Energy= 0.655861

Thermal correction to Enthalpy= 0.656805

Thermal correction to Gibbs Free Energy= 0.525436

Sum of electronic and zero-point Energies= -2719.376095

Sum of electronic and thermal Energies= -2719.330734

Sum of electronic and thermal Enthalpies= -2719.329790

Sum of electronic and thermal Free Energies= -2719.461158

A-int4

H	-1.0340552	-0.3570824	3.4762045
H	-1.1620492	1.2917606	2.8481545
H	-2.5453972	0.1779566	2.7257075
H	3.5948118	3.1752436	-4.6060375
H	3.7651708	1.4059756	-4.6245345
H	2.1747098	2.1411256	-4.3122545
H	5.3139308	2.3959206	-1.3654745
H	5.5901848	1.5375616	-2.9041255
H	5.4398008	3.3056206	-2.8805045
H	3.0910208	3.4589106	-0.8948745
H	1.7680858	3.3547046	-2.0861895
H	3.1817238	4.3867216	-2.4086245
H	3.7963698	0.5742486	-1.3769715
H	0.9947048	-1.6654324	2.2608245
H	1.0640388	0.2952736	3.6766535
H	1.8754148	3.1511636	1.2631865
H	0.2229688	1.8804936	-0.0708435
H	1.3974218	-1.5271044	-1.9905315
H	4.1665038	-1.9484084	-1.7235545
H	3.8930598	-2.0190484	3.6564745
H	6.5072058	-2.9352194	-0.5175085
H	7.4204338	-3.5197574	1.7205395
H	6.1167948	-3.0645234	3.7705275

C	-1.4547602	0.2487916	2.6610355
C	3.2493128	2.2441106	-4.1403395
C	5.0636678	2.3782476	-2.4345805
C	2.8526648	3.4382876	-1.9662335
C	3.5595328	2.2693316	-2.6475705
N	3.1452028	0.9922016	-2.0307735
O	0.9190028	1.0849686	-2.5413965
C	1.8640658	0.5462766	-1.9906245
O	3.3093548	2.0698696	3.1552935
C	1.5018428	-0.7793084	1.8429115
C	1.9216968	0.1242706	3.0098395
C	2.4100648	1.4875316	2.5783515
C	1.6689538	2.1010076	1.4635585
C	0.7796238	1.4083206	0.7419885
C	0.4818358	-0.0609354	0.9147225
C	-0.9778782	-0.2291444	1.3355035
C	-1.7088032	-0.8141424	0.3607765
O	-1.0282112	-1.7370824	-1.8008225
C	-0.7871412	-1.1441474	-0.7630385
N	0.4593128	-0.6803344	-0.3982585
C	1.6351568	-0.7784174	-1.2154335
C	2.6871308	-1.2502394	1.0431875
C	2.7357188	-1.2353384	-0.3232695
N	3.9513768	-1.7247444	-0.7636715
C	4.4548248	-2.1929764	2.7413465
C	3.9226758	-1.8413924	1.4920805
C	4.6857318	-2.1304654	0.3338185

C	5.9431278	-2.7261384	0.3891505
C	6.4427328	-3.0508004	1.6399555
C	5.7026308	-2.7898884	2.8034225
Au	-3.6723842	-1.3957804	0.1349105
C	-7.2855562	-2.9772924	-1.4854265
C	-7.8315252	-2.2909054	-0.4538045
H	-7.7395982	-3.5723754	-2.2647155
H	-8.8605472	-2.1568834	-0.1527135
C	-5.5990242	-2.0159464	-0.3396485
N	-6.7833912	-1.7129114	0.2370405
N	-5.9182472	-2.7959824	-1.4002335
C	-4.4493312	3.8935776	0.8946155
F	-3.5213282	4.2463906	1.7616825
F	-5.6386922	4.2643406	1.3385885
F	-4.2144172	4.4537136	-0.2740185
S	-4.4849522	2.0625546	0.7233835
O	-3.0032552	1.9385486	0.1801895
O	-5.4681712	1.7444476	-0.2905925
O	-4.6064752	1.5068506	2.0588345
C	-6.9477362	-0.8325164	1.3817295
H	-5.9677592	-0.6383424	1.8234995
H	-7.3754522	0.1230186	1.0638315
H	-7.5988852	-1.3069864	2.1215725
C	-4.9563702	-3.3745904	-2.3250995
H	-5.2706022	-3.1762694	-3.3536555
H	-3.9772852	-2.9155144	-2.1577265
H	-4.8787462	-4.4550094	-2.1694195

H	2.7072028	-0.3329164	3.6180985
H	-2.6807762	0.9929566	0.2019065

Zero-point correction= 0.608959 (Hartree/Particle)

Thermal correction to Energy= 0.654909

Thermal correction to Enthalpy= 0.655853

Thermal correction to Gibbs Free Energy= 0.524180

Sum of electronic and zero-point Energies= -2719.375873

Sum of electronic and thermal Energies= -2719.329923

Sum of electronic and thermal Enthalpies= -2719.328979

Sum of electronic and thermal Free Energies= -2719.460653

A-ts4

H	-1.9320258	-2.8934842	2.2085299
H	-1.6802638	-1.5444432	3.3226829
H	-3.2893768	-1.8357462	2.6176919
H	2.5082302	5.8694958	0.0274929
H	1.9835012	5.0432148	-1.4535041
H	0.9758452	4.9639248	0.0115749
H	4.8097612	2.9746488	-0.1139301
H	4.2087192	3.8557228	-1.5439461
H	4.6700952	4.7404908	-0.0756461
H	3.3694862	2.7224068	1.9076749
H	1.7674302	3.5149968	1.9929179
H	3.2538882	4.4884078	2.0537209
H	2.8285712	1.8105178	-0.8304081
H	-0.1884208	-2.4896202	0.0203429
H	0.2549572	-3.1059522	2.2579649
H	1.3636072	0.4651378	3.7424229

H	-0.3014898	1.2826368	2.0980249
H	-0.0941308	1.2125368	-1.9354381
H	2.5124902	-0.8627852	0.3022379
H	2.1863032	0.3745388	-3.0749721
H	2.5305672	-4.1457412	-0.1554811
H	3.8236102	-1.5699672	-4.2566681
H	4.6366732	-3.8988922	-3.8952741
H	3.9707412	-5.1627882	-1.8850851
C	-2.2139088	-1.8500562	2.4127449
C	2.0033572	4.9755378	-0.3584981
C	4.2017462	3.8217938	-0.4466751
C	2.7877972	3.6024628	1.6044289
C	2.7760192	3.7368968	0.0839019
N	2.1651392	2.5174218	-0.5126721
O	0.0444942	2.8439448	0.2829369
C	0.8756912	2.1791618	-0.3100961
O	2.2111072	-1.9906972	3.8082849
C	0.4432472	-1.7679002	0.5636909
C	1.0161632	-2.4549482	1.8071999
C	1.4998382	-1.5494122	2.9271769
C	0.9936912	-0.1702252	2.9405329
C	0.0976772	0.2694308	2.0485029
C	-0.4667548	-0.5623822	0.9266859
C	-1.9099938	-0.9608522	1.2591249
C	-2.7910908	-0.4072102	0.4032959
O	-2.4123888	0.9899158	-1.5743711
C	-2.0224728	0.3753078	-0.5940331

N	-0.6870218	0.2645898	-0.2451801
C	0.3704062	0.8702878	-0.9940861
C	1.5406482	-1.3401442	-0.4146841
C	1.3360352	-0.2208482	-1.2746731
N	2.0560812	-0.3558702	-2.3861241
C	2.7985952	-3.5783362	-1.0431401
C	2.3327822	-2.2805272	-1.2361311
C	2.7033952	-1.5982332	-2.4048351
C	3.5383382	-2.1345412	-3.3727851
C	3.9861202	-3.4316662	-3.1607251
C	3.6108642	-4.1457072	-2.0178041
Au	-4.8261528	-0.4421382	0.1861269
C	-8.7732398	0.3197988	-1.2604231
C	-9.1141088	-0.5173782	-0.2528391
H	-9.3790078	0.8407458	-1.9880591
H	-10.0772738	-0.8775412	0.0792669
C	-6.8652268	-0.3123502	-0.2332181
N	-7.9335478	-0.8929122	0.3628709
N	-7.3957348	0.4327048	-1.2332781
C	5.9579762	-1.2067342	0.3008609
F	6.2870142	-1.7034012	1.4795209
F	7.0341772	-0.6955192	-0.2778171
F	5.4757492	-2.1775762	-0.4647631
S	4.6991052	0.1116138	0.5012299
O	3.5446202	-0.6325512	1.1385099
O	4.3731002	0.5127498	-0.8773771
O	5.3065632	1.1007688	1.3734739

C	-7.8529088	-1.7893002	1.5003329
H	-6.7992878	-1.9146152	1.7614059
H	-8.3889878	-1.3678992	2.3561299
H	-8.2808058	-2.7640602	1.2470829
C	-6.6261508	1.2528788	-2.1565401
H	-6.8992568	2.3059138	-2.0410201
H	-5.5606888	1.1333628	-1.9374471
H	-6.8188958	0.9370468	-3.1860401
H	1.8585952	-3.1100602	1.5570909

Zero-point correction= 0.603519 (Hartree/Particle)

Thermal correction to Energy= 0.649226

Thermal correction to Enthalpy= 0.650170

Thermal correction to Gibbs Free Energy= 0.518438

Sum of electronic and zero-point Energies= -2719.366826

Sum of electronic and thermal Energies= -2719.321119

Sum of electronic and thermal Enthalpies= -2719.320175

Sum of electronic and thermal Free Energies= -2719.451908

A-2

H	-0.0821954	3.2636664	-3.1645095
H	1.3667056	2.6236514	-3.9801565
H	-0.2505734	2.4387964	-4.7104375
H	5.3276846	-3.9654206	0.9416635
H	3.9682036	-3.4742046	1.9761535
H	3.6554436	-4.1958366	0.3770485
H	5.2546966	-0.2019246	0.6894985
H	4.8900746	-1.1415606	2.1584895
H	6.2666936	-1.5901186	1.1332485

H	4.9032616	-1.2229516	-1.5763625
H	4.2000286	-2.8520916	-1.7394285
H	5.8674626	-2.6502656	-1.1450915
H	2.8955006	-0.6476466	0.7772035
H	-0.2108274	2.3393214	-0.8751095
H	1.6971466	3.5613544	-1.6223555
H	4.4352766	0.9896204	-2.0298805
H	2.5076116	-0.3015506	-2.8880345
H	-0.1687844	-1.9139966	-0.0849005
H	0.3980486	-1.3563526	2.6014905
H	0.3577356	3.9624494	1.7022305
H	0.0704676	0.1583024	4.9519945
H	-0.1199094	2.5150704	5.7190765
H	0.0116536	4.3820394	4.1058875
C	0.3066296	2.4323554	-3.7697515
C	4.3197986	-3.5324456	0.9387855
C	5.2382266	-1.2126816	1.1199975
C	4.8568726	-2.2240696	-1.1306765
C	4.3495276	-2.1445306	0.3067105
N	2.9946556	-1.5601016	0.3461135
O	1.9056476	-3.0493466	-1.0095285
C	1.9239866	-2.0319776	-0.3348805
O	4.1818046	2.8262254	-0.1965655
C	0.7500616	1.8461614	-0.6911795
C	1.8434936	2.9250364	-0.7364405
C	3.2415766	2.3695904	-0.8203495
C	3.4113076	1.2471574	-1.7613095

C	2.3660906	0.5483344	-2.2157125
C	0.9301666	0.7860124	-1.8218345
C	0.1074036	1.1527294	-3.0485275
C	-0.8089574	0.2069124	-3.2831875
O	-1.4696264	-1.7970086	-2.0721535
C	-0.7303924	-0.8385176	-2.2540365
N	0.3498556	-0.5089206	-1.4636825
C	0.6398636	-1.1782286	-0.2166215
C	0.6546376	1.1971984	0.6567755
C	0.6129076	-0.1531706	0.8569495
N	0.4450106	-0.4345596	2.1974995
C	0.3225196	3.1285124	2.3989355
C	0.4533296	1.8084414	1.9449995
C	0.3404376	0.7555804	2.8865845
C	0.1458096	0.9838764	4.2471165
C	0.0378226	2.3003504	4.6647385
C	0.1171176	3.3607374	3.7482195
Au	-3.3486414	-0.2917536	-0.0915795
C	-5.1668334	-4.0447336	0.4927025
C	-6.2590394	-3.2442416	0.5213615
H	-5.0683004	-5.1171796	0.5772965
H	-7.3084254	-3.4739876	0.6354795
C	-4.4598384	-1.9320856	0.2213785
N	-5.8066484	-1.9497126	0.3533835
N	-4.0728054	-3.2230326	0.3056765
C	-2.6306734	4.0277794	0.0239525
F	-1.3397344	4.3178654	-0.1530145

F	-2.8238894	3.7006764	1.2904625
F	-3.3471214	5.1029714	-0.2636575
S	-3.1204904	2.6501724	-1.0915685
O	-2.6262034	3.0441044	-2.4039965
O	-4.5548884	2.4774824	-0.8905345
O	-2.3011534	1.5214964	-0.4798045
C	-6.6702234	-0.7784986	0.3237935
H	-7.0851894	-0.5898276	1.3182635
H	-6.0859384	0.0900114	0.0065775
H	-7.4840694	-0.9415146	-0.3880175
C	-2.6909374	-3.6775436	0.2170525
H	-2.1715914	-3.4770566	1.1605425
H	-2.6883534	-4.7532936	0.0281495
H	-2.1847074	-3.1589616	-0.6048505
H	1.7878836	3.5779744	0.1401805
H	-1.5711774	0.2128824	-4.0539375

Zero-point correction= 0.611092 (Hartree/Particle)

Thermal correction to Energy= 0.656398

Thermal correction to Enthalpy= 0.657342

Thermal correction to Gibbs Free Energy= 0.529567

Sum of electronic and zero-point Energies= -2719.410547

Sum of electronic and thermal Energies= -2719.365241

Sum of electronic and thermal Enthalpies= -2719.364297

Sum of electronic and thermal Free Energies= -2719.492072

A-ts5

H	-1.8077235	-2.8242469	2.2186816
H	-1.9129615	-1.4612779	3.3281476

H	-3.3572915	-1.9683339	2.4233496
H	2.6785165	5.8529261	0.1634606
H	2.0411575	5.0671571	-1.2945944
H	1.1266755	4.9827971	0.2296656
H	4.8974575	2.9090541	-0.1715794
H	4.2447525	3.8661311	-1.5333414
H	4.8132535	4.6761051	-0.0591844
H	3.5875105	2.6520811	1.9241606
H	1.9944465	3.4484791	2.1194686
H	3.4876395	4.4123681	2.1259726
H	2.8914815	1.7828361	-0.7256454
H	-0.2302045	-2.4009989	-0.0304404
H	0.8224095	-3.2785659	3.0196056
H	1.0078175	0.2669981	4.0361286
H	-0.2612605	1.3276531	2.1485336
H	-0.0682765	1.3411831	-1.8595344
H	2.3450585	-0.8175709	0.3832006
H	1.9296615	0.2620771	-3.1638914
H	2.6557255	-4.0183079	0.0352466
H	3.4721045	-1.7427679	-4.3547754
H	4.3594845	-4.0340579	-3.9151594
H	3.9348125	-5.1483569	-1.7586454
C	-2.2720485	-1.8384179	2.3608956
C	2.1291095	4.9778751	-0.2044194
C	4.2989895	3.7861861	-0.4398584
C	2.9931715	3.5410701	1.6783776
C	2.9021835	3.7165181	0.1652986

N	2.2437705	2.5206901	-0.4289774
O	0.1394985	2.8771741	0.4119496
C	0.9544605	2.2176531	-0.2102764
O	1.0666965	-2.5150319	4.0126536
C	0.4018465	-1.7369999	0.5807586
C	0.9410975	-2.4387509	1.8138566
C	0.9603595	-1.6946779	3.0347106
C	0.7318365	-0.2760689	3.1366926
C	0.0418455	0.2816941	2.1266236
C	-0.4889315	-0.5115569	0.9563036
C	-1.9430345	-0.9155519	1.2424936
C	-2.7982835	-0.3538159	0.3647556
O	-2.3602455	1.0665561	-1.5833394
C	-2.0039835	0.4455481	-0.5947664
N	-0.6758635	0.3428371	-0.2014414
C	0.3939235	0.9475351	-0.9375444
C	1.5768535	-1.2635329	-0.3067764
C	1.3065225	-0.1710219	-1.2518884
N	1.9065355	-0.3981109	-2.3939684
C	2.8228235	-3.5182879	-0.9151284
C	2.3245105	-2.2466999	-1.1520394
C	2.5654235	-1.6512859	-2.3918514
C	3.2920995	-2.2437839	-3.4073564
C	3.7823715	-3.5207509	-3.1508824
C	3.5424435	-4.1491599	-1.9284104
Au	-4.8267905	-0.3978829	0.0904316
C	-8.7533605	0.3730741	-1.4067524

C	-9.1061255	-0.4716219	-0.4096004
H	-9.3505025	0.9001941	-2.1370604
H	-10.0732685	-0.8334579	-0.0911664
C	-6.8577615	-0.2684119	-0.3626904
N	-7.9330315	-0.8527969	0.2166856
N	-7.3761475	0.4847981	-1.3629194
C	6.1391195	-1.1320969	-0.0576484
F	6.7888105	-1.6386559	0.9805216
F	7.0032395	-0.4944919	-0.8371534
F	5.6023725	-2.1328559	-0.7543804
S	4.8277015	0.0159121	0.5092246
O	3.9650165	-0.8295749	1.3604136
O	4.1745805	0.3987641	-0.7718274
O	5.5433365	1.0924211	1.1876246
C	-7.8666195	-1.7566209	1.3494456
H	-6.8164075	-1.8849139	1.6225616
H	-8.4123535	-1.3398399	2.2013566
H	-8.2925145	-2.7291919	1.0849116
C	-6.5956165	1.3121561	-2.2701234
H	-5.5334645	1.1957951	-2.0340144
H	-6.7704515	1.0005881	-3.3041314
H	-6.8747945	2.3635451	-2.1540924
H	1.9668065	-2.8060229	1.6751056

Zero-point correction= 0.604111 (Hartree/Particle)

Thermal correction to Energy= 0.649175

Thermal correction to Enthalpy= 0.650119

Thermal correction to Gibbs Free Energy= 0.521254

Sum of electronic and zero-point Energies= -2719.265043

Sum of electronic and thermal Energies= -2719.219979

Sum of electronic and thermal Enthalpies= -2719.219035

Sum of electronic and thermal Free Energies= -2719.347900

A-int5

H	-2.0451400	-2.9008335	2.2094878
H	-1.7299680	-1.5536955	3.3107918
H	-3.3516940	-1.7808175	2.6120448
H	2.4606390	5.8614375	0.0617878
H	1.8654610	5.0231605	-1.3848942
H	0.9371160	4.9430995	0.1309178
H	4.7794990	2.9892205	-0.1755932
H	4.1209270	3.9069595	-1.5619802
H	4.6364710	4.7537005	-0.0888242
H	3.4490700	2.7312615	1.9051108
H	1.8193610	3.4617925	2.0552658
H	3.2691570	4.4890795	2.0737418
H	2.8306270	1.7835045	-0.7323122
H	-0.1754690	-2.4800515	-0.0565742
H	0.0979680	-3.1276735	2.2480288
H	1.3694280	0.3837515	3.7400248
H	-0.2803310	1.2503565	2.1025598
H	-0.0768360	1.2030365	-1.9242832
H	2.3649890	-0.8430425	0.4224188
H	1.9444610	0.1646115	-3.1608672
H	2.8936440	-3.9941565	0.1428228
H	3.5663000	-1.7873295	-4.3008662

H	4.5712500	-4.0209415	-3.8113782
H	4.2134160	-5.0967155	-1.6221842
C	-2.2783750	-1.8440735	2.4050028
C	1.9439740	4.9610105	-0.2921012
C	4.1580990	3.8428345	-0.4667382
C	2.8222070	3.5894855	1.6320658
C	2.7537330	3.7347675	0.1147578
N	2.1509840	2.5043545	-0.4675612
O	0.0100500	2.8063175	0.3011508
C	0.8679360	2.1611855	-0.2755232
O	2.1002420	-2.1094325	3.8336518
C	0.4202370	-1.7981215	0.5702248
C	0.9114560	-2.5292905	1.8173558
C	1.4261210	-1.6414915	2.9389108
C	0.9770720	-0.2401375	2.9399768
C	0.0891450	0.2261455	2.0522098
C	-0.4896060	-0.5932655	0.9274748
C	-1.9414650	-0.9790525	1.2415408
C	-2.8070160	-0.4315195	0.3652938
O	-2.3888880	0.9352615	-1.6256762
C	-2.0217440	0.3335895	-0.6294902
N	-0.6899680	0.2273055	-0.2535412
C	0.3739100	0.8499455	-0.9807412
C	1.6199330	-1.3164995	-0.2744952
C	1.3272400	-0.2470735	-1.2450262
N	1.9378820	-0.4813845	-2.3787272
C	3.0009270	-3.5163015	-0.8264642

C	2.4175970	-2.2874275	-1.0963352
C	2.6398210	-1.7086055	-2.3479352
C	3.4045460	-2.2812055	-3.3464202
C	3.9622610	-3.5235475	-3.0615412
C	3.7573100	-4.1309545	-1.8229822
Au	-4.8417950	-0.4402315	0.1354798
C	-8.7755730	0.3938455	-1.3064732
C	-9.1297130	-0.4373765	-0.2985462
H	-9.3731800	0.9272915	-2.0317912
H	-10.0987610	-0.7788255	0.0361928
C	-6.8775240	-0.2762565	-0.2853332
N	-7.9550270	-0.8365145	0.3133728
N	-7.3960670	0.4797125	-1.2833682
C	6.1787120	-0.9811085	0.0124758
F	6.8547030	-1.4175825	1.0642888
F	7.0022420	-0.3071695	-0.7807822
F	5.7109790	-2.0312045	-0.6615342
S	4.7923630	0.0915515	0.5461958
O	3.9673590	-0.7985175	1.3889078
O	4.1381680	0.4242485	-0.7492502
O	5.4307930	1.2157365	1.2236448
C	-7.8894210	-1.7342515	1.4509048
H	-6.8379080	-1.8826215	1.7082488
H	-8.4128620	-1.3009115	2.3085228
H	-8.3395680	-2.6993855	1.1995478
C	-6.6138550	1.2872635	-2.2070702
H	-6.8635740	2.3454145	-2.0856462

H	-5.5501730	1.1440555	-1.9938622
H	-6.8186870	0.9802005	-3.2368712
H	1.7124010	-3.2398955	1.5891848

Zero-point correction= 0.610004 (Hartree/Particle)

Thermal correction to Energy= 0.655141

Thermal correction to Enthalpy= 0.656085

Thermal correction to Gibbs Free Energy= 0.527039

Sum of electronic and zero-point Energies= -2719.362601

Sum of electronic and thermal Energies= -2719.317465

Sum of electronic and thermal Enthalpies= -2719.316521

Sum of electronic and thermal Free Energies= -2719.445567

A-ts6

H	-1.9320258	-2.8934842	2.2085299
H	-1.6802638	-1.5444432	3.3226829
H	-3.2893768	-1.8357462	2.6176919
H	2.5082302	5.8694958	0.0274929
H	1.9835012	5.0432148	-1.4535041
H	0.9758452	4.9639248	0.0115749
H	4.8097612	2.9746488	-0.1139301
H	4.2087192	3.8557228	-1.5439461
H	4.6700952	4.7404908	-0.0756461
H	3.3694862	2.7224068	1.9076749
H	1.7674302	3.5149968	1.9929179
H	3.2538882	4.4884078	2.0537209
H	2.8285712	1.8105178	-0.8304081
H	-0.1884208	-2.4896202	0.0203429
H	0.2549572	-3.1059522	2.2579649

H	1.3636072	0.4651378	3.7424229
H	-0.3014898	1.2826368	2.0980249
H	-0.0941308	1.2125368	-1.9354381
H	2.5124902	-0.8627852	0.3022379
H	2.1863032	0.3745388	-3.0749721
H	2.5305672	-4.1457412	-0.1554811
H	3.8236102	-1.5699672	-4.2566681
H	4.6366732	-3.8988922	-3.8952741
H	3.9707412	-5.1627882	-1.8850851
C	-2.2139088	-1.8500562	2.4127449
C	2.0033572	4.9755378	-0.3584981
C	4.2017462	3.8217938	-0.4466751
C	2.7877972	3.6024628	1.6044289
C	2.7760192	3.7368968	0.0839019
N	2.1651392	2.5174218	-0.5126721
O	0.0444942	2.8439448	0.2829369
C	0.8756912	2.1791618	-0.3100961
O	2.2111072	-1.9906972	3.8082849
C	0.4432472	-1.7679002	0.5636909
C	1.0161632	-2.4549482	1.8071999
C	1.4998382	-1.5494122	2.9271769
C	0.9936912	-0.1702252	2.9405329
C	0.0976772	0.2694308	2.0485029
C	-0.4667548	-0.5623822	0.9266859
C	-1.9099938	-0.9608522	1.2591249
C	-2.7910908	-0.4072102	0.4032959
O	-2.4123888	0.9899158	-1.5743711

C	-2.0224728	0.3753078	-0.5940331
N	-0.6870218	0.2645898	-0.2451801
C	0.3704062	0.8702878	-0.9940861
C	1.5406482	-1.3401442	-0.4146841
C	1.3360352	-0.2208482	-1.2746731
N	2.0560812	-0.3558702	-2.3861241
C	2.7985952	-3.5783362	-1.0431401
C	2.3327822	-2.2805272	-1.2361311
C	2.7033952	-1.5982332	-2.4048351
C	3.5383382	-2.1345412	-3.3727851
C	3.9861202	-3.4316662	-3.1607251
C	3.6108642	-4.1457072	-2.0178041
Au	-4.8261528	-0.4421382	0.1861269
C	-8.7732398	0.3197988	-1.2604231
C	-9.1141088	-0.5173782	-0.2528391
H	-9.3790078	0.8407458	-1.9880591
H	-10.0772738	-0.8775412	0.0792669
C	-6.8652268	-0.3123502	-0.2332181
N	-7.9335478	-0.8929122	0.3628709
N	-7.3957348	0.4327048	-1.2332781
C	5.9579762	-1.2067342	0.3008609
F	6.2870142	-1.7034012	1.4795209
F	7.0341772	-0.6955192	-0.2778171
F	5.4757492	-2.1775762	-0.4647631
S	4.6991052	0.1116138	0.5012299
O	3.5446202	-0.6325512	1.1385099
O	4.3731002	0.5127498	-0.8773771

O	5.3065632	1.1007688	1.3734739
C	-7.8529088	-1.7893002	1.5003329
H	-6.7992878	-1.9146152	1.7614059
H	-8.3889878	-1.3678992	2.3561299
H	-8.2808058	-2.7640602	1.2470829
C	-6.6261508	1.2528788	-2.1565401
H	-6.8992568	2.3059138	-2.0410201
H	-5.5606888	1.1333628	-1.9374471
H	-6.8188958	0.9370468	-3.1860401
H	1.8585952	-3.1100602	1.5570909

Zero-point correction= 0.604683 (Hartree/Particle)

Thermal correction to Energy= 0.649650

Thermal correction to Enthalpy= 0.650594

Thermal correction to Gibbs Free Energy= 0.522404

Sum of electronic and zero-point Energies= -2719.360521

Sum of electronic and thermal Energies= -2719.315554

Sum of electronic and thermal Enthalpies= -2719.314610

Sum of electronic and thermal Free Energies= -2719.442800

A-int6

H	-0.2043645	-3.6160487	0.0537293
H	-0.3338045	-3.2761017	-1.6789807
H	1.2270255	-3.7541917	-0.9721057
H	3.1243285	4.9053923	0.7610143
H	2.5642245	3.2662533	0.3504913
H	3.0488795	4.3813873	-0.9331987
H	-0.5655455	5.3541593	1.2082413
H	0.3301915	3.9181063	1.7458903

H	1.0182725	5.5233003	1.9790823
H	0.1891765	6.7363243	-0.7120367
H	1.7141365	6.3616713	-1.5556337
H	1.7467435	6.9452433	0.1156343
H	0.3719185	4.5855293	-2.0082277
H	-5.3689635	-2.3063567	-1.1357477
H	-1.1158855	-1.0375657	1.3413583
H	-2.0979495	-2.7187887	-0.1381967
H	-2.3772765	-0.7785657	-3.4727997
H	-0.1104435	-0.0926337	-2.7410667
H	0.6429085	2.2761103	0.7552483
H	-1.9085505	3.8574103	0.0892433
H	-4.7442755	-0.5901047	1.2969933
H	-4.5730235	4.3920893	0.8023663
H	-6.6940585	3.2242543	1.3841273
H	-6.7419675	0.7615863	1.6256913
C	0.3186735	-3.1662097	-0.8025027
C	2.5438205	4.3176423	0.0386423
C	0.4331465	4.9061513	1.2870393
C	1.1946885	6.3147303	-0.5897987
C	1.1292255	4.8802973	-0.0712387
N	0.3389965	4.1375423	-1.0959917
O	0.1203635	2.3302033	-2.4374437
C	0.2295025	2.7779943	-1.3108947
O	-4.1738545	-1.6919827	-1.8774217
C	-1.5197745	-0.6923997	0.3760013
C	-2.5464025	-1.7163097	-0.1113677

C	-3.0263015	-1.4303027	-1.5041397
C	-2.0543175	-0.8843447	-2.4399467
C	-0.8289315	-0.5080447	-2.0368367
C	-0.3356065	-0.6056597	-0.6178537
C	0.6874045	-1.7464487	-0.5420817
C	1.9208865	-1.2872247	-0.2514957
O	2.6923355	0.9745163	0.2588963
C	1.8200535	0.1757263	-0.0642277
N	0.5101995	0.5356683	-0.3006797
C	0.0502205	1.8769033	-0.0805147
C	-2.1231455	0.6829903	0.5142673
C	-1.3987095	1.8180173	0.2702343
N	-2.1903735	2.9347333	0.3893123
C	-4.6757615	0.4861623	1.1609853
C	-3.4690675	1.1176793	0.8116403
C	-3.4702535	2.5325283	0.7014443
C	-4.6099615	3.3088763	0.8993823
C	-5.7836095	2.6513543	1.2245663
C	-5.8103745	1.2546003	1.3582823
Au	3.7570615	-2.1552357	0.0059733
C	7.9168455	-2.7578537	0.7830063
C	7.5945075	-4.0471457	0.5259573
H	8.8590765	-2.2992617	1.0470053
H	8.1967235	-4.9443667	0.5194863
C	5.7096225	-2.8218077	0.3137663
N	6.2409465	-4.0651897	0.2413243
N	6.7527995	-2.0241147	0.6485473

C	-5.1293795	-5.0325707	-0.1013117
F	-4.8630065	-5.8223227	0.9232363
F	-3.9873315	-4.6060567	-0.6342657
F	-5.8117295	-5.6986047	-1.0114487
S	-6.0895285	-3.5836017	0.4920683
O	-7.3883385	-4.0685607	0.8838823
O	-6.2284425	-2.7801987	-0.8379347
O	-5.2069125	-2.9116547	1.4296553
C	5.4910965	-5.2616197	-0.0915397
H	4.4502355	-4.9756687	-0.2614467
H	5.8920485	-5.7213637	-0.9999357
H	5.5379815	-5.9809737	0.7316213
C	6.6683135	-0.5848187	0.8419643
H	7.3208365	-0.0717577	0.1292913
H	5.6350225	-0.2638097	0.6780263
H	6.9674185	-0.3255407	1.8618723
H	-3.4006385	-1.7997547	0.5638203

Zero-point correction= 0.610362 (Hartree/Particle)

Thermal correction to Energy= 0.654548

Thermal correction to Enthalpy= 0.655492

Thermal correction to Gibbs Free Energy= 0.531224

Sum of electronic and zero-point Energies= -2719.390777

Sum of electronic and thermal Energies= -2719.346592

Sum of electronic and thermal Enthalpies= -2719.345648

Sum of electronic and thermal Free Energies= -2719.469916

A-int7

H	0.5525897	-0.0455625	-3.7826243

H	1.4166557	1.3152565	-3.0759623
H	2.1033227	-0.3212305	-2.9424363
H	0.0637757	2.4873395	3.5006127
H	-0.4908433	1.1592785	2.4871787
H	0.1567657	2.6362495	1.7355487
H	-3.6945713	2.7972145	3.6836057
H	-2.9131723	1.2216745	3.4592067
H	-2.2520103	2.3687715	4.6309277
H	-2.6133473	4.9164745	2.9131917
H	-1.0076323	4.8747165	2.1400457
H	-1.1772953	4.5184425	3.8713957
H	-2.9144573	3.7628385	0.9678377
H	-2.1084463	-1.0040075	-2.1929733
H	-3.1595213	0.2489795	-4.0706593
H	-1.1981943	3.9002355	-2.7599173
H	-0.1367923	2.6624805	-0.8728323
H	-2.1706733	0.3404315	1.7353007
H	-5.1147983	0.1883345	-0.7565693
H	-2.2168633	-2.1027635	1.2621017
H	-6.9216023	-2.1551755	-1.3847413
H	-3.3524783	-4.7220865	1.0294907
H	-5.3382823	-5.8785425	0.0834007
H	-7.0948763	-4.6123305	-1.1065223
C	1.1713367	0.2547285	-2.9270523
C	-0.4530013	2.2507445	2.5624277
C	-2.7258923	2.2852495	3.6450707
C	-1.6478193	4.3945095	2.8902147

C	-1.8311893	2.9113075	2.5760827
N	-2.4937753	2.8841665	1.2520907
O	-3.7709453	2.1384475	-0.4383953
C	-2.9911913	1.8821505	0.4646577
O	-2.6955533	2.7644915	-4.5462903
C	-1.9098823	0.0549485	-2.3654523
C	-2.4708303	0.7248745	-3.3766113
C	-2.2170923	2.1604475	-3.5990583
C	-1.3430473	2.8321495	-2.6147153
C	-0.7823253	2.1678955	-1.6014613
C	-0.9272633	0.6850575	-1.4211683
C	0.4517307	0.0428505	-1.6442343
C	0.8572937	-0.6514605	-0.5587963
O	-0.3016293	-1.1171715	1.5388867
C	-0.2194153	-0.5506525	0.4525827
N	-1.1837703	0.3133505	-0.0314973
C	-2.4548263	0.4707795	0.6832577
C	-4.6185083	-0.6645705	-0.3156713
C	-3.4246693	-0.6194285	0.3525477
N	-3.0700613	-1.8985235	0.7529747
C	-6.1443853	-2.7078245	-0.8603603
C	-5.0327813	-2.0345535	-0.3346813
C	-4.0369923	-2.7828035	0.3421997
C	-4.1267063	-4.1656525	0.5052247
C	-5.2373943	-4.8008305	-0.0254873
C	-6.2367713	-4.0796305	-0.7025903
Au	2.6008697	-1.7061875	-0.2461133

C	6.6320337	-3.0902515	-0.3469523
C	6.4698817	-3.0121055	0.9959547
H	7.4958577	-3.3386315	-0.9462413
H	7.1641067	-3.1756125	1.8073167
C	4.4873247	-2.5274285	0.0456887
N	5.1488417	-2.6738745	1.2146337
N	5.4056537	-2.7947395	-0.9099083
C	5.0220777	2.9918975	-0.4588743
F	6.3398197	2.9282835	-0.5336703
F	4.6671027	3.6898985	0.6007737
F	4.5390887	3.5479615	-1.5510253
S	4.4089657	1.2632075	-0.3094863
O	4.7244087	0.5891395	-1.5541733
O	2.8729457	1.6614215	-0.2407673
O	4.8900717	0.7488575	0.9560557
C	4.5799737	-2.3469645	2.5115587
H	3.5200177	-2.6116265	2.5150547
H	5.0986927	-2.9143775	3.2883737
H	4.6809427	-1.2730045	2.6988537
C	5.1524627	-2.6537045	-2.3349443
H	5.9326807	-3.1790725	-2.8910003
H	4.1811147	-3.0928495	-2.5759403
H	5.1472707	-1.5927135	-2.6068453
H	2.2878997	0.8604075	-0.3376263

Zero-point correction= 0.607496 (Hartree/Particle)

Thermal correction to Energy= 0.653905

Thermal correction to Enthalpy= 0.654849

Thermal correction to Gibbs Free Energy= 0.523408

Sum of electronic and zero-point Energies= -2719.344888

Sum of electronic and thermal Energies= -2719.298479

Sum of electronic and thermal Enthalpies= -2719.297535

Sum of electronic and thermal Free Energies= -2719.428976

A-ts7

H	1.2543919	0.0723933	3.3929714
H	0.9815379	-1.6621247	3.2497174
H	2.4609089	-0.9358297	2.5489834
H	-0.3918931	-3.4369467	-2.9584796
H	-0.6288601	-1.8190277	-2.3223796
H	-0.3311861	-3.1785277	-1.2105966
H	-4.1057111	-2.8996097	-3.3166836
H	-2.9727331	-1.5356937	-3.3746116
H	-2.5874141	-3.0317877	-4.2336056
H	-3.5682421	-4.9889397	-2.0336776
H	-2.0066361	-5.1375897	-1.1850256
H	-2.0661641	-5.1520547	-2.9589736
H	-3.6356451	-3.3936527	-0.4257936
H	-1.3553571	1.3625023	1.9134974
H	-2.6449391	0.7681733	3.9577874
H	-2.0728011	-3.4578337	3.1165944
H	-0.7722291	-2.8888937	1.0729224
H	-2.1176101	-0.4303417	-1.7949006
H	-4.7208311	0.9040283	0.7460804
H	-1.4634001	1.9626863	-1.7010796
H	-5.7192891	3.7352163	1.1074334

H	-1.7875391	4.8084943	-1.8161066
H	-3.2698001	6.6093573	-0.9572336
H	-5.2051191	6.0786813	0.4836764
C	1.3908859	-0.7903787	2.7265754
C	-0.8440941	-2.8746857	-2.1328446
C	-3.0435271	-2.6282477	-3.3213566
C	-2.5074961	-4.7070577	-2.0610786
C	-2.3393031	-3.1895097	-2.0873246
N	-3.0075101	-2.7180297	-0.8490026
O	-4.0697031	-1.3704967	0.6009354
C	-3.2456791	-1.4930477	-0.2910026
O	-2.9982841	-1.6790837	4.7637064
C	-1.4961881	0.3273933	2.2295814
C	-2.1868001	0.0096423	3.3276194
C	-2.4053591	-1.3911477	3.7372854
C	-1.8620701	-2.4283987	2.8362554
C	-1.1706301	-2.1220897	1.7362994
C	-0.8393321	-0.7053047	1.3547124
C	0.6831869	-0.5462847	1.4512514
C	1.2073269	-0.1711757	0.2523314
O	0.1099129	0.4824463	-1.8216296
C	0.0782669	0.0169883	-0.6895946
N	-1.0619471	-0.4336577	-0.0640086
C	-2.3648771	-0.3258487	-0.7291356
C	-4.0378301	1.5097963	0.1679594
C	-2.9679961	1.0297173	-0.5381706
N	-2.2968661	2.0859513	-1.1361636

C	-4.8633421	3.9634973	0.4753054
C	-4.0393951	2.9316953	0.0044144
C	-2.9324121	3.2606773	-0.8176866
C	-2.6373361	4.5764403	-1.1771896
C	-3.4703741	5.5727523	-0.6949816
C	-4.5723161	5.2701593	0.1244894
Au	2.9341969	1.1320723	0.1775644
C	6.7764279	2.8600793	-0.1349236
C	6.0835799	4.0054233	0.0748504
H	7.8309469	2.6867663	-0.2934236
H	6.4082989	5.0336493	0.1411054
C	4.6128209	2.3043813	0.0967094
N	4.7568419	3.6432183	0.2138454
N	5.8601479	1.8286153	-0.1157606
C	2.8246909	-3.9629027	0.3643764
F	3.4966949	-4.7362227	1.1988394
F	2.4635169	-4.6659157	-0.6961866
F	1.7181169	-3.5286017	0.9791174
S	3.8434649	-2.5204537	-0.1359366
O	4.1088349	-1.8127917	1.1212864
O	2.8557749	-1.7725497	-1.0096676
O	4.9728359	-3.0512097	-0.8761446
C	3.6758239	4.5802483	0.4599224
H	2.7358169	4.0243583	0.4857154
H	3.8230119	5.0856673	1.4189034
H	3.6323469	5.3233143	-0.3415116
C	6.1783309	0.4196543	-0.3359136

H	7.2601569	0.2903313	-0.2646916
H	5.6867609	-0.2009967	0.4199254
H	5.8399779	0.1046193	-1.3277306
H	2.1382309	-0.8861487	-0.2983426

Zero-point correction= 0.603239 (Hartree/Particle)

Thermal correction to Energy= 0.648715

Thermal correction to Enthalpy= 0.649660

Thermal correction to Gibbs Free Energy= 0.521448

Sum of electronic and zero-point Energies= -2719.335686

Sum of electronic and thermal Energies= -2719.290211

Sum of electronic and thermal Enthalpies= -2719.289266

Sum of electronic and thermal Free Energies= -2719.417477

A-int8

H	1.3415469	-2.6306007	2.2104587
H	0.9836209	-4.0100647	1.1624197
H	2.4208319	-2.9938637	0.8420507
H	-4.2981741	-2.6245077	-3.3339783
H	-2.9818051	-1.6971397	-2.6240373
H	-3.6263141	-3.1187967	-1.7678073
H	-6.0700721	0.4296603	-1.9743133
H	-4.4039321	0.5205243	-2.5704863
H	-5.6092201	-0.3965677	-3.4791483
H	-7.0289671	-1.6837037	-1.0615583
H	-6.0468641	-3.1708207	-1.0112173
H	-6.5977151	-2.5148527	-2.5653513
H	-5.2918201	-1.3092117	0.4151057
H	-0.2073821	0.2954253	1.6795457

H	-0.8321451	-0.3274907	3.9958067
H	-2.5969331	-4.0280437	2.5552207
H	-1.8957921	-3.4632667	0.2301377
H	-2.6827191	0.0006323	-1.6418653
H	-2.4816731	2.0518283	1.6775247
H	-0.7565101	1.4558823	-2.1178593
H	-1.0247441	4.6554323	2.2167977
H	0.8366869	3.8070743	-2.3635193
H	1.5478399	5.7903873	-1.0421493
H	0.6295579	6.2032753	1.2144807
C	1.3759819	-2.9846697	1.1731837
C	-3.8949811	-2.2523387	-2.3845163
C	-5.2731171	-0.1385827	-2.4675903
C	-6.2335811	-2.2447557	-1.5686453
C	-4.9595071	-1.4107497	-1.6817803
N	-4.5877211	-1.0939937	-0.2831273
O	-3.6073951	-0.1036247	1.4802067
C	-3.5872741	-0.3673417	0.2874077
O	-1.9732601	-2.5831657	4.6200627
C	-0.6650261	-0.6665047	1.9106177
C	-0.9996461	-1.0018877	3.1592507
C	-1.6865341	-2.2669897	3.4780547
C	-2.0243431	-3.1322037	2.3264747
C	-1.6548211	-2.8253027	1.0819537
C	-0.8341341	-1.6043587	0.7477047
C	0.5427259	-2.1250507	0.2957307
C	0.7220699	-1.8446517	-1.0351163

O	-0.6428491	-0.6444687	-2.6577543
C	-0.4619981	-1.1073827	-1.5416843
N	-1.3354351	-0.9759357	-0.4815533
C	-2.4026651	0.0352283	-0.5840123
C	-1.9014541	2.2332573	0.7827657
C	-1.8552271	1.3999813	-0.3031573
N	-1.0001641	1.9322443	-1.2567723
C	-0.6156371	4.4601733	1.2275507
C	-1.0164681	3.3249393	0.5084007
C	-0.4655811	3.1025913	-0.7783073
C	0.4490039	3.9809683	-1.3610003
C	0.8337599	5.0863273	-0.6197533
C	0.3084799	5.3223673	0.6633967
Au	1.9349579	-0.1219517	-0.1004953
C	4.6514809	2.4608083	1.8180547
C	4.7087989	2.9879543	0.5711377
H	5.2012709	2.6964653	2.7171677
H	5.3254289	3.7717673	0.1570637
C	3.1543869	1.3837743	0.5549357
N	3.7704719	2.3202393	-0.1867163
N	3.6818309	1.4788813	1.7901517
C	6.1590919	-2.6510767	-0.9113773
F	7.1570439	-2.5661817	-0.0402843
F	6.6327479	-2.4179197	-2.1288323
F	5.6670319	-3.8852127	-0.8752643
S	4.8491709	-1.4369327	-0.4969633
O	4.4306309	-1.8323247	0.8654687

O	3.8179189	-1.6914747	-1.5288083
O	5.5141499	-0.1314137	-0.5941503
C	3.6663089	2.3972323	-1.6323693
H	3.9324029	3.4051923	-1.9618043
H	4.3376099	1.6521033	-2.0739783
H	2.6332309	2.1873763	-1.9248283
C	3.3987179	0.5428493	2.8680827
H	2.3158109	0.4480063	2.9977167
H	3.8306249	-0.4323387	2.6132367
H	3.8364099	0.9252623	3.7928347
H	1.5119659	-2.2363957	-1.6742313

Zero-point correction= 0.607390 (Hartree/Particle)

Thermal correction to Energy= 0.653699

Thermal correction to Enthalpy= 0.654643

Thermal correction to Gibbs Free Energy= 0.522949

Sum of electronic and zero-point Energies= -2719.367441

Sum of electronic and thermal Energies= -2719.321132

Sum of electronic and thermal Enthalpies= -2719.320188

Sum of electronic and thermal Free Energies= -2719.451882

A-ts8

C	2.3740123	0.5777495	3.3396324
C	1.9814493	-0.6605245	3.8707694
C	0.9429113	-1.3937225	3.3067764
C	0.3211633	-0.8526255	2.1867874
C	0.7080233	0.3830975	1.6266914
C	1.7383313	1.1121005	2.2262714
N	-0.7542847	-1.3235625	1.4476404

C	-1.0439357	-0.4536815	0.4447834
C	-0.1548467	0.6347015	0.4985564
C	-1.8892817	-0.8747375	-0.7208936
N	-1.0081557	-1.7435625	-1.5066326
C	0.1505493	-1.0981035	-2.1451806
C	-0.6177297	-2.9574905	-0.9306516
C	0.7466523	-3.2246135	-1.3882686
C	1.2666343	-2.1430685	-1.9800306
C	-0.0128217	-0.9330075	-3.6627126
C	0.7846403	-0.1081025	-4.3460266
C	1.7634263	0.7895075	-3.6585316
C	1.4608693	1.0920755	-2.2025206
C	0.3222603	0.3404155	-1.7391906
O	-1.2482817	-3.5884535	-0.1031756
O	2.6663813	1.3161435	-4.2738756
C	-3.2965597	-1.4252755	-0.4428396
O	-3.7473547	-2.3958885	-1.0154926
N	-3.9486897	-0.6152475	0.4358454
C	-5.4233357	-0.5914315	0.5688474
C	-5.9037937	-1.9080735	1.1643154
C	-6.0688147	-0.3262495	-0.7890716
C	-5.7266297	0.5611765	1.5180024
C	2.6367533	-2.0797915	-2.5553976
H	3.1801073	1.1319605	3.8169854
H	2.4850003	-1.0468365	4.7544764
H	0.6207863	-2.3407125	3.7327544
H	2.0247553	2.0837685	1.8278764

H	-1.1522517	-2.2587445	1.4828644
H	-0.3569047	1.6247355	0.0901744
H	-2.1337287	0.0145795	-1.3135466
H	1.2533173	-4.1613125	-1.1834066
H	-0.7365657	-1.5992415	-4.1285036
H	0.7783223	-0.0626675	-5.4323676
H	1.2237053	2.1662255	-2.1593436
H	-0.6044757	0.9126945	-1.7233416
H	-3.5383007	0.3147265	0.5119364
H	-6.9920397	-1.8770205	1.3008794
H	-5.4385457	-2.0788945	2.1429204
H	-5.6549397	-2.7461275	0.5069214
H	-5.6665337	0.5980865	-1.2217896
H	-5.8735467	-1.1520405	-1.4801826
H	-7.1547417	-0.2179925	-0.6743736
H	-6.8081497	0.6480805	1.6724554
H	-5.3652787	1.5131225	1.1052054
H	-5.2501927	0.4005495	2.4933864
H	2.6136323	-1.9018115	-3.6366946
H	3.2407043	-1.2719755	-2.1185736
H	3.1525233	-3.0288385	-2.3788806
Au	3.1668163	0.9198725	-0.9258056
C	6.1001763	-0.0386275	2.0166574
C	6.5390193	1.2012075	1.6947154
H	6.4610613	-0.7560095	2.7396474
H	7.3593123	1.7893525	2.0804264
C	4.7569083	0.7532955	0.3922994

N	5.7047923	1.6686845	0.6958454
N	5.0113063	-0.2970345	1.2059854
C	-2.8686027	3.6785065	0.5652284
F	-2.4553887	2.7537445	1.4432694
F	-4.1703097	3.8673235	0.7569734
F	-2.2303137	4.8108945	0.8231624
S	-2.5484867	3.1045715	-1.1485376
O	-1.0695877	3.0066115	-1.1937406
O	-3.1474127	4.1199975	-1.9996696
O	-3.2090247	1.7774305	-1.1358526
C	5.8290933	2.9758995	0.0733924
H	6.8229543	3.0876225	-0.3691036
H	5.0751363	3.0595035	-0.7128046
H	5.6674083	3.7654195	0.8130464
C	4.2397763	-1.5281165	1.2469604
H	3.3077533	-1.3768105	0.6950904
H	4.8052623	-2.3499635	0.7964484
H	3.9861493	-1.7674425	2.2841104

Zero-point correction= 0.608086 (Hartree/Particle)

Thermal correction to Energy= 0.652743

Thermal correction to Enthalpy= 0.653687

Thermal correction to Gibbs Free Energy= 0.528340

Sum of electronic and zero-point Energies= -2719.296221

Sum of electronic and thermal Energies= -2719.251565

Sum of electronic and thermal Enthalpies= -2719.250621

Sum of electronic and thermal Free Energies= -2719.375968

A-int9

C	-1.3467054	-3.0391841	1.7946542
C	-0.2427074	-3.0894731	2.6441712
C	0.8756386	-2.2943281	2.4055852
C	0.8098226	-1.4409831	1.3206382
C	-0.2944194	-1.3437051	0.4690622
C	-1.3718574	-2.1883081	0.6878552
N	1.8074626	-0.5590291	0.8499832
C	1.4396566	0.0345629	-0.2573908
C	0.0890926	-0.4498641	-0.6826468
C	1.9060956	1.3869259	-0.6794068
N	0.8681866	2.1608969	0.0076222
C	-0.5435874	2.0402879	-0.4303138
C	0.9507626	2.2148839	1.4109992
C	-0.4150214	2.4117459	1.8884002
C	-1.2920434	2.2248559	0.8928702
C	-0.9537534	3.1778749	-1.3333198
C	-1.8812624	3.0184879	-2.2845328
C	-2.5674404	1.7228209	-2.5667158
C	-2.0703404	0.5073679	-1.8602188
C	-0.6870494	0.7405219	-1.2675468
O	1.9634076	2.0215519	2.0553862
O	-3.5049124	1.7088109	-3.3570248
C	3.3188156	1.8835199	-0.3150878
O	3.5173416	3.0758339	-0.1996318
N	4.2296236	0.8850369	-0.1835628
C	5.6505626	1.1334869	0.1389492
C	5.7345296	1.7912869	1.5115832

C	6.3118856	2.0017119	-0.9277518
C	6.3134466	-0.2365531	0.1729012
C	-2.7660304	2.3405849	1.0430632
H	-2.1930524	-3.6975411	1.9797672
H	-0.2412984	-3.7742611	3.4881892
H	1.7629966	-2.3509091	3.0302392
H	-2.2150254	-2.1974631	-0.0014908
H	2.6751136	-0.3180661	1.3251992
H	0.2869226	-1.1568551	-1.5148978
H	1.8064826	1.5046549	-1.7634688
H	-0.6432594	2.6159049	2.9286352
H	-0.4959764	4.1450229	-1.1249658
H	-2.2047444	3.8532729	-2.9038068
H	-1.9839444	-0.2750501	-2.6312008
H	-0.0645754	0.9863439	-2.1463028
H	4.0204566	0.0279529	-0.7034378
H	6.7854276	1.9353619	1.7911002
H	5.2587976	1.1555099	2.2694122
H	5.2322246	2.7625419	1.5147102
H	6.2339366	1.5245959	-1.9123108
H	5.8403376	2.9870519	-0.9752478
H	7.3763666	2.1314729	-0.6954298
H	7.3676016	-0.1379231	0.4554142
H	6.2665946	-0.7206541	-0.8102278
H	5.8206716	-0.8969951	0.8985992
H	-3.2352634	2.8157069	0.1748812
H	-3.2274404	1.3480399	1.1461042

H	-3.0094864	2.9221299	1.9385452
Au	-3.7664714	-0.2360791	-0.8094898
C	-7.1994204	-1.7742381	1.2756672
C	-7.7571084	-1.4684751	0.0807182
H	-7.6273194	-2.1929541	2.1752502
H	-8.7710574	-1.5719661	-0.2782558
C	-5.5704034	-0.9327951	-0.0388878
N	-6.7464274	-0.9528281	-0.7090148
N	-5.8598804	-1.4405681	1.1822792
C	3.9259226	-3.1528921	-0.9534298
F	3.7181816	-2.6361641	0.2701052
F	5.1791186	-2.8779101	-1.2986928
F	3.7816506	-4.4648671	-0.8774048
S	2.7474816	-2.4297211	-2.1635838
O	1.4416106	-2.9040591	-1.6849928
O	3.2139176	-2.9121151	-3.4524808
O	2.9389616	-0.9629421	-1.9341248
C	-6.9266774	-0.5166461	-2.0861338
H	-7.7843454	0.1588659	-2.1481818
H	-6.0273954	0.0134589	-2.4134248
H	-7.0925374	-1.3785661	-2.7390948
C	-4.9076434	-1.5733091	2.2695882
H	-3.8989684	-1.4154071	1.8770162
H	-5.1092294	-0.8321531	3.0496442
H	-4.9710234	-2.5771441	2.7003392

Zero-point correction= 0.610607 (Hartree/Particle)

Thermal correction to Energy= 0.655027

Thermal correction to Enthalpy= 0.655971

Thermal correction to Gibbs Free Energy= 0.531158

Sum of electronic and zero-point Energies= -2719.343404

Sum of electronic and thermal Energies= -2719.298984

Sum of electronic and thermal Enthalpies= -2719.298039

Sum of electronic and thermal Free Energies= -2719.422853

A-ts9

C	-0.2167956	4.3288392	0.0087205
C	-1.4947646	4.6618502	0.4816995
C	-2.5320846	3.7432172	0.4455095
C	-2.2433896	2.4790312	-0.0576785
C	-0.9670546	2.1217462	-0.5459075
C	0.0559234	3.0759732	-0.5191075
N	-3.0810046	1.3708072	-0.1783835
C	-2.3990216	0.3475942	-0.7334325
C	-1.0887746	0.7596142	-1.0369305
C	-2.6637846	-1.1283818	-0.5423155
N	-1.6542436	-1.5248438	0.4514475
C	-0.2097056	-1.4110028	0.1141825
C	-1.8820286	-0.9224918	1.7125855
C	-0.5795316	-0.7741588	2.3427805
C	0.3974124	-1.0150998	1.4549125
C	0.4558314	-2.6559268	-0.4313645
C	1.2314774	-2.6624048	-1.5291635
C	1.5360614	-1.4961108	-2.4240115
C	1.1350584	-0.1743718	-1.8341955
C	-0.1820996	-0.4296918	-1.0945405

O	-2.9762586	-0.5473198	2.0926795
O	2.0676414	-1.6319098	-3.5055375
C	-4.0657036	-1.6042078	-0.1308065
O	-4.2204796	-2.6613808	0.4392455
N	-5.0743146	-0.7702438	-0.5275465
C	-6.5056906	-1.0270568	-0.2534635
C	-6.7079616	-1.1023098	1.2561825
C	-6.9690236	-2.3094698	-0.9367675
C	-7.2625676	0.1684542	-0.8168865
C	1.8427224	-1.0582988	1.7513105
H	0.5750174	5.0730252	0.0502215
H	-1.6755306	5.6564252	0.8810775
H	-3.5259516	3.9935792	0.8080175
H	1.0519374	2.8333072	-0.8912965
H	-3.9475386	1.2275222	0.3303665
H	-0.0316756	0.5614012	-2.2370025
H	-2.4567626	-1.6738908	-1.4733635
H	-0.4565276	-0.4860668	3.3803765
H	0.3471054	-3.5641438	0.1608255
H	1.7250804	-3.5816678	-1.8371405
H	1.1413394	0.6694442	-2.6018985
H	-0.7170776	-1.0736358	-1.8084465
H	-4.8710856	-0.0992988	-1.2580835
H	-7.7726116	-1.2378058	1.4815135
H	-6.3654116	-0.1761238	1.7347105
H	-6.1461466	-1.9353158	1.6863295
H	-6.8224906	-2.2451718	-2.0223035

H	-6.4134636	-3.1710398	-0.5569595
H	-8.0374256	-2.4696688	-0.7471215
H	-8.3353656	0.0580232	-0.6257155
H	-7.1258576	0.2530982	-1.9037625
H	-6.9305656	1.1039772	-0.3468735
H	2.2683314	-2.0555358	1.5571705
H	2.4240544	-0.3861048	1.1057445
H	2.0278244	-0.7885178	2.7959745
Au	2.8819124	0.7278362	-0.9424415
C	6.1996634	2.3126332	1.2127535
C	6.8400474	1.7741062	0.1479345
H	6.5753264	2.8008002	2.1000635
H	7.8922144	1.6936442	-0.0829445
C	4.6406054	1.4754502	-0.1744955
N	5.8691064	1.2710552	-0.6916755
N	4.8474664	2.1295022	0.9899215
C	5.6343104	-1.8441668	1.1119775
F	6.6630404	-1.2472358	0.4990665
F	6.1145364	-2.5896878	2.0950785
F	4.8860794	-0.8695568	1.6641715
S	4.6615224	-2.8483278	-0.0861845
O	4.1483784	-1.8001138	-1.0040185
O	3.6263514	-3.4636818	0.7552705
O	5.6659474	-3.7375588	-0.6566135
C	6.1280084	0.5381902	-1.9273845
H	7.2011704	0.3482212	-1.9967735
H	5.5915764	-0.4171268	-1.8949095

H	5.8033314	1.1286962	-2.7889315
C	3.8128864	2.4371972	1.9574545
H	2.8484134	2.4881522	1.4438625
H	3.7697774	1.6549942	2.7231645
H	4.0232804	3.4007172	2.4300735

Zero-point correction= 0.602722 (Hartree/Particle)

Thermal correction to Energy= 0.646911

Thermal correction to Enthalpy= 0.647855

Thermal correction to Gibbs Free Energy= 0.526381

Sum of electronic and zero-point Energies= -2719.221971

Sum of electronic and thermal Energies= -2719.177783

Sum of electronic and thermal Enthalpies= -2719.176838

Sum of electronic and thermal Free Energies= -2719.298313

A-2'

C	2.5371447	-0.4995413	2.7591288
C	2.2595687	-1.8666013	2.5429418
C	1.0123737	-2.2743323	2.1109908
C	0.0440657	-1.2988053	1.8594848
C	0.2733627	0.0825057	2.0902928
C	1.5591947	0.4919297	2.5423928
N	-1.2309333	-1.4409243	1.3471698
C	-1.7861843	-0.1900793	1.2303508
C	-0.9105023	0.7650177	1.6919228
C	-2.9567233	0.2849917	0.4166728
N	-2.3525353	1.1618677	-0.5989242
C	-1.6173593	2.3437367	-0.1083782
C	-1.5393773	0.4524737	-1.4990832

C	-0.4565533	1.3532417	-1.8911512
C	-0.4092043	2.3937397	-1.0504262
C	-2.3829823	3.6297957	-0.2617102
C	-2.1353443	4.6857837	0.5265878
C	-1.1175463	4.6683247	1.6057278
C	-0.4784933	3.3288787	1.9508418
C	-1.3082253	2.1742497	1.4251898
O	-1.6772693	-0.7257013	-1.7742142
O	-0.8011823	5.6857377	2.1895488
C	-3.9292833	-0.7164663	-0.2169792
O	-4.5803363	-0.4230213	-1.1976002
N	-4.0275403	-1.8961913	0.4631968
C	-4.9197173	-3.0062073	0.0648668
C	-4.5458533	-3.4596893	-1.3425092
C	-6.3813863	-2.5751953	0.1326238
C	-4.6595173	-4.1324253	1.0565728
C	0.6336007	3.4548957	-1.0702852
H	3.5193287	-0.2127903	3.1265858
H	3.0584797	-2.5886103	2.6729818
H	0.8049767	-3.3260213	1.9277058
H	1.7365257	1.5159807	2.8690528
H	-1.5678913	-2.2446963	0.8324948
H	-3.5955883	0.9235847	1.0476998
H	0.2538437	1.1227707	-2.6798362
H	-3.1046253	3.6761827	-1.0767292
H	-2.6505743	5.6346817	0.3924778
H	-0.3864153	3.2870687	3.0432188

H	-2.3011083	2.3112887	1.8872008
H	-3.6636653	-1.9256863	1.4074998
H	-5.1534863	-4.3275333	-1.6259802
H	-3.4877203	-3.7463453	-1.3828892
H	-4.7102783	-2.6589863	-2.0681612
H	-6.6456093	-2.2589193	1.1495658
H	-6.5694683	-1.7456853	-0.5546672
H	-7.0329913	-3.4134683	-0.1428502
H	-5.2775833	-5.0021433	0.8090628
H	-4.9089283	-3.8282363	2.0823718
H	-3.6078483	-4.4479813	1.0296628
H	0.2461927	4.4443537	-0.8059852
H	1.4424587	3.2019267	-0.3671702
H	1.0892707	3.5152117	-2.0641842
Au	2.5698107	0.4860667	0.4375348
C	3.2559347	-0.1199473	-3.6614062
C	4.0652797	0.9536567	-3.4965692
H	3.0682477	-0.7445143	-4.5223062
H	4.7405367	1.4478117	-4.1792432
C	3.0580577	0.5595647	-1.5393522
N	3.9142297	1.3692837	-2.1891412
N	2.6350747	-0.3427023	-2.4478152
C	6.0319497	-0.9286543	1.4091448
F	7.3478557	-0.7890333	1.4458468
F	5.6512467	-1.6382063	2.4755728
F	5.4910637	0.2988487	1.5412208
S	5.4873167	-1.7277633	-0.1587072

O	5.7421737	-0.6717263	-1.1518772
O	4.0490297	-1.9762993	0.1066188
O	6.3196587	-2.9217743	-0.2356892
C	4.8011447	2.3043417	-1.5196062
H	5.1719627	3.0333407	-2.2444212
H	4.2517357	2.8238327	-0.7295502
H	5.6306937	1.7378907	-1.0822052
C	1.7936467	-1.4920503	-2.1315652
H	0.8028747	-1.1698913	-1.7887562
H	1.6710757	-2.0890013	-3.0379542
H	2.2999457	-2.0838873	-1.3603072
H	0.5468947	3.3228797	1.5561588

Zero-point correction= 0.610115 (Hartree/Particle)

Thermal correction to Energy= 0.654273

Thermal correction to Enthalpy= 0.655217

Thermal correction to Gibbs Free Energy= 0.531805

Sum of electronic and zero-point Energies= -2719.372490

Sum of electronic and thermal Energies= -2719.328332

Sum of electronic and thermal Enthalpies= -2719.327388

Sum of electronic and thermal Free Energies= -2719.450799

B-1

Au	4.1008807	-0.2453596	0.6217556
C	7.3948917	-1.7231986	-1.5576964
C	8.0459957	-1.4404526	-0.4041824
H	7.7480937	-2.1390966	-2.4903934
H	9.0830917	-1.5573496	-0.1243044
C	5.8922267	-0.8869266	-0.1220934

N	7.1050487	-0.9282896	0.4683216
N	6.0720257	-1.3770756	-1.3666204
C	7.4075957	-0.4951326	1.8230746
H	6.4775617	-0.2012526	2.3144876
H	7.8646607	-1.3153476	2.3828676
H	8.0900107	0.3589294	1.8022786
C	5.0396877	-1.5265266	-2.3876374
H	5.0116337	-2.5651426	-2.7269654
H	4.0628047	-1.2606176	-1.9722584
H	5.2618607	-0.8717696	-3.2345034
C	-6.0232173	-3.0522336	2.0280186
C	-5.0997273	-4.0708476	2.3253306
C	-3.7351063	-3.8531436	2.2485616
C	-3.3144083	-2.5803516	1.8621856
C	-4.2233563	-1.5408856	1.5585236
C	-5.5999673	-1.7925366	1.6480486
N	-2.0431623	-2.0720356	1.7011436
C	-2.1264323	-0.7499326	1.2956136
C	-3.4457063	-0.3929006	1.2062826
C	-0.8682763	-0.0021846	1.0281156
N	-0.1902153	-0.4657246	-0.2222174
C	1.1694527	-0.4480216	-0.3370954
C	-0.9514453	-0.6884166	-1.4242274
O	1.7992977	-0.8016486	-1.3232794
C	1.8939857	0.0884174	0.8326186
C	2.2793167	0.7858534	1.7755316
C	-1.7680023	-1.8117036	-1.5636434

C	-2.5137303	-1.9920106	-2.7159104
C	-2.4419323	-1.0562876	-3.7503354
C	-1.6185273	0.0644464	-3.6190344
C	-0.8783013	0.2435344	-2.4590624
O	-3.1904993	-1.2908546	-4.8451944
H	-0.1726023	-0.2120986	1.8494176
C	-1.0279443	1.5247284	1.0482946
O	-0.4356723	2.1871354	1.8936166
N	-1.8077573	2.0310444	0.0730816
C	-2.1336483	3.4631384	-0.1170314
C	-0.8583993	4.2465064	-0.4084374
C	-3.0726283	3.5207824	-1.3142384
C	-2.8353343	4.0012374	1.1251746
C	2.5129837	1.6274804	2.9326006
H	-7.0868043	-3.2638356	2.1012316
H	-5.4662783	-5.0501406	2.6227096
H	-3.0225343	-4.6411156	2.4817616
H	-6.3190143	-1.0085696	1.4215296
H	-1.1855553	-2.5768116	1.8647036
H	-3.8256433	0.5840054	0.9331596
H	-1.8258373	-2.5447066	-0.7632794
H	-3.1604923	-2.8557876	-2.8394244
H	-1.5550273	0.7938384	-4.4256014
H	-0.2348083	1.1153454	-2.3505884
H	-3.0588423	-0.5937806	-5.4974554
H	-2.2285213	1.3737464	-0.5739904
H	-0.3626683	3.8560174	-1.3064854

H	-1.0999093	5.3013714	-0.5841954
H	-0.1641633	4.1850694	0.4348166
H	-3.3548193	4.5581844	-1.5219914
H	-3.9931643	2.9538954	-1.1209824
H	-2.5937523	3.1126874	-2.2146754
H	-3.1133173	5.0503774	0.9703506
H	-2.1844153	3.9389044	2.0017036
H	-3.7513203	3.4321824	1.3273106
H	1.5461217	2.0921644	3.1695046
H	3.2470417	2.4105814	2.7209146
H	2.8566147	1.0405014	3.7903866

Zero-point correction= 0.575586 (Hartree/Particle)

Thermal correction to Energy= 0.614300

Thermal correction to Enthalpy= 0.615244

Thermal correction to Gibbs Free Energy= 0.499823

Sum of electronic and zero-point Energies= -1757.956918

Sum of electronic and thermal Energies= -1757.918204

Sum of electronic and thermal Enthalpies= -1757.917260

Sum of electronic and thermal Free Energies= -1758.032681

B-ts1

H	-1.2815279	4.2456491	0.4622912
H	-2.2675429	4.2251391	-1.0233378
H	-2.9955119	3.8212631	0.5582012
H	2.4493491	-4.2830019	-1.8337828
H	1.8823031	-3.0013739	-0.7782768
H	1.3372531	-3.0684449	-2.4835338
H	5.3878971	-1.9251269	-1.5109118

H	4.1655231	-2.0739699	-0.2310468
H	4.8003461	-3.5289019	-1.0304118
H	4.7976301	-2.4455169	-3.9227368
H	3.1463971	-2.9678569	-4.3364788
H	4.2263831	-4.0391439	-3.4154548
H	3.7042001	-0.5946589	-3.2674698
H	0.8706231	1.7897031	1.4856792
H	1.5784891	4.1749611	1.7589492
H	0.8737801	4.8624691	-2.4298808
H	0.1941921	2.4822881	-2.7041838
H	0.8978691	-1.2969329	-1.0964338
H	3.8748261	0.8578261	0.1981992
H	0.6874851	-1.6306219	1.3940792
H	5.2276091	0.8721551	2.9006872
H	1.3532901	-2.0689099	4.1347762
H	3.0811011	-1.4596979	5.8097022
H	4.9856101	-0.0124059	5.2018682
C	-2.0959759	3.7283521	-0.0626238
C	2.1878221	-3.2192049	-1.8076548
C	4.5018481	-2.4855469	-1.1893238
C	3.9205561	-2.9977289	-3.5610338
C	3.4042161	-2.4121829	-2.2478558
N	3.0876881	-0.9948629	-2.5664028
O	2.4051741	1.1409271	-2.4837298
C	2.3245711	0.0009541	-2.0443108
O	1.6769721	5.8996791	-0.0991688
C	0.8627711	2.4743771	0.6394752

C	1.2482251	3.7880821	0.7993412
C	1.2624901	4.6469761	-0.3128528
C	0.8484221	4.1912381	-1.5732728
C	0.4651111	2.8754371	-1.7291498
C	0.4334901	2.0017271	-0.6225568
C	-1.7988969	2.3227911	-0.2231018
C	-2.0390789	1.0699901	-0.2693638
O	-1.1616829	-1.1564919	-0.3319458
C	-0.9798999	0.0418711	-0.4680678
N	0.2306571	0.6062651	-0.8215388
C	1.3758051	-0.3341979	-0.8991258
C	3.2410551	0.2324311	0.8171662
C	2.0996181	-0.3976939	0.4002012
N	1.5397571	-1.0906099	1.4584492
C	4.3836841	0.2381061	3.1632222
C	3.4181701	-0.0915559	2.2003202
C	2.3324561	-0.9219689	2.5738972
C	2.1900491	-1.4279599	3.8665542
C	3.1589471	-1.0834549	4.7926722
C	4.2443961	-0.2583489	4.4457452
Au	-3.9986999	0.3519671	0.0004882
C	-7.3189639	-2.2502369	0.4422122
C	-7.9882589	-1.0765269	0.5285662
H	-7.6665189	-3.2723489	0.4882282
H	-9.0388209	-0.8643509	0.6660822
C	-5.8109489	-0.5952859	0.2427012
N	-7.0464179	-0.0727289	0.4038782

N	-5.9851339	-1.9357759	0.2672482
C	-7.3639539	1.3446271	0.4443942
H	-6.4414349	1.9121061	0.3041782
H	-8.0657689	1.5952121	-0.3558468
H	-7.8043529	1.6046161	1.4109962
C	-4.9307599	-2.9300339	0.1260672
H	-5.1160089	-3.5467639	-0.7576358
H	-3.9692629	-2.4216159	0.0129822
H	-4.8983409	-3.5660709	1.0148822
H	1.6976551	6.4009231	-0.9238798

Zero-point correction= 0.575761 (Hartree/Particle)

Thermal correction to Energy= 0.614030

Thermal correction to Enthalpy= 0.614974

Thermal correction to Gibbs Free Energy= 0.499022

Sum of electronic and zero-point Energies= -1757.946021

Sum of electronic and thermal Energies= -1757.907752

Sum of electronic and thermal Enthalpies= -1757.906808

Sum of electronic and thermal Free Energies= -1758.022760

B-int1

H	-1.4892102	3.6898219	1.4885596
H	-1.9219202	4.1538189	-0.1605854
H	-3.0456572	3.1826759	0.8072996
H	3.1639898	-3.4877021	-2.7920184
H	2.3819878	-2.6221651	-1.4792194
H	1.9448328	-2.2694041	-3.1825634
H	5.7933798	-1.0713411	-1.6204254
H	4.5475388	-1.7215131	-0.5292094

H	5.3692538	-2.7917351	-1.6859444
H	5.3319328	-0.8524321	-4.1042764
H	3.7602968	-1.3693521	-4.7621034
H	4.9248308	-2.5709451	-4.1618654
H	4.0894748	0.5837099	-2.8669894
H	0.5861378	1.1488749	1.7993426
H	1.7823168	3.2022549	2.5950226
H	1.2928018	5.0335249	-1.2867454
H	0.2148558	2.9502269	-2.1365234
H	1.0886308	-1.0314561	-1.5559594
H	3.7681008	0.5573449	0.7528516
H	0.3904628	-1.9661511	0.7260386
H	4.6579518	-0.2025691	3.5393126
H	0.5974668	-3.1452361	3.3276936
H	2.0279378	-3.0810901	5.3562596
H	4.0236848	-1.6334481	5.4589716
C	-1.9884762	3.3416299	0.5749706
C	2.7675218	-2.5095781	-2.4983724
C	4.9630898	-1.7836631	-1.5412094
C	4.5107418	-1.5718881	-3.9896084
C	3.8970818	-1.4937411	-2.5935594
N	3.4417828	-0.0816881	-2.4533864
O	2.4966288	1.8262649	-1.7648684
C	2.4937758	0.5914209	-1.7700724
O	2.1396028	5.2764189	1.2200106
C	0.7630088	1.9980849	1.1413346
C	1.3836988	3.1164279	1.5885416

C	1.5407048	4.2222039	0.7071866
C	1.0925128	4.1913929	-0.6280034
C	0.5326678	3.0404319	-1.1010094
C	0.1482198	1.9338749	-0.2076224
C	-1.4131212	2.0722209	0.0618786
C	-2.0242912	0.9146569	-0.2306954
O	-1.1102212	-1.2537361	-0.8620474
C	-0.9989752	-0.0513271	-0.6771604
N	0.2122208	0.6306449	-0.8264884
C	1.4320298	-0.1606561	-0.9870314
C	3.0342928	-0.1735511	1.0749926
C	1.9648578	-0.6121251	0.3338626
N	1.2367548	-1.5246051	1.0681706
C	3.7736628	-0.8341501	3.4893266
C	2.9775818	-0.8523721	2.3340236
C	1.8357848	-1.6909031	2.2991976
C	1.4743418	-2.5039131	3.3737196
C	2.2789378	-2.4614811	4.4990296
C	3.4163968	-1.6355011	4.5574796
Au	-3.9870362	0.3024339	-0.1082064
C	-7.6206722	-1.9371611	-0.1885524
C	-8.1348402	-0.7554121	0.2255206
H	-8.0937452	-2.8882631	-0.3867934
H	-9.1478262	-0.4639231	0.4632456
C	-5.9135522	-0.4737421	-0.0343564
N	-7.0744882	0.1272879	0.3138286
N	-6.2607032	-1.7455631	-0.3418754

C	-7.2053712	1.5127329	0.7282366
H	-6.2171662	1.9775459	0.6970376
H	-7.8768592	2.0477789	0.0505966
H	-7.5978432	1.5673539	1.7477686
C	-5.3407822	-2.7829441	-0.7816074
H	-5.6095822	-3.1219341	-1.7861204
H	-4.3268252	-2.3737381	-0.8002004
H	-5.3743802	-3.6300041	-0.0905464
H	2.2277818	5.9910469	0.5725126

Zero-point correction= 0.578622 (Hartree/Particle)

Thermal correction to Energy= 0.616235

Thermal correction to Enthalpy= 0.617179

Thermal correction to Gibbs Free Energy= 0.505012

Sum of electronic and zero-point Energies= -1757.963455

Sum of electronic and thermal Energies= -1757.925843

Sum of electronic and thermal Enthalpies= -1757.924899

Sum of electronic and thermal Free Energies= -1758.037066

B-ts2

H	-0.3311323	-2.0415147	3.0173084
H	-0.4726753	-0.4311977	3.7242624
H	-1.8798783	-1.1799867	2.9407204
H	-0.5328293	4.6434013	0.1618984
H	-0.0859423	2.9652523	0.5231484
H	0.6887547	4.3080053	1.4024754
H	1.6504077	3.6155763	-2.7479566
H	0.2302187	2.8039613	-2.0140466
H	0.1873827	4.5251603	-2.3484506

H	2.7096987	5.5979603	-1.4622406
H	2.3632697	5.8011813	0.2736834
H	1.1270287	6.1995833	-0.9261276
H	3.2915367	3.7579353	0.2456494
H	3.6123337	-2.6240077	4.1481194
H	1.2254767	-2.0743977	0.2971324
H	2.6830687	-3.0588547	2.0624704
H	2.8325207	0.7493023	4.0759424
H	1.3774087	1.7825163	2.3244044
H	1.4949057	1.3346353	-1.8256136
H	4.0905937	-0.7503437	0.2919994
H	1.2820807	-0.8665717	-2.8073516
H	4.8219797	-3.7144127	0.1032704
H	1.6524007	-3.5199847	-3.7835986
H	2.8678717	-5.6167037	-3.2267146
H	4.4268537	-5.7102887	-1.3211186
C	-0.7943133	-1.0554107	2.8812514
C	0.3036217	3.9855923	0.4265894
C	0.8419227	3.7127713	-2.0128396
C	1.9360887	5.5000993	-0.6918176
C	1.3958517	4.0723773	-0.6374686
N	2.5667637	3.2433433	-0.2456526
O	3.9735647	1.5522783	0.2013454
C	2.9171367	1.9325383	-0.2865356
O	3.4064627	-1.6838587	4.2415934
C	1.7348147	-1.4200907	1.0072994
C	2.3829837	-2.0128397	2.1112184

C	2.7456207	-1.2277177	3.1842194
C	2.4263187	0.1791723	3.2455454
C	1.6498077	0.7287543	2.2984634
C	1.0408767	-0.0890537	1.2130154
C	-0.4463183	-0.4503957	1.5701204
C	-1.2643263	-0.1692197	0.5380954
O	-0.7116223	0.5992033	-1.7172016
C	-0.4342423	0.3875903	-0.5473666
N	0.8399557	0.6460843	-0.0183526
C	1.9531997	0.9253213	-0.9188406
C	3.3812737	-1.1847907	-0.4001876
C	2.5640187	-0.3956517	-1.2265776
N	2.0414677	-1.1667877	-2.2054816
C	4.1219297	-3.6717777	-0.7285656
C	3.4408727	-2.4898607	-1.0248226
C	2.5629237	-2.4597947	-2.1261526
C	2.3318377	-3.5642907	-2.9364316
C	3.0162777	-4.7295407	-2.6170586
C	3.9010607	-4.7827017	-1.5310446
Au	-3.2881143	-0.4290807	0.2682514
C	-7.3128673	-0.6261507	-1.1661276
C	-7.5300953	-1.0652787	0.0956754
H	-7.9919043	-0.4711957	-1.9923136
H	-8.4372133	-1.3718197	0.5964954
C	-5.3235483	-0.6459007	-0.1048946
N	-6.3012083	-1.0707077	0.7288424
N	-5.9576733	-0.3748977	-1.2698456

C	-6.1035443	-1.4747367	2.1095434
H	-5.0377223	-1.4071687	2.3405694
H	-6.6601733	-0.8144217	2.7808494
H	-6.4390953	-2.5059147	2.2525914
C	-5.3151033	0.1188393	-2.4769056
H	-5.7233243	1.0969263	-2.7471196
H	-4.2422753	0.2162193	-2.2902436
H	-5.4753013	-0.5822627	-3.3009896

Zero-point correction= 0.578740 (Hartree/Particle)

Thermal correction to Energy= 0.615499

Thermal correction to Enthalpy= 0.616443

Thermal correction to Gibbs Free Energy= 0.506455

Sum of electronic and zero-point Energies= -1757.949440

Sum of electronic and thermal Energies= -1757.912681

Sum of electronic and thermal Enthalpies= -1757.911736

Sum of electronic and thermal Free Energies= -1758.021724

B-int2

H	-0.5112259	-2.5976267	2.3890553
H	-0.5344359	-1.1566927	3.4008263
H	-2.0102519	-1.6564427	2.5378873
H	-0.9590359	4.2383593	1.0765343
H	-0.3582949	2.5751923	0.9900153
H	0.3627621	3.7300443	2.1412403
H	1.1115931	4.2259493	-2.0790887
H	-0.0970599	3.0157853	-1.5453827
H	-0.4480459	4.7307763	-1.4128887
H	2.0470171	5.8945473	-0.3930727

H	1.7986401	5.6262393	1.3529343
H	0.4535211	6.1637733	0.3375063
H	3.0035101	3.8428933	0.5639803
H	3.0370121	-3.2251277	3.9713733
H	1.2012111	-2.1307167	-0.0750937
H	2.3981081	-3.3957087	1.6902573
H	2.5769911	0.2076063	4.0340933
H	1.2572811	1.4549663	2.3384933
H	1.2903601	1.4682293	-1.8460767
H	3.7088371	-0.4829347	0.5691863
H	2.6441041	-0.1430707	-3.2655797
H	4.6048871	-3.4735807	0.4996163
H	3.9757211	-2.3646937	-4.3494827
H	5.1964451	-4.4271077	-3.6575007
H	5.5049161	-4.9625927	-1.2738127
C	-0.9204339	-1.5816097	2.4658983
C	-0.0566629	3.6183963	1.1333253
C	0.3536121	3.9889033	-1.3219387
C	1.3414931	5.5240163	0.3602433
C	0.9469361	4.0759353	0.0797223
N	2.2239761	3.3115453	0.1869003
O	3.8824091	1.8562623	-0.2888047
C	2.6857201	2.1461623	-0.3074257
O	2.8950081	-2.2813437	4.1129033
C	1.7835921	-1.5192257	0.6313033
C	2.2141451	-2.3296637	1.8133753
C	2.4460391	-1.7024567	2.9840913

C	2.1973011	-0.2704627	3.1345213
C	1.4891301	0.3990263	2.2163813
C	0.8953991	-0.3110557	1.0291103
C	-0.5575039	-0.7556647	1.2845103
C	-1.3938749	-0.3406197	0.3086003
O	-0.8907369	0.8772443	-1.7534137
C	-0.5945279	0.4196893	-0.6622617
N	0.6971041	0.5734663	-0.1169577
C	1.7658061	1.0910293	-0.9262467
C	3.0701181	-1.0171107	-0.1464627
C	2.6399901	-0.0833637	-1.2127207
N	2.9048011	-0.5849027	-2.3886547
C	4.4499971	-3.2370637	-0.5498847
C	3.7603121	-2.0949607	-0.9255167
C	3.6138491	-1.8149737	-2.2856157
C	4.1052231	-2.6146047	-3.2999227
C	4.7864721	-3.7629087	-2.9021297
C	4.9580081	-4.0655547	-1.5509677
Au	-3.4061449	-0.6239137	-0.0074167
C	-7.4378719	-0.7273027	-1.4430137
C	-7.6283039	-1.3727637	-0.2687197
H	-8.1294869	-0.4637757	-2.2303657
H	-8.5199169	-1.7875727	0.1792063
C	-5.4381969	-0.8488717	-0.4060027
N	-6.3938519	-1.4373537	0.3507953
N	-6.0929039	-0.4148637	-1.5089757
C	-6.1679189	-2.0544717	1.6454963

H	-5.1060569	-1.9680637	1.8885843
H	-6.7561659	-1.5461467	2.4150213
H	-6.4461619	-3.1119197	1.6141853
C	-5.4771839	0.2878673	-2.6224237
H	-5.9384599	1.2718373	-2.7468407
H	-4.4116609	0.4139843	-2.4123437
H	-5.5969819	-0.2888637	-3.5441697

Zero-point correction= 0.580414 (Hartree/Particle)

Thermal correction to Energy= 0.617197

Thermal correction to Enthalpy= 0.618142

Thermal correction to Gibbs Free Energy= 0.508555

Sum of electronic and zero-point Energies= -1757.963108

Sum of electronic and thermal Energies= -1757.926325

Sum of electronic and thermal Enthalpies= -1757.925381

Sum of electronic and thermal Free Energies= -1758.034967

B-ts3

H	-2.0757231	-1.4505159	2.9660086
H	-0.3887301	-1.9556049	3.2135116
H	-0.9124591	-0.3650019	3.7512666
H	-0.4999941	4.6311551	-0.1447434
H	-0.1963111	2.9395821	0.2892726
H	0.6432869	4.2507641	1.1585586
H	1.7119799	3.2993291	-2.9117524
H	0.2073389	2.6291691	-2.1925814
H	0.3024029	4.3268641	-2.6246394
H	2.8546939	5.2803651	-1.6801924
H	2.4532239	5.5930281	0.0281326

H	1.2966249	6.0101531	-1.2424904
H	3.2571749	3.4906181	0.1131786
H	4.8002469	-1.0585389	3.6518376
H	1.0117209	-2.3240949	1.4900306
H	3.4394859	-2.3368139	2.2484756
H	2.5614339	1.5706101	3.7926406
H	0.5497109	1.7487421	2.3629056
H	1.2619519	1.0366991	-1.8350744
H	3.3746609	-1.1061569	0.7370776
H	3.1811119	-0.5776109	-2.9918914
H	2.8188039	-4.4267969	0.7795046
H	4.3360289	-3.0246469	-3.7950554
H	4.7298569	-5.3358549	-2.9668494
H	3.9730469	-6.0236689	-0.7253544
C	-1.0369821	-1.1072249	2.9504996
C	0.2725169	3.9237291	0.1789156
C	0.8834829	3.4912031	-2.2183394
C	2.0462409	5.2719961	-0.9397454
C	1.4068109	3.8888101	-0.8412404
N	2.5049939	3.0033871	-0.3648124
O	3.7667339	1.2180311	0.1716536
C	2.7434979	1.6747711	-0.3314544
O	4.2410429	-0.2763489	3.7556036
C	1.6389369	-1.4511229	1.2661446
C	2.8969329	-1.3957589	2.1323776
C	3.1556999	-0.3566649	2.9978506
C	2.2816689	0.7866221	3.0945036

C	1.1964039	0.8720551	2.3162906
C	0.7468169	-0.1584229	1.3169656
C	-0.7055491	-0.5295319	1.6207936
C	-1.5341251	-0.2396199	0.5990866
O	-1.0198901	0.6954031	-1.6021064
C	-0.7105411	0.3547231	-0.4739904
N	0.5994289	0.5041901	0.0219366
C	1.7035099	0.6885951	-0.8928934
C	2.3614539	-1.6093429	-0.0602054
C	2.3469449	-0.6400799	-1.0776914
N	2.9756719	-1.1144919	-2.1593264
C	3.1547389	-4.1106459	-0.2065234
C	2.9313289	-2.8129569	-0.6601304
C	3.3541289	-2.4480919	-1.9510554
C	4.0103199	-3.3257229	-2.8027794
C	4.2254539	-4.6141459	-2.3304664
C	3.7988209	-5.0028539	-1.0544344
Au	-3.5493821	-0.4960979	0.2895746
C	-7.5028641	-0.6157709	-1.3309354
C	-7.7865021	-1.1085559	-0.1026924
H	-8.1379491	-0.4207909	-2.1832014
H	-8.7192791	-1.4314759	0.3369606
C	-5.5704231	-0.6927569	-0.1703904
N	-6.5915761	-1.1480889	0.5921396
N	-6.1433491	-0.3674829	-1.3535834
C	-6.4632371	-1.6165379	1.9601576
H	-5.4130811	-1.5427369	2.2524756

H	-7.0683311	-0.9990669	2.6304106
H	-6.7865091	-2.6588959	2.0350766
C	-5.4368501	0.1716541	-2.5045454
H	-5.8426351	1.1527001	-2.7678154
H	-4.3777901	0.2764151	-2.2527114
H	-5.5383041	-0.5047769	-3.3581234

Zero-point correction= 0.574830 (Hartree/Particle)

Thermal correction to Energy= 0.611635

Thermal correction to Enthalpy= 0.612580

Thermal correction to Gibbs Free Energy= 0.502338

Sum of electronic and zero-point Energies= -1757.916204

Sum of electronic and thermal Energies= -1757.879399

Sum of electronic and thermal Enthalpies= -1757.878454

Sum of electronic and thermal Free Energies= -1757.988696

B-int3

H	-1.2847439	-3.8709997	0.1364262
H	-1.1145339	-3.5495387	1.8709532
H	-2.6556179	-3.2361537	1.0507042
H	0.2872521	5.1380823	-0.1080398
H	-0.0701209	3.4030753	-0.0292978
H	0.0308851	4.3535493	1.4605952
H	3.7163111	3.7265953	-0.6826198
H	2.2153981	3.0797433	-1.4177488
H	2.4878901	4.8131853	-1.3389708
H	3.6915701	4.9955333	1.4495462
H	2.1612561	5.2650423	2.3256282
H	2.4541361	6.0760753	0.7814602

H	2.6120341	2.9884203	2.3475912
H	0.6582381	-2.4404707	-1.1557558
H	0.8949871	-4.1742327	0.4431742
H	1.8356911	-2.2001287	3.6960552
H	0.1479651	-0.6647737	2.7220822
H	0.9914471	1.6863633	-0.6557308
H	3.8877821	1.5541543	-0.9756268
H	3.6344571	-3.7795347	-1.8002988
H	6.2030921	0.5062213	-2.1623998
H	7.1590141	-1.6376137	-2.9768028
H	5.8732181	-3.7394047	-2.7987558
C	-1.5681989	-3.1771027	0.9420912
C	0.4682411	4.2204573	0.4642312
C	2.6331231	3.8756433	-0.7907178
C	2.6108561	5.1432673	1.3324432
C	1.9700001	3.9803723	0.5800402
N	2.2530431	2.7807473	1.4201732
O	1.9350321	0.7521753	2.3351202
C	1.8284571	1.5009103	1.3630652
O	2.9788201	-4.1273227	2.2643752
C	1.2429511	-2.1416997	-0.2715568
C	1.7092751	-3.4331407	0.4209162
C	2.1221731	-3.2385057	1.8290902
C	1.5735871	-2.2574777	2.6412592
C	0.6986691	-1.3506137	2.0851372
C	0.2993241	-1.3360817	0.6504292
C	-1.1730269	-1.7768147	0.6233102

C	-1.9783269	-0.7580717	0.2567382
O	-1.4400789	1.5497883	-0.3525778
C	-1.1253479	0.4287163	0.0047242
N	0.1930561	0.0435763	0.2371892
C	1.3264541	0.9042893	0.0369432
C	2.4006831	-1.2847627	-0.6938528
C	2.4272081	0.0753683	-0.5396978
N	3.6219251	0.5808743	-0.9875608
C	4.1892851	-2.8434647	-1.8300588
C	3.6387431	-1.6507037	-1.3332918
C	4.3844721	-0.4561057	-1.4835098
C	5.6512301	-0.4256007	-2.0629368
C	6.1742261	-1.6236677	-2.5173798
C	5.4453211	-2.8191157	-2.4097998
Au	-4.0004989	-0.5973717	-0.0689358
C	-7.9176529	0.8105893	-1.0259268
C	-8.2523819	-0.4558037	-0.6842428
H	-8.5230739	1.6403723	-1.3615048
H	-9.2090559	-0.9576497	-0.6603608
C	-6.0192149	-0.2566727	-0.4433208
N	-7.0772269	-1.0926867	-0.3307718
N	-6.5482119	0.9135363	-0.8721058
C	-7.0026599	-2.4762977	0.1021082
H	-5.9575599	-2.7159127	0.3118042
H	-7.5955009	-2.6214717	1.0098862
H	-7.3739189	-3.1394177	-0.6846538
C	-5.7908899	2.1257363	-1.1426558

H	-6.1447199	2.9388233	-0.5023748
H	-4.7337049	1.9384593	-0.9345218
H	-5.9049899	2.4125763	-2.1919338
H	2.5366111	-3.9080857	-0.1145708
H	3.2058661	-3.9878467	3.1975772

Zero-point correction= 0.581257 (Hartree/Particle)

Thermal correction to Energy= 0.618164

Thermal correction to Enthalpy= 0.619109

Thermal correction to Gibbs Free Energy= 0.508288

Sum of electronic and zero-point Energies= -1757.979505

Sum of electronic and thermal Energies= -1757.942597

Sum of electronic and thermal Enthalpies= -1757.941653

Sum of electronic and thermal Free Energies= -1758.052474

B-ts4

H	-1.0471707	-3.6662399	1.1780730
H	-1.6043007	-2.8852179	2.6623730
H	-2.6740737	-2.9696159	1.2614670
H	1.1543453	5.1868321	0.3142390
H	0.5388103	3.5315991	0.3848910
H	1.0394513	4.3563921	1.8755520
H	4.1096243	3.1734321	-0.9121680
H	2.3880733	3.0227941	-1.3965400
H	3.1318553	4.6069741	-1.2768100
H	4.7082403	4.4294071	1.2149690
H	3.4282783	4.8614011	2.3800840
H	3.5565103	5.7252831	0.8426110
H	3.4842053	2.5501991	2.2468400

H	0.6507343	-2.8742549	-0.1023760
H	2.6242293	-3.8143829	0.7908760
H	1.6242753	-1.7473649	4.2861980
H	0.1480463	-0.0674479	3.0365300
H	1.1298023	1.7740191	-0.4520140
H	3.3745953	1.1962281	-2.0549490
H	2.7047373	-4.1444429	-1.6543840
H	4.9722013	-0.2560979	-3.8711620
H	5.4264013	-2.5862879	-4.5936000
H	4.3113633	-4.4958849	-3.4983800
C	-1.6334777	-2.8213549	1.5649640
C	1.2779173	4.2192241	0.8146060
C	3.1085173	3.6125801	-0.8174020
C	3.6621583	4.7435941	1.3147470
C	2.7195303	3.7426451	0.6531320
N	2.9365043	2.4676321	1.3951470
O	2.4596653	0.4352171	2.2303490
C	2.3205503	1.2769701	1.3307010
O	1.1330393	-4.1595609	3.0156690
C	1.2871653	-2.1056339	0.3591310
C	2.3129563	-2.8881499	1.2800950
C	1.6342053	-3.1069259	2.5515180
C	1.1291463	-1.9776479	3.3403480
C	0.5897663	-0.9485569	2.5740180
C	0.3345793	-1.1047269	1.1196110
C	-1.1611787	-1.5052429	1.0555700
C	-1.8976917	-0.5217019	0.4963980

O	-1.2259437	1.6555911	-0.3997280
C	-0.9841407	0.5919311	0.1400680
N	0.2963333	0.2166311	0.5442130
C	1.4829983	0.9000881	0.1059070
C	2.0848873	-1.4089229	-0.6900620
C	2.2417863	-0.0529619	-0.7609210
N	3.1531793	0.2647431	-1.7379420
C	3.2012943	-3.2929249	-2.1180830
C	2.9333133	-1.9843189	-1.6937520
C	3.5842373	-0.9054749	-2.3367040
C	4.4833093	-1.0962739	-3.3836800
C	4.7298013	-2.4001389	-3.7804070
C	4.0957553	-3.4873249	-3.1556390
Au	-3.8837957	-0.3530089	-0.0025050
C	-7.6660057	0.9877171	-1.4621030
C	-8.0736517	-0.1925579	-0.9393040
H	-8.2137847	1.7660251	-1.9738270
H	-9.0494237	-0.6552029	-0.9009290
C	-5.8556037	-0.0200329	-0.5747170
N	-6.9514887	-0.7942639	-0.4009070
N	-6.3067587	1.0757581	-1.2292710
C	-6.9628437	-2.0867789	0.2603890
H	-5.9452227	-2.3181329	0.5835510
H	-7.6211277	-2.0592899	1.1335570
H	-7.3068887	-2.8619249	-0.4304230
C	-5.4848337	2.2021881	-1.6438730
H	-5.8529477	3.1232431	-1.1831050

H	-4.4538967	2.0274091	-1.3236340
H	-5.5103047	2.3043031	-2.7325410
H	3.1766463	-2.2331799	1.4450800
H	0.4915363	-3.1785979	3.7003710

Zero-point correction= 0.574096 (Hartree/Particle)

Thermal correction to Energy= 0.610050

Thermal correction to Enthalpy= 0.610995

Thermal correction to Gibbs Free Energy= 0.503672

Sum of electronic and zero-point Energies= -1757.891186

Sum of electronic and thermal Energies= -1757.855232

Sum of electronic and thermal Enthalpies= -1757.854287

Sum of electronic and thermal Free Energies= -1757.961610

B-int4

H	-0.9416728	-2.8621608	-2.1758529
H	-0.7529618	-4.0528338	-0.8823089
H	-2.2932108	-3.2136608	-1.0893319
H	1.7202272	-1.3515708	-1.8217849
H	1.3083092	-3.7074118	-1.5648269
H	-0.0427968	-4.4387438	1.0130321
H	-0.1757048	-1.7893028	2.0077831
H	4.0177202	1.3211562	1.8114641
H	4.9028762	-2.8760908	-1.4968309
H	6.7483282	0.5860302	1.6192601
H	8.2446502	-0.9979938	0.4202591
H	7.3106582	-2.6970418	-1.1107549
C	-1.2059878	-3.0910438	-1.1369419
O	2.7831112	-4.7348068	0.8526561

C	1.8501572	-1.7470668	-0.8013259
C	2.0574102	-3.2641998	-0.8940909
C	1.9599172	-3.9575328	0.4423341
C	0.7024022	-3.6705818	1.2686681
C	0.1760422	-2.2817788	1.1007601
C	0.6077372	-1.4108368	0.0038121
C	-0.8020618	-1.9598368	-0.2347469
C	-1.7072908	-0.9403618	0.1185001
O	-1.3504298	1.2193772	1.1706581
C	-0.9077838	0.2367112	0.6100701
N	0.4218792	-0.0124708	0.3297661
C	1.4678542	0.6733852	1.0816361
C	2.9789112	-1.0435198	-0.0928939
C	2.7642802	0.0166062	0.7534691
N	3.9453382	0.4711022	1.2651101
C	5.2740262	-2.1275588	-0.8011569
C	4.4059252	-1.2524358	-0.1283909
C	4.9726122	-0.2804318	0.7349031
C	6.3449652	-0.1700698	0.9501971
C	7.1687442	-1.0543378	0.2776621
C	6.6368152	-2.0209268	-0.5911969
Au	-3.7264418	-0.7579948	0.1042351
C	-7.7059438	0.6333272	0.6955681
C	-8.0075078	-0.5371638	0.0817751
H	-8.3416658	1.4170092	1.0823231
H	-8.9587628	-0.9804878	-0.1758809
C	-5.7676768	-0.4001998	0.2180321

N	-6.8072288	-1.1555168	-0.2021699
N	-6.3304098	0.6996862	0.7698141
C	-6.6980738	-2.4448028	-0.8650239
H	-5.6403288	-2.6976228	-0.9660949
H	-7.1975738	-3.2157358	-0.2719699
H	-7.1528478	-2.3964978	-1.8581869
C	-5.6061568	1.8130312	1.3692281
H	-5.8853058	1.9150312	2.4213301
H	-4.5314428	1.6239192	1.3012051
H	-5.8417728	2.7389012	0.8377401
H	3.0356722	-3.4978268	-1.3176479
H	0.9444832	-3.8436908	2.3230171
C	1.6057522	2.1805322	0.8004001
O	2.2418882	2.8293302	1.6195891
N	1.0886692	2.6326102	-0.3517109
H	0.5768002	1.9698992	-0.9186829
C	1.0296082	4.0602962	-0.7480759
C	2.4405832	4.6152742	-0.9013829
C	0.3038872	4.0963322	-2.0856209
C	0.2401952	4.8366722	0.3005641
H	2.9835172	4.5674472	0.0465181
H	2.9987932	4.0503012	-1.6571989
H	2.3917512	5.6622232	-1.2230709
H	-0.7163778	3.6998012	-1.9937549
H	0.2289572	5.1288852	-2.4420769
H	0.8437112	3.5175332	-2.8460499
H	0.1228332	5.8797432	-0.0158599

H	-0.7557428	4.3950132	0.4312151
H	0.7553182	4.8232302	1.2655461
H	1.2478422	0.6237502	2.1627911

Zero-point correction= 0.582175 (Hartree/Particle)

Thermal correction to Energy= 0.618435

Thermal correction to Enthalpy= 0.619379

Thermal correction to Gibbs Free Energy= 0.510218

Sum of electronic and zero-point Energies= -1757.982274

Sum of electronic and thermal Energies= -1757.946014

Sum of electronic and thermal Enthalpies= -1757.945070

Sum of electronic and thermal Free Energies= -1758.054231

B-ts5

H	-1.2123357	-3.9020631	0.4248279
H	-1.2683647	-3.4942601	2.1445729
H	-2.6952677	-3.2392371	1.1255399
H	0.3030033	5.0797209	-0.0830621
H	-0.0382727	3.3501839	0.0878379
H	0.2180383	4.3517039	1.5299849
H	3.6496573	3.6193959	-0.9740141
H	2.0752113	2.9523859	-1.5112601
H	2.3603953	4.6850459	-1.5424751
H	3.8561793	4.9969229	1.0842499
H	2.4319913	5.3035899	2.1149499
H	2.5473963	6.0472819	0.5148889
H	2.9450093	3.0230559	2.1572799
H	0.6251293	-2.6685861	-0.8096641
H	1.0068243	-4.0739801	1.1503879

H	1.9986783	-1.8650571	3.9144929
H	0.0083873	-0.7001361	2.9265889
H	0.9812473	1.5972529	-0.5427781
H	3.7826593	1.3899919	-1.2586321
H	3.4080743	-3.9834731	-1.6501791
H	5.9274153	0.2324909	-2.6539031
H	6.7562523	-1.9754981	-3.4321531
H	5.5013003	-4.0432991	-2.9369221
C	-1.6032477	-3.1726841	1.1483179
C	0.5453973	4.1821789	0.4977439
C	2.5620113	3.7724369	-0.9709141
C	2.7684223	5.1390239	1.0840219
C	2.0506753	3.9478509	0.4559409
N	2.4267893	2.7837529	1.3156819
O	2.3968313	0.7927479	2.3183709
C	2.0733883	1.4935999	1.3393059
O	3.5487853	-3.4544601	2.4860789
C	1.2394803	-2.2395001	-0.0024081
C	1.8168273	-3.4076841	0.8144249
C	2.5382953	-2.9595141	2.0574909
C	1.8228933	-1.8746501	2.8368609
C	0.6479873	-1.3433961	2.3167419
C	0.2974843	-1.3762121	0.8760909
C	-1.1837627	-1.7827091	0.8144649
C	-1.9570377	-0.7527441	0.4164629
O	-1.3490427	1.5178799	-0.2470451
C	-1.0783497	0.4121629	0.1769059

N	0.2372593	0.0305309	0.5130689
C	1.3836503	0.8361439	0.1379439
C	2.3296433	-1.4057691	-0.6038891
C	2.3839083	-0.0418221	-0.5366971
N	3.5169713	0.4218279	-1.1604601
C	3.9542223	-3.0605751	-1.8341941
C	3.4784813	-1.8271511	-1.3636911
C	4.2037543	-0.6558741	-1.6846131
C	5.3855833	-0.6814211	-2.4222551
C	5.8377603	-1.9158841	-2.8543491
C	5.1254733	-3.0924261	-2.5688601
Au	-3.9679277	-0.5887191	0.0137879
C	-7.8666517	0.7322599	-1.1243501
C	-8.1953017	-0.5217021	-0.7343061
H	-8.4721797	1.5370359	-1.5159421
H	-9.1458337	-1.0352921	-0.7154281
C	-5.9739527	-0.2802331	-0.4371781
N	-7.0237097	-1.1252521	-0.3170941
N	-6.5039697	0.8615039	-0.9350381
C	-6.9467107	-2.4871391	0.1808689
H	-7.2843377	-3.1896981	-0.5864401
H	-5.9065107	-2.7039841	0.4349999
H	-7.5671287	-2.5985391	1.0747579
C	-5.7547827	2.0702259	-1.2401651
H	-6.1420247	2.9086429	-0.6542491
H	-4.7034297	1.9093259	-0.9862441
H	-5.8353887	2.3026909	-2.3058571

H	2.5048823	-4.0147861	0.2212679
H	2.2158143	-0.7454301	2.4895089

Zero-point correction= 0.574074 (Hartree/Particle)

Thermal correction to Energy= 0.610017

Thermal correction to Enthalpy= 0.610961

Thermal correction to Gibbs Free Energy= 0.502975

Sum of electronic and zero-point Energies= -1757.941827

Sum of electronic and thermal Energies= -1757.905884

Sum of electronic and thermal Enthalpies= -1757.904939

Sum of electronic and thermal Free Energies= -1758.012925

B-int5

H	-1.3484778	-3.8618750	0.1835637
H	-1.1849718	-3.5499780	1.9178157
H	-2.7048548	-3.1687330	1.0778037
H	0.1177222	5.1122360	-0.1707113
H	-0.1866508	3.3717570	0.0142977
H	-0.0556148	4.4131890	1.4467677
H	3.5551512	3.7219760	-0.8112193
H	2.0240642	3.0505350	-1.4633863
H	2.3055062	4.7835880	-1.4642013
H	3.5938132	5.1215680	1.2501317
H	2.0977442	5.3867940	2.1921847
H	2.2988182	6.1455940	0.6111837
H	2.6350672	3.1248270	2.2630397
H	0.6247242	-2.3765000	-1.1209403
H	0.7676722	-4.1363520	0.5853737
H	2.0693372	-2.4542380	3.6590887

H	0.2580082	-0.9264120	2.9201677
H	0.9787962	1.6008680	-0.6036663
H	3.8741772	1.4862430	-1.1096633
H	3.7255282	-3.8837780	-1.5744913
H	6.2306912	0.4185400	-2.1277703
H	7.2069912	-1.7455700	-2.8646883
H	5.9525332	-3.8544150	-2.5785283
C	-1.6140458	-3.1584140	0.9856437
C	0.3415832	4.2315550	0.4416997
C	2.4695302	3.8678460	-0.8864473
C	2.5049122	5.2370820	1.1847317
C	1.8501042	4.0460730	0.4938747
N	2.1875242	2.8698960	1.3828037
O	2.3901362	0.8982630	2.3166807
C	1.9776912	1.5847330	1.2897157
O	3.4029032	-3.9626460	1.9693957
C	1.2331902	-2.1798670	-0.2237733
C	1.6564792	-3.5268880	0.3751677
C	2.3986322	-3.3519160	1.6756347
C	1.7512962	-2.4033550	2.6188157
C	0.7863432	-1.5659240	2.2078127
C	0.3313512	-1.4055460	0.7776407
C	-1.1509768	-1.7764530	0.6821317
C	-1.9241698	-0.7337560	0.3151087
O	-1.2801938	1.5333350	-0.3245833
C	-1.0355738	0.4178330	0.1035627
N	0.2671482	0.0296980	0.4720197

C	1.3825492	0.8525410	0.0933167
C	2.4227382	-1.3495850	-0.6270103
C	2.4589252	0.0112050	-0.5024113
N	3.6680652	0.5137840	-0.9369953
C	4.2502192	-2.9380530	-1.6704913
C	3.6758362	-1.7302270	-1.2383703
C	4.4196692	-0.5395340	-1.4206703
C	5.6865532	-0.5144950	-2.0007103
C	6.2207762	-1.7225950	-2.4087583
C	5.5070072	-2.9211830	-2.2450943
Au	-3.9458988	-0.5761950	-0.0298333
C	-7.9447248	0.5519580	-1.0643713
C	-8.2016468	-0.6921100	-0.5974863
H	-8.6005998	1.3098360	-1.4682593
H	-9.1274048	-1.2425000	-0.5096763
C	-5.9803018	-0.3449560	-0.4122863
N	-6.9879248	-1.2243220	-0.2034503
N	-6.5815228	0.7462240	-0.9425783
C	-6.8312248	-2.5539690	0.3586457
H	-5.7728898	-2.7134730	0.5788507
H	-7.4093418	-2.6446010	1.2828277
H	-7.1684008	-3.3092940	-0.3571143
C	-5.8974268	1.9645390	-1.3422213
H	-6.3009248	2.8192660	-0.7916713
H	-4.8330768	1.8597410	-1.1155973
H	-6.0219868	2.1318740	-2.4160323
H	2.2781642	-4.1038410	-0.3111373

H	2.2551552	-0.0714510	2.2087977

Zero-point correction= 0.580529 (Hartree/Particle)

Thermal correction to Energy= 0.617617

Thermal correction to Enthalpy= 0.618562

Thermal correction to Gibbs Free Energy= 0.506500

Sum of electronic and zero-point Energies= -1757.976959

Sum of electronic and thermal Energies= -1757.939871

Sum of electronic and thermal Enthalpies= -1757.938927

Sum of electronic and thermal Free Energies= -1758.050988

B-ts6

H	-1.5836003	-3.8265859	-0.8194580
H	-0.5131193	-3.9870209	0.5894640
H	-2.1865743	-3.3622799	0.7632410
H	0.5287017	5.1938821	-1.1066730
H	0.1992887	3.4668101	-1.3501950
H	-0.7271553	4.3781761	-0.1545880
H	3.4380897	3.6608551	0.6951090
H	2.7874177	3.0839851	-0.8798140
H	2.9683187	4.8016631	-0.5634730
H	2.0056167	4.8554051	2.3413980
H	0.2978807	5.2045021	1.9636560
H	1.5850977	6.0172311	1.0682950
H	0.3005007	2.9470151	2.0403510
H	1.4467907	-2.0537429	-2.1809740
H	1.2035527	-4.1739449	-0.9811600
H	1.9769347	-2.8156909	2.6827710
H	0.5608697	-1.0032959	1.9275980

H	1.2595697	1.6391801	-1.2392760
H	3.8948697	1.7218331	0.3601950
H	4.7837467	-3.3070269	-1.3979300
H	6.5764237	1.0008091	0.4291020
H	8.0815827	-0.9125179	-0.0719500
H	7.1737207	-3.0268489	-0.9724560
C	-1.2882733	-3.3654379	0.1352060
C	0.2687357	4.2594741	-0.5964530
C	2.7019827	3.8464201	-0.0983500
C	1.2975237	5.0685621	1.5322540
C	1.3037397	3.9612231	0.4845040
N	0.8799267	2.7247411	1.2326140
O	-0.3254293	0.8623791	1.4096790
C	0.5832247	1.5000631	0.7969110
O	3.0639057	-4.5981419	1.1552370
C	1.7361147	-2.0959789	-1.1218480
C	2.0668237	-3.5338479	-0.7443300
C	2.3713057	-3.6992599	0.7265900
C	1.7477497	-2.7030559	1.6249440
C	0.9833837	-1.6874839	1.1996140
C	0.5766977	-1.5269769	-0.2812730
C	-0.8624823	-1.9820789	-0.1472480
C	-1.7173883	-0.8798419	-0.1771250
O	-1.3657383	1.1963421	-1.4168270
C	-0.9611433	0.1537861	-0.9495690
N	0.3792047	-0.1868759	-0.8436170
C	1.2621367	0.8673161	-0.4541240

C	2.8472247	-1.0936639	-0.8227570
C	2.6094077	0.1971761	-0.3831670
N	3.7917897	0.7949311	-0.0198330
C	5.1442037	-2.3645559	-0.9962040
C	4.2664317	-1.2999389	-0.7175530
C	4.8204497	-0.1005779	-0.2069400
C	6.1836417	0.0659991	0.0357480
C	7.0127437	-1.0027309	-0.2466450
C	6.4952217	-2.2053029	-0.7592730
Au	-3.7864023	-0.7628959	-0.0662750
C	-7.8864783	0.2917521	-0.5971240
C	-8.0648733	-0.7473679	0.2519250
H	-8.5978863	0.9490061	-1.0762930
H	-8.9632023	-1.1816659	0.6667220
C	-5.8487863	-0.5215419	-0.0855880
N	-6.8059443	-1.2320749	0.5534200
N	-6.5239783	0.4153391	-0.7913550
C	-6.5625963	-2.3557479	1.4410460
H	-7.0339603	-3.2595089	1.0444700
H	-5.4840943	-2.5134969	1.5131400
H	-6.9623803	-2.1436589	2.4366870
C	-5.9169853	1.4157611	-1.6557420
H	-6.2342283	2.4157571	-1.3472110
H	-4.8289623	1.3429741	-1.5749760
H	-6.2117143	1.2449431	-2.6950400
H	2.8981137	-3.9424549	-1.3243930
H	-1.1172783	-0.0901749	0.8131880

Zero-point correction= 0.573872 (Hartree/Particle)

Thermal correction to Energy= 0.610320

Thermal correction to Enthalpy= 0.611265

Thermal correction to Gibbs Free Energy= 0.501932

Sum of electronic and zero-point Energies= -1757.904445

Sum of electronic and thermal Energies= -1757.867997

Sum of electronic and thermal Enthalpies= -1757.867052

Sum of electronic and thermal Free Energies= -1757.976385

B-2

H	-0.2905108	3.5398815	3.0484390
H	-0.3702998	2.0345895	3.9693570
H	1.1911202	2.8517975	3.7290800
H	-1.3422818	-5.7104695	-0.6125870
H	-1.0733028	-4.5976535	-1.9689290
H	-0.0939668	-4.4500365	-0.4890980
H	-4.2776998	-3.3836445	-0.4609310
H	-3.5077368	-3.9779385	-1.9571460
H	-3.7922468	-5.0798635	-0.5992220
H	-2.9340058	-3.1603655	1.6445290
H	-1.1965898	-3.5716965	1.6628100
H	-2.4183098	-4.8553575	1.5377030
H	-2.6120378	-1.7888945	-1.0431950
H	-1.3342318	3.0674115	0.5159820
H	-2.3936228	2.8638955	2.7049050
H	-2.7635248	-0.9297825	3.1576780
H	-0.4709148	-0.8092435	2.2395990
H	0.0461442	-0.2467895	-1.7736480

H	-2.4223538	-0.3804435	-3.0702620
H	-4.4573538	3.6941935	-0.2010010
H	-4.8612738	0.5608925	-4.0901130
H	-6.5072158	2.3888405	-3.7368620
H	-6.2926728	3.9255395	-1.8151560
C	0.2393442	2.6001805	3.2540210
C	-1.0913858	-4.6762175	-0.8754010
C	-3.5081128	-4.0557315	-0.8627090
C	-2.1694558	-3.8318275	1.2337890
C	-2.1354378	-3.7341675	-0.2880400
N	-1.8353898	-2.3379545	-0.6920650
O	0.2644662	-2.1457065	0.2006900
C	-0.6997128	-1.6813635	-0.3886030
O	-4.5638048	0.9090765	2.7427930
C	-1.7985738	2.0960705	0.7571120
C	-2.8397978	2.3187115	1.8610590
C	-3.4033638	1.0296375	2.4124180
C	-2.4248338	-0.0642715	2.5911710
C	-1.1882568	-0.0010305	2.0897570
C	-0.6724478	1.1486005	1.2505550
C	0.4539252	1.8296015	2.0063610
C	1.6200552	1.5894685	1.3830660
O	2.1773282	0.4067875	-0.6967140
C	1.3710402	0.8063465	0.1778550
N	0.0502112	0.5934385	0.0996430
C	-0.6190768	-0.2129475	-0.8963690
C	-2.4183808	1.5337115	-0.4937690

C	-1.8909608	0.4938475	-1.2076340
N	-2.7003908	0.1911905	-2.2855040
C	-4.5384938	2.9903955	-1.0259160
C	-3.6034678	1.9584865	-1.1971080
C	-3.7431008	1.1038745	-2.3152540
C	-4.7769018	1.2328585	-3.2391240
C	-5.6878898	2.2555885	-3.0354110
C	-5.5664168	3.1270835	-1.9416880
Au	4.2824942	0.4283385	-0.5270930
C	8.3926812	-0.2731475	0.0119660
C	8.4605632	0.9109075	-0.6407040
H	9.1683972	-0.9199815	0.3959120
H	9.3076372	1.5092495	-0.9439690
C	6.2900952	0.3825445	-0.4205800
N	7.1602622	1.2996325	-0.8981700
N	7.0526042	-0.5827385	0.1389930
C	6.8100602	2.5239695	-1.6019940
H	7.1814912	2.4852715	-2.6295990
H	5.7228452	2.6247465	-1.6167980
H	7.2443862	3.3850465	-1.0871940
C	6.5631602	-1.7923645	0.7838350
H	6.9189732	-2.6736125	0.2434700
H	6.9139372	-1.8300385	1.8185840
H	5.4712162	-1.7830165	0.7743170
H	-3.6765978	2.9251625	1.5066400
H	2.6099682	1.9214285	1.6814720

Zero-point correction= 0.580634 (Hartree/Particle)

Thermal correction to Energy= 0.617694

Thermal correction to Enthalpy= 0.618638

Thermal correction to Gibbs Free Energy= 0.507188

Sum of electronic and zero-point Energies= -1758.025126

Sum of electronic and thermal Energies= -1757.988066

Sum of electronic and thermal Enthalpies= -1757.987122

Sum of electronic and thermal Free Energies= -1758.098572

C-1

Au	1.7455956	-2.8504939	-0.8447307
C	4.8444506	-0.3478949	0.5410243
C	4.5974906	-1.0563719	1.6708983
H	5.4358046	0.5376811	0.3568683
H	4.9881996	-0.9547759	2.6728223
C	3.3146036	-1.9066059	0.0466033
N	3.6521666	-2.0111309	1.3489443
N	4.0518866	-0.8905699	-0.4484417
C	3.0031736	-2.9051449	2.2964273
H	1.9283786	-2.6890739	2.3282973
H	3.1631886	-3.9466419	2.0028443
H	3.4406636	-2.7430099	3.2839513
C	4.0679836	-0.4234619	-1.8342297
H	4.9156066	-0.8711159	-2.3609247
H	3.1401036	-0.7249249	-2.3286337
H	4.1569716	0.6688581	-1.8503607
C	-7.3026924	0.9979401	0.1873253
C	-7.3031504	0.6858441	-1.1833747
C	-6.1860834	0.1472021	-1.7997887

C	-5.0618554	-0.0733299	-1.0049017
C	-5.0348664	0.2412221	0.3736693
C	-6.1821824	0.7819241	0.9694373
N	-3.8288364	-0.5952459	-1.3308607
C	-3.0162524	-0.5809349	-0.2124837
C	-3.7260284	-0.0897029	0.8516013
C	-1.6452704	-1.1703949	-0.3066077
N	-0.9868724	-0.7414359	-1.5597167
C	-0.3993904	-1.6310099	-2.4249977
C	-0.5371094	0.6267941	-1.6542287
O	0.0935596	-1.3411269	-3.4952217
C	-0.2606424	-3.0325479	-1.9502547
C	-0.0378134	-4.2276989	-1.7654637
C	-1.3699684	1.6968201	-1.9700167
C	-0.8611544	2.9912521	-1.9590157
C	0.4837776	3.2306911	-1.6409367
C	1.3087876	2.1489201	-1.2980507
C	0.7927736	0.8717891	-1.3162297
O	0.9355196	4.4838751	-1.6581047
H	-1.7278234	-2.2654449	-0.3585157
C	-0.7368264	-0.9214149	0.9138743
O	-0.0567324	-1.8502019	1.3537883
N	-0.7273184	0.3347931	1.3851703
C	0.1163736	0.8626481	2.4814693
C	1.5974226	0.7203131	2.1440933
C	-0.2449544	2.3367141	2.6030533
C	-0.2208164	0.1237051	3.7723853

C	0.0682486	-5.6679859	-1.5981137
H	-8.1995974	1.4182011	0.6358843
H	-8.1988044	0.8707511	-1.7715967
H	-6.1862854	-0.0951739	-2.8602197
H	-6.1875184	1.0290701	2.0289433
H	-3.5025344	-0.8010509	-2.2633007
H	-3.3608824	0.0100491	1.8666423
H	-2.4145804	1.5264031	-2.2228657
H	-1.4905384	3.8404621	-2.2115167
H	2.3360226	2.3149691	-0.9900947
H	1.4246806	0.0339921	-1.0191097
H	1.9002546	4.4879201	-1.4659207
H	-1.2876914	1.0116441	0.8780393
H	1.8713836	1.3198141	1.2676533
H	2.2021066	1.0708281	2.9897853
H	1.8495086	-0.3262389	1.9465903
H	0.3504606	2.8069351	3.3927383
H	-1.3067254	2.4636311	2.8532353
H	-0.0360024	2.8657061	1.6633333
H	0.3515536	0.5494641	4.6052853
H	0.0200256	-0.9409729	3.6884253
H	-1.2886674	0.2221961	4.0056563
H	-0.8008734	-6.1543419	-2.0543407
H	0.1005186	-5.9427419	-0.5389247
H	0.9694256	-6.0524509	-2.0867657
B	4.5318756	3.3120391	-1.1688987
F	5.7812496	3.8375261	-1.0127637

F	4.2909466	2.3110121	-0.1818057
F	4.3539226	2.7158611	-2.4138457
F	3.5386736	4.3151981	-0.9905847

Zero-point correction= 0.593289 (Hartree/Particle)

Thermal correction to Energy= 0.637698

Thermal correction to Enthalpy= 0.638642

Thermal correction to Gibbs Free Energy= 0.513427

Sum of electronic and zero-point Energies= -2182.458719

Sum of electronic and thermal Energies= -2182.414311

Sum of electronic and thermal Enthalpies= -2182.413366

Sum of electronic and thermal Free Energies= -2182.538582

C-ts1

H	2.2244691	-1.4054953	-4.1172109
H	3.5660991	-0.2610823	-4.1251789
H	3.5743091	-1.6483753	-3.0212379
H	-2.8800649	4.9927767	0.4457271
H	-1.7588289	3.6898927	0.0892241
H	-2.2985169	4.7357087	-1.1946099
H	-5.1551589	1.9892817	0.5206381
H	-3.5819429	2.1358887	1.2713371
H	-4.7192789	3.4514807	1.3940921
H	-5.8339769	3.5646537	-1.3743709
H	-4.6440599	4.6485207	-2.0929769
H	-5.2508299	4.9569167	-0.4790069
H	-3.9208389	2.5012847	-2.5054989
H	1.8559461	-5.2609833	-1.3678329
H	0.6052201	-1.4245083	0.8761931

H	1.3678341	-3.7191203	0.4806861
H	-0.4788379	-3.6816603	-3.3602939
H	-1.2570669	-1.3401533	-2.9565399
H	-1.7337249	1.5463547	0.2254071
H	-4.1868889	-1.0553823	-1.2046399
H	-1.8240169	-0.1992593	2.1502781
H	-5.9063409	-3.0779563	0.2050621
H	-3.0110929	-1.8990203	4.0901941
H	-4.8014009	-3.5813423	4.3104081
H	-6.2318839	-4.1638583	2.3957941
C	2.9595131	-0.9025353	-3.5009999
C	-2.6115319	4.2371347	-0.2851529
C	-4.3469819	2.6765387	0.7335241
C	-4.9617799	4.1752797	-1.1697979
C	-3.8254759	3.3257757	-0.5635399
N	-3.5042319	2.3182807	-1.6163399
O	-2.4591209	0.7111657	-2.7866249
C	-2.6435619	1.2722137	-1.6978619
O	1.0143621	-5.0725223	-1.7853749
C	0.3582361	-1.9125453	-0.0462619
C	0.7882361	-3.2137653	-0.2617479
C	0.5227321	-3.8252293	-1.4862559
C	-0.2537829	-3.1726933	-2.4451329
C	-0.6863879	-1.8680593	-2.2208259
C	-0.3397029	-1.2243863	-1.0344539
C	2.2366131	-0.1230393	-2.4861619
C	1.6077941	0.5058167	-1.6533639

O	0.2766951	2.2957287	-0.8609679
C	0.3837851	1.0845757	-1.0800289
N	-0.6018119	0.1837197	-0.8302639
C	-1.9226589	0.7300967	-0.4502689
C	-3.8059439	-1.0503393	-0.2079679
C	-2.7736809	-0.2945263	0.2468961
N	-2.5583749	-0.5706483	1.5961131
C	-5.2846349	-2.8159723	1.0389221
C	-4.2701699	-1.8569573	0.8996041
C	-3.4633009	-1.5357223	2.0072241
C	-3.6353829	-2.1456093	3.2534801
C	-4.6432649	-3.0907513	3.3698311
C	-5.4649119	-3.4252083	2.2708011
Au	3.5434451	0.8092907	-0.4249909
C	6.7913931	1.4067897	2.3020521
C	6.2078611	2.6186907	2.3960181
H	7.6493151	1.0114987	2.7911561
H	6.4672491	3.4707817	2.9778771
C	5.0131671	1.3968247	0.9229041
N	5.1075281	2.6012147	1.5373751
N	6.0467581	0.6656097	1.3875321
C	4.2131821	3.7468547	1.3487151
H	3.4110421	3.4732527	0.6843501
H	3.7935281	4.0445177	2.2993191
H	4.7586961	4.5757527	0.9195691
C	6.3392201	-0.7404983	1.0408021
H	5.8418251	-1.4093983	1.7235541

H	5.9991491	-0.9474273	0.0425741
H	7.4067041	-0.8933623	1.0869291
F	3.5948911	-4.4848003	-0.6155539
B	4.3262731	-3.3672273	-0.1197389
F	5.6786461	-3.6989943	0.0960731
F	3.7378091	-2.8943723	1.0895681
F	4.2619141	-2.2953773	-1.0887319

Zero-point correction= 0.639782 (Hartree/Particle)

Thermal correction to Energy= 0.682984

Thermal correction to Enthalpy= 0.683928

Thermal correction to Gibbs Free Energy= 0.555600

Sum of electronic and zero-point Energies= -2170.316775

Sum of electronic and thermal Energies= -2170.273574

Sum of electronic and thermal Enthalpies= -2170.272630

Sum of electronic and thermal Free Energies= -2170.400957

C-int1

H	1.6788766	-3.0307337	1.6034709
H	2.1219706	-3.4831247	-0.0199331
H	3.1696416	-2.3703977	0.8987449
H	-3.4835204	3.5709443	-3.0569311
H	-2.6694514	2.8625173	-1.6688121
H	-2.1955894	2.3874003	-3.3284101
H	-5.9946854	1.1315023	-1.6981741
H	-4.7853614	1.9093113	-0.6522941
H	-5.6459024	2.8619963	-1.8845861
H	-5.4989844	0.7292583	-4.1494761
H	-3.9551954	1.2801323	-4.8413681

H	-5.1889394	2.4605873	-4.3391701
H	-4.2151924	-0.5312557	-2.7639661
H	-0.7478124	-0.7063587	1.8563469
H	-1.6272924	-2.8950437	2.6971349
H	-0.7052294	-4.7603467	-1.0890281
H	-0.0496624	-2.5403137	-2.0192011
H	-1.3393464	1.3369073	-1.5809661
H	-3.8990554	-0.1862687	0.8854369
H	-0.6467884	2.4693763	0.5863049
H	-4.8469094	0.8314263	3.5714059
H	-0.9413524	3.9352453	3.0438219
H	-2.3758734	4.0190813	5.0707379
H	-4.2981014	2.4899503	5.3280749
C	2.1303776	-2.6398227	0.6837129
C	-3.0390414	2.6440663	-2.6764861
C	-5.1973464	1.8845673	-1.6675951
C	-4.7210754	1.5017883	-4.0893791
C	-4.1103854	1.5615333	-2.6905511
N	-3.5847614	0.1972393	-2.4404931
O	-2.6440564	-1.5902567	-1.4701001
C	-2.6485364	-0.3753747	-1.6350891
O	-1.4525594	-5.0685677	1.4188769
C	-0.7706414	-1.5964457	1.2287149
C	-1.2337734	-2.7727347	1.6924189
C	-1.1291704	-3.9483007	0.8731659
C	-0.7132694	-3.8591477	-0.4867491
C	-0.3439034	-2.6578317	-0.9785631

C	-0.1310474	-1.4818217	-0.1089551
C	1.4235336	-1.4456897	0.1586179
C	1.9174466	-0.2429637	-0.1841131
O	0.7974026	1.8025843	-0.8843851
C	0.8036596	0.5978903	-0.6470301
N	-0.3400194	-0.1957427	-0.7482821
C	-1.6154604	0.4927373	-0.9414011
C	-3.2166964	0.6226483	1.1219789
C	-2.1659654	1.0309333	0.3419529
N	-1.4939534	2.0603103	0.9688589
C	-3.9986604	1.5023193	3.4517379
C	-3.2011484	1.4361163	2.3002989
C	-2.1021554	2.3236203	2.1747859
C	-1.7882174	3.2623873	3.1581509
C	-2.5940504	3.3012233	4.2834389
C	-3.6883324	2.4300963	4.4296339
Au	3.8472286	0.4497873	-0.1105801
C	7.5891766	2.5422123	-0.1903431
C	8.0455926	1.3103223	0.1354829
H	8.1101126	3.4755293	-0.3490591
H	9.0466396	0.9474283	0.3196099
C	5.8017696	1.1695393	-0.0631731
N	6.9384306	0.4852453	0.2086249
N	6.2155236	2.4359443	-0.3076291
C	6.9980496	-0.9300617	0.5307829
H	5.9825656	-1.3332887	0.5094909
H	7.6094156	-1.4600827	-0.2053251

H	7.4217736	-1.0736937	1.5290189
C	5.3379876	3.5414153	-0.6505641
H	5.6102796	3.9495143	-1.6284171
H	4.3102606	3.1706293	-0.6896331
H	5.4089356	4.3290943	0.1055129
H	-1.0646964	-5.8386827	0.8809689
B	1.2158116	-6.3522537	0.1819209
F	1.9354816	-7.4975157	0.3131879
F	-0.2079994	-6.7099397	0.0095809
F	1.5758196	-5.6103857	-0.9355551
F	1.2634036	-5.5499117	1.3197629

Zero-point correction= 0.595415 (Hartree/Particle)

Thermal correction to Energy= 0.638389

Thermal correction to Enthalpy= 0.639334

Thermal correction to Gibbs Free Energy= 0.514318

Sum of electronic and zero-point Energies= -2182.465375

Sum of electronic and thermal Energies= -2182.422400

Sum of electronic and thermal Enthalpies= -2182.421456

Sum of electronic and thermal Free Energies= -2182.546472

C-ts2

H	-0.3493076	-2.5202959	-2.1151099
H	0.0246694	-1.2863769	-3.3129689
H	1.3489764	-2.1546729	-2.4975349
H	2.2735364	3.9753191	-1.7813969
H	1.2385964	2.5670981	-1.4708849
H	0.7726574	3.7626481	-2.7037549
H	0.5632924	4.8506371	1.4649011

H	1.4043934	3.3411021	0.9983191
H	2.1265304	4.9013881	0.6336411
H	-0.0540976	6.5390081	-0.3595749
H	-0.0493996	6.0349761	-2.0690119
H	1.4816354	6.2906211	-1.2186059
H	-1.5735286	4.6734091	-1.1173719
H	-4.3619216	-2.2955429	-2.7487369
H	-1.3685906	-1.2945799	0.5863161
H	-3.2393616	-2.3420389	-0.6669409
H	-2.8540846	0.7034311	-3.6994939
H	-0.9140396	1.7273291	-2.5151799
H	-0.3101586	2.4424431	1.5483321
H	-3.6513116	0.8166521	0.1706081
H	-0.8078666	0.7776551	3.2327991
H	-5.1326436	-1.6476919	1.1317791
H	-1.9232806	-1.1937609	4.9744131
H	-3.7186326	-2.9190929	5.0006061
H	-5.2832066	-3.1499289	3.1007551
C	0.3556424	-1.7155449	-2.3589429
C	1.2327824	3.6346241	-1.7154499
C	1.1712774	4.3658381	0.6905191
C	0.4586664	5.9166211	-1.1027419
C	0.4801024	4.4517711	-0.6670949
N	-0.9480646	4.0570831	-0.6088439
O	-2.9217286	3.1460851	-0.0636239
C	-1.7040616	3.1133071	0.0238711
O	-3.9326846	-1.4696869	-3.1262199

C	-1.8171246	-0.7518339	-0.2509289
C	-2.7229126	-1.4699849	-1.0663949
C	-3.0680376	-0.9459339	-2.3005489
C	-2.4445616	0.2787871	-2.7865089
C	-1.4071676	0.8308791	-2.1438119
C	-0.8221746	0.1823661	-0.9314889
C	0.4140234	-0.6936659	-1.2831979
C	1.4469834	-0.4244149	-0.4595819
O	1.5617644	1.0868171	1.4584231
C	1.0133124	0.6452491	0.4563181
N	-0.2114296	1.1311691	-0.0113119
C	-1.0149046	2.0062581	0.8283681
C	-3.0247616	0.3884981	0.9442531
C	-1.9741536	1.1178361	1.5353731
N	-1.6594906	0.5676521	2.7265571
C	-4.4579426	-1.5308479	1.9762551
C	-3.4567456	-0.5641559	1.9563611
C	-2.5573226	-0.4628499	3.0328221
C	-2.6252586	-1.2860939	4.1490701
C	-3.6326206	-2.2446429	4.1519531
C	-4.5282386	-2.3685389	3.0822201
Au	3.3107364	-1.2520879	-0.2455329
C	7.2478204	-2.3366319	1.0327291
C	7.1316914	-3.2117309	0.0066901
H	8.0533564	-2.1623409	1.7316171
H	7.8143114	-3.9581069	-0.3735809
C	5.2175654	-2.0189269	0.0988791

N	5.8838044	-3.0017699	-0.5514559
N	6.0683424	-1.6165069	1.0735871
C	5.3604434	-3.7463029	-1.6824369
H	4.3587814	-3.3714399	-1.9067699
H	6.0021314	-3.6074239	-2.5575859
H	5.2998014	-4.8113729	-1.4399919
C	5.7869794	-0.5683849	2.0405651
H	6.5040084	0.2504061	1.9290091
H	4.7765174	-0.1886639	1.8638201
H	5.8473404	-0.9693729	3.0566051
B	-5.5384786	-3.4195229	-0.9282729
F	-4.8467566	-3.6401649	-2.1792039
F	-4.6591586	-3.7847289	0.0909761
F	-5.7707566	-2.0381409	-0.8576699
F	-6.6945026	-4.1391679	-0.9035559

Zero-point correction= 0.595349 (Hartree/Particle)

Thermal correction to Energy= 0.637614

Thermal correction to Enthalpy= 0.638558

Thermal correction to Gibbs Free Energy= 0.515079

Sum of electronic and zero-point Energies= -2182.445898

Sum of electronic and thermal Energies= -2182.403633

Sum of electronic and thermal Enthalpies= -2182.402689

Sum of electronic and thermal Free Energies= -2182.526168

C-int2

H	-0.1670759	-2.7515561	-1.6283781
H	0.0930271	-1.6594411	-2.9777971
H	1.4981341	-2.3507651	-2.1214391

H	2.2419171	3.6924959	-2.2338991
H	1.2294111	2.3543659	-1.6617801
H	0.6841731	3.3686799	-3.0187361
H	0.7500901	5.0513619	0.9516779
H	1.4731961	3.4359529	0.6842569
H	2.2703981	4.8730429	0.0592359
H	0.0585741	6.4703629	-1.0400001
H	-0.0423759	5.7369159	-2.6626841
H	1.5375671	6.0641239	-1.9341791
H	-1.5510879	4.6453399	-1.3335201
H	-3.9609979	-2.7665671	-2.6316151
H	-1.3028219	-1.2330691	0.7731029
H	-3.0288469	-2.5224371	-0.4553321
H	-2.6702429	0.2847069	-3.6946931
H	-0.8492889	1.5151009	-2.5343141
H	-0.2422789	2.5163069	1.5055929
H	-3.3882569	0.8199689	-0.1542901
H	-1.5815769	1.5580039	3.3971329
H	-5.0087829	-1.6741291	0.7466379
H	-3.1895499	0.0074889	5.1245229
H	-4.9587929	-1.7539221	5.0544779
H	-5.8253479	-2.5811411	2.8915439
C	0.4861981	-1.9502201	-1.9959681
C	1.2072121	3.3760489	-2.0540371
C	1.2884191	4.4177199	0.2351639
C	0.5150951	5.7377279	-1.7168681
C	0.5331441	4.3456719	-1.0876241

N	-0.9004499	4.0062109	-0.8879401
O	-2.8097099	3.3306299	0.0938479
C	-1.5989189	3.1979669	-0.0526981
O	-3.5787339	-1.9586531	-3.0599151
C	-1.8031439	-0.7037201	-0.0528041
C	-2.5805479	-1.6385811	-0.9052281
C	-2.8441659	-1.2819081	-2.1874051
C	-2.2761379	-0.0470271	-2.7363611
C	-1.2994849	0.6207289	-2.1083681
C	-0.7196249	0.0842119	-0.8277611
C	0.5157441	-0.8030551	-1.0531221
C	1.5515801	-0.4330661	-0.2678251
O	1.6704631	1.3156929	1.4366409
C	1.1175161	0.7295259	0.5151439
N	-0.1346269	1.1289319	0.0186279
C	-0.9224919	2.0854919	0.7531089
C	-2.8265179	0.3333769	0.6501049
C	-2.0002389	1.2870249	1.4008489
N	-2.1365739	1.0878169	2.6898099
C	-4.6080159	-1.3014251	1.6876419
C	-3.6153679	-0.3360741	1.7262069
C	-3.1315689	0.1092449	2.9595819
C	-3.5829279	-0.3594901	4.1798449
C	-4.5720839	-1.3402391	4.1266309
C	-5.0690529	-1.8009881	2.9061649
Au	3.4104181	-1.2508571	0.0145349
C	7.3758731	-2.3308771	1.2328669

C	7.1610211	-3.3283001	0.3434839
H	8.2285031	-2.1053851	1.8572669
H	7.7869681	-4.1524661	0.0326589
C	5.3078461	-2.0386761	0.3747189
N	5.8919611	-3.1322641	-0.1701951
N	6.2324541	-1.5534681	1.2381349
C	5.2710441	-3.9945571	-1.1596671
H	4.2712571	-3.6085021	-1.3738131
H	5.8606551	-4.0003821	-2.0812261
H	5.1870041	-5.0147861	-0.7738371
C	6.0531821	-0.3727251	2.0653579
H	6.7929401	0.3894089	1.8024719
H	5.0491361	0.0249229	1.8932469
H	6.1599791	-0.6343291	3.1222859
B	-5.2282959	-3.8656921	-0.7663041
F	-4.3188309	-4.1423591	-1.8389781
F	-4.4999059	-3.9227521	0.4277559
F	-5.6766489	-2.5475741	-0.9561351
F	-6.2607139	-4.7591431	-0.7755991

Zero-point correction= 0.597217 (Hartree/Particle)

Thermal correction to Energy= 0.639529

Thermal correction to Enthalpy= 0.640473

Thermal correction to Gibbs Free Energy= 0.518166

Sum of electronic and zero-point Energies= -2182.450147

Sum of electronic and thermal Energies= -2182.407836

Sum of electronic and thermal Enthalpies= -2182.406892

Sum of electronic and thermal Free Energies= -2182.529199

C-ts3

H	-0.1027688	-2.7782490	-2.0581718
H	0.4785752	-1.6322750	-3.2567998
H	1.6494952	-2.5584920	-2.2853518
H	2.3170872	3.8840240	-1.6606448
H	1.3854862	2.4048230	-1.3660498
H	0.9143702	3.5061770	-2.6815928
H	0.2853492	4.7277350	1.4053442
H	1.2648292	3.2621690	1.0686382
H	1.9073232	4.8581240	0.7050282
H	-0.3175898	6.2877220	-0.5279908
H	-0.1332418	5.7254710	-2.2096158
H	1.2974572	6.1400030	-1.2529528
H	-1.6252468	4.2891940	-1.2874148
H	-4.7477378	-1.6894640	-2.7716048
H	-1.1345988	-2.0515740	0.0153992
H	-3.4687938	-2.2730880	-0.8920648
H	-2.4523778	0.7480940	-3.7817858
H	-0.3511268	1.2650510	-2.5918948
H	-0.3682788	2.1308000	1.5201142
H	-3.3210298	-0.3653980	-0.1121988
H	-2.6790888	1.9138370	2.9761922
H	-3.7989318	-3.0768340	1.2399242
H	-4.3733758	0.5054660	4.7118652
H	-5.4804608	-1.7157780	4.9547102
H	-5.1738388	-3.4666580	3.2436142
C	0.6864542	-2.0389420	-2.2577828

C	1.3067262	3.4569800	-1.6576558
C	0.9891382	4.2584230	0.7058422
C	0.3025232	5.6848480	-1.2024648
C	0.4098492	4.2440720	-0.7052538
N	-0.9813618	3.7314080	-0.7359448
O	-2.9044558	2.6874290	-0.2295678
C	-1.6875798	2.7488640	-0.1155568
O	-4.1566408	-0.9606930	-3.1227638
C	-1.6388428	-1.1322040	-0.3132538
C	-2.8594848	-1.4174100	-1.1798848
C	-3.0945128	-0.7816950	-2.3771728
C	-2.1728588	0.2324740	-2.8664828
C	-1.0408018	0.5096900	-2.2147998
C	-0.5769838	-0.1821750	-0.9611318
C	0.7039222	-0.9657130	-1.2312518
C	1.7133802	-0.5776980	-0.4271758
O	1.7521212	1.1130520	1.3388732
C	1.2015622	0.5195460	0.4217222
N	-0.0879908	0.8231690	-0.0175858
C	-0.9816708	1.6717790	0.7297532
C	-2.3856758	-0.4677760	0.8343222
C	-2.0244298	0.7978920	1.3433842
N	-2.6683188	1.0266840	2.4908762
C	-3.8607788	-2.3142340	2.0125082
C	-3.2112568	-1.0891810	1.8894392
C	-3.4144118	-0.0990480	2.8652582
C	-4.2244948	-0.2822920	3.9772662

C	-4.8372608	-1.5217050	4.1000982
C	-4.6575638	-2.5170370	3.1320462
Au	3.6355002	-1.2287670	-0.1479058
C	7.6243972	-1.8477760	1.2719272
C	7.6248062	-2.7853400	0.2956562
H	8.3887542	-1.5547020	1.9773542
H	8.3889092	-3.4784600	-0.0259218
C	5.5992152	-1.7879570	0.2762302
N	6.3782202	-2.7330310	-0.3012578
N	6.3785442	-1.2488560	1.2447592
C	5.9627152	-3.5861910	-1.3991988
H	4.9358162	-3.3249420	-1.6662648
H	6.6116892	-3.4320190	-2.2664798
H	6.0003122	-4.6374210	-1.0982838
C	5.9661702	-0.1837330	2.1444132
H	6.6151632	0.6879230	2.0179582
H	4.9355192	0.0977360	1.9091452
H	6.0161812	-0.5276650	3.1817362
B	-5.7603428	-3.1340440	-0.9192938
F	-5.5766798	-2.9395800	-2.3358308
F	-4.6548628	-3.8958620	-0.4803308
F	-5.7035658	-1.8794040	-0.3229248
F	-6.9362498	-3.7792980	-0.6858448

Zero-point correction= 0.591585 (Hartree/Particle)

Thermal correction to Energy= 0.633875

Thermal correction to Enthalpy= 0.634819

Thermal correction to Gibbs Free Energy= 0.511968

Sum of electronic and zero-point Energies= -2182.408004

Sum of electronic and thermal Energies= -2182.365715

Sum of electronic and thermal Enthalpies= -2182.364770

Sum of electronic and thermal Free Energies= -2182.487621

C-int3

H	-1.1468234	-3.5762121	-1.6901767
H	-0.6278574	-3.9414301	-0.0348257
H	-2.3401264	-3.6324981	-0.3901827
H	-0.9750314	5.2291679	0.9777793
H	-1.0529884	3.4718529	0.7090803
H	-0.8923924	4.1062629	2.3501173
H	2.5045976	4.6170159	-0.2563057
H	1.0656936	3.8409329	-0.9508277
H	1.0202826	5.5460259	-0.5078337
H	2.6063666	5.3235579	2.1198993
H	1.1768436	5.1711879	3.1729303
H	1.1648076	6.3181569	1.8240913
H	1.7678526	3.0247209	2.7010673
H	0.4801646	-1.1403951	-2.4161077
H	0.9593196	-3.4348181	-1.8015577
H	2.3946676	-2.9988531	1.8255863
H	0.5160796	-1.4104571	1.8817693
H	0.2359666	2.1391379	-0.4600667
H	3.2700706	2.4665869	-0.0595767
H	3.9326336	-1.8391171	-3.2580467
H	5.7889316	2.3781529	-1.3027147
H	7.1722646	0.9222679	-2.7720487

H	6.2261236	-1.1512091	-3.7309187
C	-1.3163564	-3.3283911	-0.6318637
C	-0.5821924	4.2597009	1.3092093
C	1.4094866	4.5662579	-0.2067567
C	1.5095146	5.3271349	2.1387463
C	0.9411356	4.2553719	1.2122993
N	1.5024376	2.9694199	1.7207353
O	1.1153466	0.8325359	2.3579893
C	1.0768206	1.6783579	1.4848893
O	3.3811296	-3.9131211	-0.4956647
C	1.1205226	-1.2884971	-1.5318637
C	1.7400966	-2.6834941	-1.6167227
C	2.4219246	-3.0966731	-0.3586797
C	1.9302856	-2.6489851	0.9041933
C	0.9072296	-1.7620351	0.9285713
C	0.2194336	-1.1953661	-0.2798617
C	-1.1577254	-1.8698021	-0.3724127
C	-2.1519304	-0.9847511	-0.1580887
O	-2.0749334	1.4285009	0.2271233
C	-1.5345764	0.3454579	0.0418983
N	-0.1673034	0.1826279	-0.0397837
C	0.7362196	1.2948249	0.0367123
C	2.1714626	-0.2126851	-1.4368697
C	1.9863846	0.9170709	-0.6852867
N	3.1186976	1.6926309	-0.6918697
C	4.3128436	-0.9273851	-2.8042277
C	3.5150276	-0.1375071	-1.9591917

C	4.0802546	1.0589549	-1.4476717
C	5.3857246	1.4588979	-1.7218547
C	6.1467466	0.6446779	-2.5417027
C	5.6097526	-0.5335941	-3.0823647
Au	-4.1951774	-1.1062951	-0.0846587
C	-8.3304874	-0.1148141	0.3276013
C	-8.4845384	-1.4452021	0.1308763
H	-9.0559594	0.6677749	0.4978223
H	-9.3710554	-2.0619841	0.0942283
C	-6.2726844	-1.0001171	0.0545983
N	-7.2147624	-1.9684101	-0.0341007
N	-6.9724424	0.1384189	0.2778503
C	-6.9333994	-3.3727271	-0.2658257
H	-5.8511404	-3.4943201	-0.3542697
H	-7.2964964	-3.9760751	0.5715993
H	-7.4115564	-3.7086351	-1.1908777
C	-6.3822724	1.4573809	0.4470903
H	-6.6465564	1.8623669	1.4283223
H	-5.2936734	1.3724149	0.3756863
H	-6.7420894	2.1325699	-0.3348897
H	2.4479006	-2.7794991	-2.4427977
H	3.8220536	-4.2374801	0.4115753
B	4.7590186	-3.5783331	2.4230453
F	5.9320526	-3.9365891	2.9976603
F	4.8651146	-2.5272281	1.5319503
F	3.7380126	-3.3586921	3.3297183
F	4.2892326	-4.7246951	1.5770323

Zero-point correction= 0.595741 (Hartree/Particle)

Thermal correction to Energy= 0.638405

Thermal correction to Enthalpy= 0.639349

Thermal correction to Gibbs Free Energy= 0.514570

Sum of electronic and zero-point Energies= -2182.480826

Sum of electronic and thermal Energies= -2182.438162

Sum of electronic and thermal Enthalpies= -2182.437218

Sum of electronic and thermal Free Energies= -2182.561996

C-int4

H	-1.2516132	-3.6014561	-1.2873517
H	-0.9672522	-3.8633651	0.4419803
H	-2.5231862	-3.2169851	-0.1232757
H	0.8506948	5.1687159	0.3981683
H	0.3741778	3.4550629	0.3367093
H	0.5115508	4.2773679	1.8951713
H	4.1835638	3.5987309	-0.2615437
H	2.6799777	3.0709659	-1.0451077
H	3.0045558	4.7899369	-0.8289767
H	4.2068848	4.6189599	1.9990173
H	2.6815567	4.9607249	2.8554423
H	3.0917068	5.8578259	1.3851643
H	2.7669827	2.6929769	2.7425473
H	1.0682418	-1.7216331	-1.9879317
H	0.8343428	-3.9895601	-1.1126207
H	1.9378258	-3.5087361	2.5861473
H	0.5153498	-1.5061471	2.2855373
H	1.4207558	1.7001399	-0.4599237

H	4.3696428	1.3871699	0.3326883
H	4.3287028	-3.4314271	-2.1077427
H	6.9161618	0.5368509	-0.4923227
H	8.0660167	-1.4147211	-1.5269987
H	6.7594668	-3.3594271	-2.3216347
C	-1.4412752	-3.1925911	-0.2854127
C	0.9572618	4.1966059	0.8960523
C	3.1100858	3.8057089	-0.3574457
C	3.1484088	4.8750539	1.8657603
C	2.4345928	3.8306699	1.0111953
N	2.6096408	2.5452049	1.7487123
O	1.6512308	0.6781549	2.5952243
C	1.9072698	1.3608069	1.6223113
O	2.9972888	-4.8307221	0.6066183
C	1.5340628	-1.9441151	-1.0132017
C	1.7689958	-3.4505631	-0.9116057
C	2.2433938	-3.8868641	0.4579243
C	1.6833318	-3.1375901	1.5957133
C	0.9174278	-2.0509581	1.4320333
C	0.5432658	-1.4797831	0.0850663
C	-0.9327782	-1.7979391	-0.1718527
C	-1.6864442	-0.6743621	-0.2002687
O	-1.0310162	1.6762639	-0.0993247
C	-0.7691742	0.4799439	-0.0516847
N	0.4969868	-0.0218941	0.1330813
C	1.6376758	0.8471969	0.2000933
C	2.8106898	-1.1549621	-0.8557647

C	2.8267948	0.0878809	-0.2834227
N	4.1094598	0.5746109	-0.2087917
C	4.8631728	-2.5560741	-1.7505127
C	4.1864358	-1.4740461	-1.1623767
C	4.9660338	-0.3712021	-0.7256017
C	6.3533578	-0.3257671	-0.8432677
C	6.9837858	-1.4138881	-1.4208837
C	6.2412748	-2.5160391	-1.8716047
Au	-3.6725432	-0.2499761	-0.5759667
C	-7.3190262	1.8193659	-1.3575647
C	-7.8442542	0.5871789	-1.1612517
H	-7.7886642	2.7662619	-1.5821437
H	-8.8670453	0.2387989	-1.1726437
C	-5.6083402	0.4099359	-0.9409107
N	-6.7818172	-0.2612331	-0.9110557
N	-5.9498842	1.6914339	-1.2176587
C	-6.9247682	-1.6717981	-0.5949807
H	-5.9362212	-2.1344551	-0.5835017
H	-7.3769492	-1.7927811	0.3936743
H	-7.5498312	-2.1572581	-1.3499497
C	-5.0070372	2.7890829	-1.3609617
H	-5.3274012	3.6331009	-0.7435107
H	-4.0195642	2.4564499	-1.0268937
H	-4.9457212	3.1050719	-2.4068767
H	2.4836878	-3.8063451	-1.6571577
B	-4.6567682	-2.3572731	2.2324273
F	-5.2808022	-1.1901341	2.0913193

F	-4.5826923	-3.1383721	1.1508943
F	-4.5980652	-2.9165251	3.4249543
F	-2.8335092	-1.7113421	2.2130103
H	-2.5601232	-1.2898981	1.3968403

Zero-point correction= 0.596110 (Hartree/Particle)

Thermal correction to Energy= 0.639209

Thermal correction to Enthalpy= 0.640153

Thermal correction to Gibbs Free Energy= 0.516189

Sum of electronic and zero-point Energies= -2182.472208

Sum of electronic and thermal Energies= -2182.429110

Sum of electronic and thermal Enthalpies= -2182.428166

Sum of electronic and thermal Free Energies= -2182.552129

C-ts4

H	-1.5555015	-3.5847752	-0.5397897
H	-0.9503355	-3.8745562	1.1001983
H	-2.5825765	-3.1944572	0.8408363
H	0.8886505	5.1267907	0.8700193
H	0.4057365	3.4162148	0.8500153
H	0.8096915	4.2023038	2.3822783
H	4.0530535	3.5663458	-0.3888927
H	2.4337755	3.0519728	-0.9072977
H	2.7973445	4.7668118	-0.7255457
H	4.4693675	4.5590138	1.8481803
H	3.1153725	4.8834417	2.9613343
H	3.2640365	5.8032277	1.4560623
H	3.1985285	2.6149338	2.7955193
H	0.6353695	-1.7274862	-1.6024047

H	0.5413105	-4.0052163	-0.7260347
H	2.2984575	-3.5682612	2.7223563
H	0.8697465	-1.5519622	2.7054413
H	1.2892665	1.6742968	-0.1256617
H	4.3283285	1.3334218	0.1066843
H	3.8020355	-3.4615922	-2.3276057
H	6.6752455	0.4706458	-1.1714547
H	7.5997925	-1.4774972	-2.4164927
H	6.1532725	-3.4039072	-2.9786867
C	-1.5472275	-3.1904632	0.4860583
C	1.0777255	4.1441688	1.3202753
C	2.9798365	3.7755658	-0.2939147
C	3.4036815	4.8137187	1.9046423
C	2.5524675	3.7801958	1.1714113
N	2.8542645	2.4843198	1.8475663
O	2.0861625	0.5891938	2.8160483
C	2.1479295	1.2979788	1.8298673
O	2.9699065	-4.8774282	0.5734663
C	1.2672215	-1.9646982	-0.7295997
C	1.5007605	-3.4738582	-0.6870147
C	2.2083135	-3.9289192	0.5709543
C	1.8680525	-3.1878592	1.7985443
C	1.0948295	-2.0946972	1.7890723
C	0.4930995	-1.5024472	0.5368043
C	-1.0037085	-1.8092152	0.5011253
C	-1.7471745	-0.6727432	0.5483633
O	-1.0599355	1.6690438	0.4884483

C	-0.8066185	0.4742098	0.5560253
N	0.4670685	-0.0438452	0.6049213
C	1.6150445	0.8118988	0.4738233
C	2.5577045	-1.1869842	-0.7971587
C	2.6882685	0.0495778	-0.2264227
N	3.9672375	0.5253648	-0.3810927
C	4.3998595	-2.5938183	-2.0642617
C	3.8515435	-1.5134412	-1.3522147
C	4.7071895	-0.4209302	-1.0542747
C	6.0502245	-0.3839472	-1.4222047
C	6.5550625	-1.4701712	-2.1151367
C	5.7331775	-2.5620392	-2.4337167
Au	-3.6309735	-0.2410812	-0.3344327
C	-6.8100765	1.5774008	-2.4881657
C	-7.4903175	0.5293158	-1.9665927
H	-7.1319535	2.3935518	-3.1187657
H	-8.5304685	0.2467398	-2.0423557
C	-5.3562575	0.3522528	-1.2812787
N	-6.5833545	-0.2106792	-1.2324257
N	-5.5034195	1.4532968	-2.0555237
C	-6.9381035	-1.3964212	-0.4650697
H	-6.0343625	-1.8465832	-0.0501427
H	-7.5921045	-1.1189822	0.3661043
H	-7.4472175	-2.1118022	-1.1171347
C	-4.4336735	2.3749868	-2.3984787
H	-4.7897945	3.4036238	-2.2946377
H	-3.5967675	2.2159328	-1.7123707

H	-4.0959015	2.2074958	-3.4259107
H	2.0692075	-3.8236252	-1.5515237
B	-4.6954415	-1.6949992	2.5180203
F	-5.4389345	-0.6051982	2.1838403
F	-4.6326235	-2.6183182	1.4968313
F	-4.9257915	-2.2120513	3.7330443
F	-3.1994325	-1.1524272	2.6088353
H	-2.6841745	-0.8798662	1.6386703

Zero-point correction= 0.592003 (Hartree/Particle)

Thermal correction to Energy= 0.634056

Thermal correction to Enthalpy= 0.635000

Thermal correction to Gibbs Free Energy= 0.514159

Sum of electronic and zero-point Energies= -2182.471939

Sum of electronic and thermal Energies= -2182.429886

Sum of electronic and thermal Enthalpies= -2182.428942

Sum of electronic and thermal Free Energies= -2182.549784

C-2

H	-1.6303140	1.0471066	-3.7076397
H	-0.1875420	0.5365796	-4.6139947
H	-1.7328940	-0.3255364	-4.8210797
H	6.3241020	-2.0486014	1.4797473
H	4.8109950	-2.1776944	2.4015593
H	4.9336130	-2.9176424	0.7865703
H	4.8050380	1.3720656	1.2002913
H	4.7502310	0.3309656	2.6525743
H	6.2497640	0.4804766	1.7156073
H	5.0387610	0.4014566	-1.0323807

H	4.9786870	-1.3687064	-1.3010867
H	6.4276650	-0.6177704	-0.5906667
H	2.8364490	0.1200886	1.0358803
H	-1.0750740	1.2886456	-1.5764807
H	0.5776180	2.4871036	-2.6723267
H	3.6179740	0.5188836	-2.8102567
H	1.9097030	-1.2343874	-3.1655877
H	0.6178470	-2.3782754	0.7313573
H	1.0838710	-0.5453144	2.9266993
H	-1.1635190	3.6015286	0.3301083
H	0.7939950	1.7340146	4.5607653
H	-0.0930860	4.0561646	4.4811283
H	-1.0313720	4.9832956	2.3964223
C	-1.0856240	0.1749826	-4.0960147
C	5.2307790	-2.0589604	1.3948843
C	5.1581830	0.4288396	1.6379633
C	5.3321880	-0.5767314	-0.6326087
C	4.7543780	-0.7540794	0.7670303
N	3.2745750	-0.7378154	0.7246243
O	2.9150630	-2.6228444	-0.5210647
C	2.5046050	-1.6516814	0.0872763
O	3.1323180	2.3772246	-0.9339767
C	-0.0736890	1.0127766	-1.2428777
C	0.8360590	2.1909046	-1.6461177
C	2.2872330	1.8051326	-1.6017587
C	2.6035370	0.6276246	-2.4326647
C	1.6802760	-0.3190554	-2.6176537

C	0.3195030	-0.3249624	-1.9618667
C	-0.7339880	-0.7307724	-2.9772517
C	-1.2370070	-1.9310614	-2.6615157
O	-0.9134520	-3.4064374	-0.7449397
C	-0.6424160	-2.4172564	-1.4059467
N	0.3189170	-1.4802754	-1.0622057
C	0.9635010	-1.4636624	0.2211533
C	-0.1039990	0.8496216	0.2670033
C	0.5005780	-0.2317614	0.9263753
N	0.7921940	0.1108206	2.2161293
C	-0.6979220	3.2187496	1.2347223
C	-0.1917480	1.9149746	1.2652103
C	0.3483400	1.4077406	2.4633133
C	0.3852540	2.1472226	3.6415533
C	-0.1120950	3.4402946	3.5853113
C	-0.6422400	3.9684976	2.3978683
Au	-2.1131390	-0.2117554	0.6645693
C	-5.3091650	-2.9181554	1.2941933
C	-6.0196260	-1.8796664	0.7900313
H	-5.6161650	-3.9015234	1.6190533
H	-7.0741450	-1.7724764	0.5817823
C	-3.8743630	-1.2381694	0.8906203
N	-5.1246820	-0.8577634	0.5528793
N	-3.9942670	-2.5055444	1.3491943
C	-5.4897080	0.4300166	-0.0324417
H	-6.5482050	0.6108336	0.1665633
H	-4.8817010	1.2195456	0.4116113

H	-5.2944460	0.4305626	-1.1069357
C	-2.8837260	-3.3218774	1.8200763
H	-2.3944510	-2.8259104	2.6637903
H	-3.2777850	-4.2853044	2.1517313
H	-2.1621190	-3.4778314	1.0107053
H	0.6592950	3.0546436	-1.0000917
H	-2.0098320	-2.4778654	-3.1890927
B	-3.2852490	2.3491376	-1.4836467
F	-2.2243990	3.0639276	-2.0423157
F	-3.1341080	2.3523656	-0.0720107
F	-3.1823180	0.9963786	-1.9109347
F	-4.5115100	2.8539376	-1.8284997

Zero-point correction= 0.598529 (Hartree/Particle)

Thermal correction to Energy= 0.640536

Thermal correction to Enthalpy= 0.641480

Thermal correction to Gibbs Free Energy= 0.524335

Sum of electronic and zero-point Energies= -2182.528924

Sum of electronic and thermal Energies= -2182.486917

Sum of electronic and thermal Enthalpies= -2182.485973

Sum of electronic and thermal Free Energies= -2182.603118

D-1

Au	-4.6178257	-0.8684025	0.1936470
C	-6.8198677	-3.4405845	-2.3182990
C	-7.8442157	-3.0359735	-1.5298990
H	-6.7940267	-4.1177605	-3.1598670
H	-8.8953637	-3.2854165	-1.5420510
C	-5.9823777	-2.0130095	-0.8081100

N	-7.3101527	-2.1568105	-0.6071360
N	-5.6845677	-2.8021715	-1.8619490
C	6.4696503	-3.8499405	-0.1258850
F	6.8613883	-3.6214825	1.1256300
F	7.4857013	-3.5837475	-0.9394200
F	6.1631633	-5.1384865	-0.2402490
S	5.0235813	-2.8010525	-0.5337040
O	4.0030953	-3.2225015	0.4355800
O	4.7311373	-3.2006125	-1.9364820
O	5.5163623	-1.4274935	-0.3927240
C	-8.0857697	-1.4916515	0.4252480
H	-7.4274877	-0.8165845	0.9765660
H	-8.8944897	-0.9123785	-0.0287780
H	-8.5061367	-2.2283825	1.1156100
C	-4.3546627	-2.9962125	-2.4365280
H	-4.4259197	-2.9435625	-3.5255400
H	-3.6759577	-2.2121375	-2.0863180
H	-3.9626017	-3.9736615	-2.1426250
C	2.5533263	6.4986435	-1.3820240
C	1.3348143	6.5825245	-2.0733040
C	0.3378103	5.6313625	-1.8998190
C	0.6179323	4.6065375	-1.0104100
C	1.8225693	4.4937735	-0.3044660
C	2.8120373	5.4637035	-0.4966260
C	0.4689023	2.7922445	0.2040750
C	1.6937123	3.3002855	0.4857130
C	-0.3060587	1.6125755	0.6687470

N	-0.5996007	0.6859025	-0.4545430
C	-1.7899677	0.0457935	-0.5476350
C	0.4862523	0.2104615	-1.2737280
O	-2.1237967	-0.7227215	-1.4421570
C	-2.7110057	0.2559335	0.5889580
C	-3.2320847	0.3060165	1.7066590
C	1.0739473	1.0117945	-2.2522170
C	2.1802903	0.5468395	-2.9444720
C	2.7152833	-0.7229615	-2.6751770
C	2.0850803	-1.5418405	-1.7207610
C	0.9892853	-1.0681215	-1.0264290
O	3.7933993	-1.1036925	-3.3494060
H	-1.2734807	1.9868375	1.0254240
C	0.2949473	0.8521375	1.8659080
O	-0.4198067	0.6275645	2.8408430
N	1.5741373	0.4695705	1.7192470
C	2.3650093	-0.3793055	2.6501370
C	1.8604283	-1.8165075	2.5792150
C	3.8017043	-0.2969445	2.1556790
C	2.2690443	0.1760975	4.0658980
C	-3.5923267	0.5258875	3.0956620
H	3.3099453	7.2611645	-1.5494750
H	1.1688373	7.4077075	-2.7614750
H	-0.6100757	5.6782305	-2.4278360
H	3.7608283	5.4027405	0.0303860
H	2.4201003	2.8765905	1.1669150
H	0.6689123	1.9997905	-2.4617950

H	2.6711743	1.1602185	-3.6952750
H	2.4833903	-2.5306205	-1.5109990
H	0.5217763	-1.6890505	-0.2622130
H	4.1956153	-1.9042655	-2.9237040
H	1.9801983	0.5766815	0.7941220
H	2.0479013	-2.2447315	1.5871370
H	2.4090403	-2.4366415	3.2983980
H	0.7917953	-1.8649195	2.8228150
H	4.4393123	-0.9686025	2.7409010
H	4.1908173	0.7254855	2.2574150
H	3.9039253	-0.6183165	1.1115740
H	2.9541873	-0.3849615	4.7124610
H	1.2554913	0.0972395	4.4669230
H	2.5716183	1.2311095	4.0852700
H	-2.6565167	0.8052005	3.5994480
H	-3.9945007	-0.3791175	3.5597950
H	-4.3239117	1.3336785	3.1971410
O	-0.2143037	3.5750135	-0.6936340

Zero-point correction= 0.593896 (Hartree/Particle)

Thermal correction to Energy= 0.641308

Thermal correction to Enthalpy= 0.642252

Thermal correction to Gibbs Free Energy= 0.504633

Sum of electronic and zero-point Energies= -2739.185740

Sum of electronic and thermal Energies= -2739.138328

Sum of electronic and thermal Enthalpies= -2739.137384

Sum of electronic and thermal Free Energies= -2739.275002

D-ts1

H	-1.0496930	-4.3437971	1.0968891
H	-2.7670470	-4.6001401	1.4967841
H	-2.1910520	-4.8646531	-0.1698159
H	0.0937780	5.3876199	-0.8129079
H	0.3688690	3.6657439	-1.0318469
H	-1.1425880	4.2387349	-0.2639599
H	2.5874200	4.4868759	1.8891051
H	2.5159940	3.5753029	0.3723441
H	2.4223020	5.3478319	0.3432921
H	0.5621970	5.6659779	2.7967711
H	-0.9682570	5.6400499	1.8830951
H	0.4332110	6.5450429	1.2668141
H	-0.0049050	3.4859019	2.8285331
H	3.5724330	-4.3480331	1.5301101
H	1.2614330	-1.4943611	-1.1640629
H	2.7638000	-3.3140381	-0.3618639
H	1.1221770	-2.9361071	3.5787521
H	-0.3360970	-1.0423301	2.7871251
H	-0.5150900	1.8462809	-0.4364429
H	2.7998990	0.3851639	1.3144701
H	5.5334080	0.1680209	-0.0046679
H	3.0390900	2.3311239	-3.7995029
H	5.4779800	1.8006919	-3.9971999
H	6.6891100	0.7265539	-2.1372979
C	-2.0791010	-4.2440661	0.7242551
C	-0.0613540	4.4054629	-0.3505969
C	2.1214950	4.4498959	0.8973831

C	0.1246610	5.6335579	1.7902041
C	0.6013210	4.3998059	1.0239011
N	0.1721290	3.2520619	1.8576221
O	-0.6110380	1.2848859	2.5855451
C	-0.1348070	1.9379449	1.6697551
O	2.8021510	-4.1983611	2.1442771
C	1.2202690	-1.8279501	-0.1272689
C	2.0479050	-2.8461931	0.3087841
C	2.0208200	-3.2429201	1.6592251
C	1.1197860	-2.6211891	2.5381641
C	0.3134590	-1.5819521	2.1024301
C	0.3642720	-1.1823091	0.7668681
C	-2.2787300	-2.8374071	0.4299201
C	-2.2127230	-1.6202101	0.2454541
O	-2.5691580	0.6818479	-0.1333929
C	-1.7711150	-0.2145711	0.1289311
N	-0.4435700	-0.0807061	0.3109651
C	0.0941410	1.2941229	0.2887531
C	2.6639670	0.8409429	0.3393831
C	1.5020490	1.3019969	-0.1849819
C	5.0125270	0.6753559	-0.8130069
C	3.6542070	0.9892429	-0.6903159
C	2.9830110	1.5627929	-1.7788479
C	3.5951740	1.8827719	-2.9811199
C	4.9471420	1.5804079	-3.0737389
C	5.6399420	0.9790189	-2.0107949
Au	-4.3670280	-1.8585261	-0.1957349

C	-8.0302640	-0.0029561	-1.1669189
C	-8.4513480	-1.2873181	-1.2500519
H	-8.5542920	0.9291479	-1.3219129
H	-9.4165670	-1.7072781	-1.4936499
C	-6.2787500	-1.3175341	-0.6893199
N	-7.3599650	-2.0819311	-0.9533969
N	-6.6935140	-0.0398421	-0.8224269
C	5.9912020	-2.7881031	-1.2380169
F	6.8395010	-1.7677901	-1.3832849
F	4.8430900	-2.4586851	-1.8348699
F	6.4994680	-3.8405401	-1.8682209
S	5.7218530	-3.1397411	0.5416871
O	7.0603200	-3.4086551	1.0526851
O	4.8246000	-4.3280701	0.4571901
O	5.0460680	-1.9280741	1.0282071
C	-7.3912260	-3.5344021	-0.9378889
H	-6.3936500	-3.9031801	-0.6893429
H	-8.1023900	-3.8879821	-0.1861789
H	-7.6788550	-3.9147021	-1.9219499
C	-5.8748110	1.1521369	-0.6167809
H	-6.2187110	1.6856249	0.2735651
H	-4.8236350	0.8729789	-0.4844509
H	-5.9625970	1.8035379	-1.4901249
O	1.6642970	1.7441439	-1.4810879

Zero-point correction= 0.593746 (Hartree/Particle)

Thermal correction to Energy= 0.640315

Thermal correction to Enthalpy= 0.641260

Thermal correction to Gibbs Free Energy= 0.506163

Sum of electronic and zero-point Energies= -2739.178826

Sum of electronic and thermal Energies= -2739.132257

Sum of electronic and thermal Enthalpies= -2739.131313

Sum of electronic and thermal Free Energies= -2739.266409

D-int1

H	0.6808907	-3.9309192	-0.5334307
H	1.1466017	-3.6159762	-2.2028277
H	2.4023047	-3.7979002	-0.9574807
H	0.3521897	5.4329018	0.6131553
H	0.0138957	3.7430588	0.9473233
H	1.2092347	4.1763298	-0.3035667
H	-3.0282703	4.6845858	-0.9777367
H	-2.4252603	3.6771838	0.3523403
H	-2.2830733	5.4451348	0.4454503
H	-1.4152583	5.8936638	-2.5150497
H	0.3368147	5.7938148	-2.2088517
H	-0.7234923	6.6832648	-1.0908407
H	-1.1472273	3.6890238	-2.8206427
H	-3.9584253	-3.6433372	-1.7445637
H	-0.7917783	-1.4891992	0.8804963
H	-2.7054933	-2.8362152	0.0505703
H	-1.4756923	-2.0889622	-4.0379627
H	0.4343367	-0.6963952	-3.2161947
H	0.4280497	2.0851688	0.0177103
H	-3.1462453	0.7421148	-1.0193327
H	-5.4880443	0.1562318	0.8892983

H	-1.9387143	1.1399908	4.3080793
H	-4.2739353	0.5598678	5.0057103
H	-6.0058773	0.0749418	3.3195193
C	1.4055957	-3.3935032	-1.1592657
C	0.2449097	4.4487088	0.1422343
C	-2.2302933	4.5836808	-0.2321447
C	-0.6506733	5.7984238	-1.7325457
C	-0.8615503	4.5296318	-0.9077787
N	-0.8163433	3.4273128	-1.8974407
O	-0.7930193	1.4035598	-2.8668357
C	-0.6345513	2.0785318	-1.8577747
O	-3.1005713	-3.3041882	-2.5193347
C	-0.9473303	-1.6602912	-0.1853847
C	-1.9729243	-2.4074582	-0.6286277
C	-2.1651263	-2.5991542	-2.0549527
C	-1.2595853	-1.9638002	-2.9808967
C	-0.2427093	-1.2045542	-2.5360647
C	0.0980577	-1.0963802	-1.0895867
C	1.4007457	-1.9333352	-0.8845277
C	2.4085917	-1.1505312	-0.4680527
O	2.4857897	1.2344228	0.0339213
C	1.8941807	0.2315858	-0.3349717
N	0.5518607	0.2248418	-0.7032777
C	-0.2469553	1.4242928	-0.5357477
C	-2.7467733	0.8833238	-0.0211207
C	-1.4652503	1.2015798	0.2872363
C	-4.7297393	0.3913818	1.6312483

C	-3.4294723	0.7224028	1.2337153
C	-2.4639713	0.9762478	2.2192693
C	-2.7187633	0.9335128	3.5810613
C	-4.0178773	0.6106788	3.9500123
C	-5.0046203	0.3402638	2.9892183
Au	4.3729597	-1.4736302	0.0201883
C	8.3995417	-0.8754762	1.3096673
C	8.4884217	-2.2026942	1.0585193
H	9.1332627	-0.1691082	1.6708203
H	9.3147537	-2.8922692	1.1550563
C	6.3781157	-1.5613662	0.5781443
N	7.2419887	-2.6031632	0.6119853
N	7.1029657	-0.5013182	1.0102313
C	-5.9251953	-2.9713522	1.1106033
F	-6.7440313	-2.0381312	1.5833463
F	-4.7359493	-2.8305452	1.6870223
F	-6.4111253	-4.1632072	1.4103433
S	-5.7855273	-2.7694982	-0.7070577
O	-7.1262803	-2.9717832	-1.2158657
O	-4.8367403	-3.9342642	-1.0047657
O	-5.1197643	-1.4854792	-0.9100757
C	6.9080717	-3.9627872	0.2313513
H	5.8609867	-3.9831042	-0.0801777
H	7.5385647	-4.2899902	-0.6008557
H	7.0452357	-4.6395922	1.0800443
C	6.5936797	0.8548398	1.1466003
H	7.1658587	1.5354858	0.5093883

H	5.5433797	0.8740538	0.8403483
H	6.6693857	1.1804958	2.1882123
O	-1.2617203	1.2643268	1.6441703

Zero-point correction= 0.594241 (Hartree/Particle)

Thermal correction to Energy= 0.639891

Thermal correction to Enthalpy= 0.640835

Thermal correction to Gibbs Free Energy= 0.508911

Sum of electronic and zero-point Energies= -2739.224066

Sum of electronic and thermal Energies= -2739.178416

Sum of electronic and thermal Enthalpies= -2739.177471

Sum of electronic and thermal Free Energies= -2739.309395

D-ts2

H	-0.5178012	-2.4383729	-1.8102706
H	-0.0511112	-1.3434939	-3.1044696
H	1.1891688	-2.3375699	-2.2991906
H	3.2087168	3.4472261	-1.9527546
H	1.9283988	2.3035641	-1.5110516
H	1.6682538	3.4653851	-2.8329256
H	1.8107318	4.9277381	1.2220434
H	2.2806918	3.2316681	0.8970854
H	3.3246188	4.5490381	0.3827824
H	1.4880898	6.5331881	-0.7287736
H	1.3366088	5.8968651	-2.3878796
H	2.9135198	5.9079481	-1.5832596
H	-0.3999782	5.0160741	-1.2096236
H	-4.2810692	-1.6085499	-2.7319276
H	-1.3460002	-0.8456889	0.7114714

H	-3.3208582	-1.6489329	-0.5800476
H	-2.3531672	1.1515001	-3.6932146
H	-0.3092272	1.9056041	-2.4804746
H	0.4027928	2.6110261	1.5868994
H	-3.0752642	1.6189261	-0.0256496
H	-5.1372062	-0.4660059	1.0703364
H	-2.1868502	0.1640921	5.1040274
H	-4.3008752	-1.1860909	5.2457304
H	-5.7263532	-1.4965919	3.2530574
C	0.2747838	-1.7559679	-2.1416416
C	2.1238388	3.3280181	-1.8438246
C	2.2755528	4.2499941	0.4949184
C	1.8404828	5.7597491	-1.4219956
C	1.5839668	4.3624751	-0.8595686
N	0.1059928	4.2704671	-0.7423986
O	-1.9587852	3.8897181	0.0544524
C	-0.7789452	3.5659691	0.0109434
O	-3.7167152	-0.8670169	-3.1208306
C	-1.7003442	-0.2282009	-0.1236716
C	-2.6681032	-0.8755119	-0.9752996
C	-2.8580432	-0.3990929	-2.2511326
C	-2.0435092	0.7067971	-2.7506346
C	-0.9497602	1.1151851	-2.0939356
C	-0.5063602	0.4172181	-0.8437706
C	0.5352578	-0.6904679	-1.1396096
C	1.6236898	-0.5649929	-0.3531696
O	2.1118598	1.0522961	1.4099414

C	1.4311688	0.6243041	0.4921574
N	0.2667538	1.2724911	0.0452384
C	-0.3345082	2.3404621	0.8173554
C	-2.5884652	1.0703071	0.7777064
C	-1.5144082	1.7067201	1.4585694
C	-4.4996702	-0.3325259	1.9450014
C	-3.3263862	0.4081191	1.8695094
C	-2.5425602	0.5534111	3.0098234
C	-2.8336302	0.0159611	4.2451274
C	-4.0107782	-0.7282619	4.3035054
C	-4.8224352	-0.8976379	3.1775624
Au	3.3039528	-1.7166669	-0.1147916
C	6.9785458	-3.4964829	1.1707314
C	6.6795138	-4.3649549	0.1765834
H	7.8128358	-3.4595819	1.8565164
H	7.1988418	-5.2414019	-0.1836826
C	5.0350748	-2.8201299	0.2436604
N	5.4879228	-3.9343589	-0.3780426
N	5.9621438	-2.5593949	1.1963504
C	-5.9344342	-3.3016889	0.3220054
F	-6.7639332	-2.9036249	1.2882434
F	-4.6837262	-3.1382769	0.7739314
F	-6.1281392	-4.5923239	0.1020094
S	-6.2124392	-2.3104299	-1.1994206
O	-7.5551002	-2.6777309	-1.6195936
O	-5.1032972	-2.7992259	-2.0702876
O	-5.9942372	-0.9287309	-0.7454416

C	4.8140038	-4.5982449	-1.4791116
H	3.8967638	-4.0478159	-1.7026076
H	5.4545238	-4.6074829	-2.3660346
H	4.5586848	-5.6255829	-1.2030086
C	5.9018268	-1.4472169	2.1304284
H	6.7762248	-0.8019269	2.0044684
H	4.9955118	-0.8686109	1.9302674
H	5.8695668	-1.8203759	3.1582824
O	-1.4164052	1.3337331	2.7162924

Zero-point correction= 0.596145 (Hartree/Particle)

Thermal correction to Energy= 0.640833

Thermal correction to Enthalpy= 0.641777

Thermal correction to Gibbs Free Energy= 0.513669

Sum of electronic and zero-point Energies= -2739.187928

Sum of electronic and thermal Energies= -2739.143241

Sum of electronic and thermal Enthalpies= -2739.142296

Sum of electronic and thermal Free Energies= -2739.270404

D-int2

H	-0.4509756	-2.5651161	-1.5806060
H	-0.0120516	-1.5451411	-2.9418330
H	1.2516534	-2.4704961	-2.0894790
H	3.1979384	3.3114319	-2.1381480
H	1.9304474	2.2039639	-1.5857280
H	1.6291144	3.2859379	-2.9661200
H	1.9127784	4.9878189	0.9867170
H	2.3196384	3.2600199	0.7597040
H	3.3939664	4.5065559	0.1410930

H	1.5558404	6.4772599	-1.0385460
H	1.3527824	5.7501489	-2.6549130
H	2.9494624	5.7829589	-1.8903530
H	-0.3643996	5.0001729	-1.3296640
H	-4.1360776	-1.8634111	-2.6640320
H	-1.3316856	-0.8046991	0.8071500
H	-3.2372406	-1.7563111	-0.4785970
H	-2.2811946	0.9094809	-3.7089660
H	-0.2755006	1.7694109	-2.5072540
H	0.4263314	2.6411859	1.5510850
H	-2.9463896	1.6045169	-0.2238080
H	-5.1318706	-0.4076261	0.8388510
H	-2.7571286	0.9429979	5.0739550
H	-4.9068366	-0.3597061	5.1494620
H	-6.0462886	-1.0147431	3.0629150
C	0.3295804	-1.8937091	-1.9595330
C	2.1169664	3.2053379	-1.9863450
C	2.3385964	4.2510339	0.2939710
C	1.8789034	5.6603789	-1.6954700
C	1.6185424	4.3011289	-1.0489820
N	0.1411824	4.2405769	-0.8843770
O	-1.8730046	3.9535789	0.0799680
C	-0.7080676	3.5887109	-0.0554900
O	-3.5918346	-1.1311441	-3.0817630
C	-1.6864236	-0.2192931	-0.0532260
C	-2.6151136	-0.9734631	-0.9039530
C	-2.7771066	-0.5865261	-2.2029870

C	-1.9775826	0.5162459	-2.7414210
C	-0.9026976	0.9830599	-2.0917520
C	-0.4631036	0.3484369	-0.8021780
C	0.5792124	-0.7660221	-1.0246670
C	1.6705764	-0.5919051	-0.2491630
O	2.1545854	1.1279399	1.4159300
C	1.4753964	0.6399219	0.5267860
N	0.3002104	1.2537479	0.0529230
C	-0.2879156	2.3636169	0.7606330
C	-2.5262106	1.0652099	0.6286440
C	-1.5313056	1.8126579	1.3632510
C	-4.6110796	-0.1181451	1.7536410
C	-3.4202536	0.5942429	1.7177480
C	-2.8084946	0.9419979	2.9149620
C	-3.2792706	0.6396099	4.1722830
C	-4.4731526	-0.0814841	4.1925180
C	-5.1201076	-0.4489671	3.0103040
Au	3.3517974	-1.7330481	0.0309340
C	7.0269134	-3.5185221	1.3185390
C	6.7030754	-4.4070861	0.3502830
H	7.8714584	-3.4751421	1.9912500
H	7.2066324	-5.2982751	0.0040570
C	5.0781374	-2.8408731	0.4028880
N	5.5088644	-3.9754351	-0.1977990
N	6.0221854	-2.5686671	1.3354440
C	-5.8680416	-3.4094971	0.4754100
F	-6.8109496	-3.0206881	1.3340500

F	-4.6819456	-3.0701141	1.0015960
F	-5.9088676	-4.7287521	0.3699810
S	-6.1157476	-2.5966461	-1.1520160
O	-7.3905146	-3.1217881	-1.6161500
O	-4.9121446	-3.0648521	-1.8966760
O	-6.0532006	-1.1645101	-0.8224020
C	4.8118094	-4.6581781	-1.2728290
H	3.9004904	-4.0998591	-1.5011890
H	5.4418534	-4.7012351	-2.1662140
H	4.5439274	-5.6735621	-0.9661460
C	5.9881484	-1.4337141	2.2424940
H	6.8713254	-0.8055461	2.0932160
H	5.0892434	-0.8464071	2.0352150
H	5.9591384	-1.7808051	3.2795690
O	-1.6269326	1.6698159	2.6513580

Zero-point correction= 0.596246 (Hartree/Particle)

Thermal correction to Energy= 0.641539

Thermal correction to Enthalpy= 0.642483

Thermal correction to Gibbs Free Energy= 0.511940

Sum of electronic and zero-point Energies= -2739.188014

Sum of electronic and thermal Energies= -2739.142721

Sum of electronic and thermal Enthalpies= -2739.141777

Sum of electronic and thermal Free Energies= -2739.272320

D-ts3

H	0.3368452	-3.4229941	0.8044672
H	-0.2658198	-3.0986251	2.4236162
H	-1.3840078	-3.6885171	1.1691612

H	-2.9857258	4.9810849	0.0724672
H	-2.4072038	3.3177079	0.2622752
H	-2.6763198	4.3303649	1.6945232
H	0.6571792	5.3262649	-0.8515328
H	-0.4385208	4.0386479	-1.3832998
H	-0.9943528	5.7088799	-1.3911438
H	0.1325322	6.7170359	1.1824412
H	-1.2275008	6.2699559	2.2471182
H	-1.5417058	6.9513109	0.6430302
H	0.3512932	4.5597769	2.2919322
H	4.6242812	-1.9274661	2.2558352
H	1.1002202	-1.6089551	-0.6000808
H	3.4710212	-1.7632241	0.2829172
H	1.8974132	-0.8110991	4.1688912
H	-0.2279738	-0.0259651	3.1701722
H	-0.6671218	2.3514349	-0.4079468
H	2.8070342	0.3281569	0.5067892
H	4.0775962	-1.3211431	-1.8709438
H	3.6857472	3.5601119	-3.0378658
H	5.4415322	2.1057709	-4.0894408
H	5.6182722	-0.2839581	-3.4822998
C	-0.5283758	-3.0328671	1.3594162
C	-2.3181648	4.3367299	0.6581402
C	-0.3844998	4.9856979	-0.8367968
C	-0.8772738	6.2886499	1.2072912
C	-0.8964418	4.8884459	0.5988772
N	0.0207292	4.0934959	1.4532832

O	1.0590012	2.3210219	2.3824202
C	0.3965392	2.7929409	1.4727502
O	3.8881932	-1.6953041	2.8958112
C	1.4235702	-0.8820341	0.1581112
C	2.6868192	-1.3114511	0.8892282
C	2.7969112	-1.3386751	2.2617082
C	1.7124852	-0.8662211	3.0996802
C	0.5701842	-0.4360051	2.5541202
C	0.2181012	-0.5564591	1.0946212
C	-0.8537728	-1.6374571	0.9654002
C	-2.0114208	-1.1502171	0.4779032
O	-2.5670378	1.0970729	-0.2998658
C	-1.8087888	0.2886349	0.2188412
N	-0.5266108	0.6255029	0.6565952
C	0.0593632	1.8817449	0.2690632
C	1.9913392	0.3744309	-0.4725818
C	1.3072642	1.6018099	-0.4669588
C	3.9630622	-0.2695681	-2.1349878
C	2.9826502	0.5352749	-1.5662138
C	2.9239572	1.8846649	-1.9109648
C	3.7704762	2.5029489	-2.8065548
C	4.7377102	1.6800669	-3.3791088
C	4.8315742	0.3252189	-3.0463498
Au	-3.8109798	-2.0063301	0.0035532
C	-7.7939188	-2.7953901	-1.3486388
C	-7.4903698	-4.0418071	-0.9169468
H	-8.6915788	-2.3977251	-1.8000868

H	-8.0680968	-4.9549851	-0.9141018
C	-5.6873738	-2.7363681	-0.5392968
N	-6.1986998	-3.9850861	-0.4257558
N	-6.6802148	-2.0117301	-1.1095028
C	7.0249022	-4.0744771	0.0279672
F	7.2135202	-4.6699211	-1.1444358
F	6.4176492	-4.9298211	0.8445722
F	8.2076132	-3.7633791	0.5432262
S	6.0030632	-2.5696201	-0.1907158
O	6.7823842	-1.7141351	-1.0820138
O	5.8695212	-2.0639251	1.2002212
O	4.7405942	-3.0936711	-0.7464078
C	-5.4881338	-5.1192421	0.1355202
H	-4.4931948	-4.7841161	0.4387632
H	-6.0204788	-5.5060311	1.0096362
H	-5.3891068	-5.9126131	-0.6113358
C	-6.5933468	-0.5971391	-1.4333728
H	-5.6074978	-0.2274821	-1.1363448
H	-6.7232028	-0.4489881	-2.5095308
H	-7.3643278	-0.0396891	-0.8931908
O	1.8890142	2.5210189	-1.2157418

Zero-point correction= 0.592209 (Hartree/Particle)

Thermal correction to Energy= 0.637373

Thermal correction to Enthalpy= 0.638317

Thermal correction to Gibbs Free Energy= 0.506882

Sum of electronic and zero-point Energies= -2739.150070

Sum of electronic and thermal Energies= -2739.104907

Sum of electronic and thermal Enthalpies= -2739.103963

Sum of electronic and thermal Free Energies= -2739.235398

D-int3

H	0.2422454	-3.5789029	-0.0459483
H	0.3574874	-3.2404629	1.6880917
H	-1.1963306	-3.7233599	0.9686207
H	-2.9695186	4.9773591	-0.9564093
H	-2.5131286	3.3203161	-0.4861723
H	-3.1687686	4.4277751	0.7214767
H	0.7739784	5.2771521	-0.8027913
H	-0.1818966	4.0351871	-1.6212923
H	-0.6638606	5.7248301	-1.7560613
H	-0.2619146	6.7092351	1.0057107
H	-1.8651206	6.2942251	1.6682877
H	-1.7280056	6.9674431	0.0362637
H	-0.5175936	4.5131321	2.1695177
H	5.4285914	-2.2532659	1.1908377
H	1.1466174	-1.0321779	-1.3278793
H	2.1565924	-2.6892199	0.1533157
H	2.4024834	-0.7404339	3.4832697
H	0.1331374	-0.0827689	2.7533057
H	-0.6295176	2.3369101	-0.7170643
H	4.8188444	-0.4985509	-1.3174673
H	4.3397274	4.4873201	-1.0142773
H	6.5273484	3.4250481	-1.6293883
H	6.7235674	0.9671021	-1.7660973
C	-0.2889196	-3.1318279	0.8069237

C	-2.5210866	4.3673551	-0.1617163
C	-0.2452616	4.9784441	-1.0700543
C	-1.2490296	6.2987561	0.7596517
C	-1.1276506	4.8937141	0.1736767
N	-0.5059426	4.0861361	1.2494167
O	0.1332424	2.2950271	2.4486787
C	-0.1477246	2.7794541	1.3624437
O	4.2166034	-1.6266909	1.8910567
C	1.5476724	-0.6758179	-0.3659383
C	2.5903334	-1.6802759	0.1253247
C	3.0650224	-1.3818469	1.5180147
C	2.0851764	-0.8470739	2.4488687
C	0.8560274	-0.4808429	2.0451057
C	0.3638734	-0.5745509	0.6259537
C	-0.6600976	-1.7129959	0.5450287
C	-1.8897326	-1.2527149	0.2428607
O	-2.6550376	1.0063401	-0.2821063
C	-1.7857566	0.2103741	0.0511847
N	-0.4759046	0.5708611	0.2988537
C	-0.0124016	1.9194551	0.0904857
C	2.1338304	0.6999231	-0.5379473
C	1.4135924	1.8254921	-0.3164883
C	4.6903294	0.5778191	-1.2346323
C	3.4631134	1.1596991	-0.8852863
C	3.3922264	2.5611991	-0.8228593
C	4.4550124	3.4092511	-1.0802623
C	5.6587204	2.8058791	-1.4194073

C	5.7688484	1.4111351	-1.4951993
Au	-3.7270746	-2.1159479	-0.0240713
C	-7.8870636	-2.6993809	-0.8109863
C	-7.5718886	-3.9899969	-0.5516333
H	-8.8264336	-2.2362469	-1.0772243
H	-8.1787466	-4.8840819	-0.5449803
C	-5.6812446	-2.7740869	-0.3377153
N	-6.2189566	-4.0146429	-0.2645163
N	-6.7195676	-1.9714359	-0.6754153
C	5.2048404	-4.9589279	0.0859157
F	4.9430234	-5.7094589	-0.9686173
F	4.0608404	-4.5448519	0.6245337
F	5.8762674	-5.6602199	0.9770107
S	6.1771214	-3.4938639	-0.4448263
O	7.4819144	-3.9668179	-0.8303793
O	6.2905944	-2.7335759	0.9126457
O	5.3111334	-2.7888709	-1.3744023
C	-5.4761226	-5.2144499	0.0717957
H	-4.4341726	-4.9337119	0.2436407
H	-5.8814886	-5.6707179	0.9799847
H	-5.5249786	-5.9348249	-0.7503593
C	-6.6277736	-0.5326159	-0.8701823
H	-7.2790996	-0.0157999	-0.1591773
H	-5.5933766	-0.2160559	-0.7048093
H	-6.9238676	-0.2730269	-1.8908543
H	3.4464734	-1.7490799	-0.5505963
O	2.1356004	2.9671201	-0.4742643

Zero-point correction= 0.598321 (Hartree/Particle)

Thermal correction to Energy= 0.643398

Thermal correction to Enthalpy= 0.644342

Thermal correction to Gibbs Free Energy= 0.514251

Sum of electronic and zero-point Energies= -2739.246888

Sum of electronic and thermal Energies= -2739.201811

Sum of electronic and thermal Enthalpies= -2739.200867

Sum of electronic and thermal Free Energies= -2739.330958

D-int4

H	1.1383371	0.5660614	-3.6503074
H	1.1909301	2.0150614	-2.6346084
H	2.5927951	0.9220804	-2.7080114
H	-2.9655179	0.9419684	5.7312996
H	-2.6982709	-0.7058606	5.1182656
H	-1.5934979	0.6064244	4.6468426
H	-5.6213989	0.4911454	3.1129646
H	-5.0391669	-0.7878286	4.2118506
H	-5.3346319	0.8501094	4.8254876
H	-4.0921429	2.3741284	2.4432186
H	-2.4276319	2.4461354	3.0694866
H	-3.8023529	2.7589524	4.1552976
H	-3.8172499	-0.7172436	2.0597926
H	-1.0692239	-0.9675846	-2.8342834
H	-0.9144159	1.2941894	-3.7392024
H	-1.7820719	3.4968454	-0.7092214
H	-0.2737299	1.8412204	0.3449276
H	-1.5697359	-2.0307186	1.1253196

H	-4.2042709	-0.4566846	-4.2374544
H	-6.7096869	-2.1351476	-0.2312214
H	-7.8363269	-1.9058246	-2.4586744
H	-6.5778169	-1.0810256	-4.4146544
C	1.4987341	0.9614134	-2.6899554
C	-2.6364459	0.3586904	4.8623136
C	-4.9642079	0.2795014	3.9667236
C	-3.4543589	2.1546974	3.3083136
C	-3.5243929	0.6716614	3.6623086
N	-3.1095579	-0.1434736	2.5025576
O	-0.9738839	0.6326424	2.2855326
C	-1.8967979	-0.0700766	1.9080686
O	-3.1054499	3.0230624	-2.9104634
C	-1.5217799	-0.1526156	-2.2454854
C	-1.8203959	1.0233314	-3.1800004
C	-2.2738669	2.2659104	-2.4457544
C	-1.5901209	2.5295794	-1.1696374
C	-0.7770469	1.6311264	-0.5994774
C	-0.5066759	0.2478934	-1.1429244
C	0.9662011	0.1688194	-1.5485064
C	1.6636641	-0.6441816	-0.7235254
O	0.9072641	-2.0623066	1.1212866
C	0.7023251	-1.2401346	0.2437016
N	-0.5388249	-0.7184316	-0.0550534
C	-1.7187959	-1.0252746	0.6954576
C	-2.7730679	-0.6716886	-1.5895764
C	-2.8332119	-1.0315616	-0.2856154

C	-4.7365689	-0.8081516	-3.3575064
C	-4.0982089	-0.9187016	-2.1163774
C	-4.8467409	-1.4041646	-1.0330094
C	-6.1797169	-1.7657586	-1.1044834
C	-6.7894489	-1.6356546	-2.3462584
C	-6.0736759	-1.1664706	-3.4552044
Au	3.6207271	-1.2711886	-0.5666874
C	7.1753201	-3.2097856	0.7713436
C	7.7591391	-2.2716036	-0.0114254
H	7.6008931	-3.9869066	1.3898156
H	8.7993191	-2.0556756	-0.2086504
C	5.5304261	-1.9926766	-0.1743254
N	6.7363221	-1.5402066	-0.5843524
N	5.8107021	-3.0221096	0.6603916
C	4.4127631	4.0307154	0.0460876
F	3.5140401	4.6017964	-0.7304014
F	5.6176041	4.4843744	-0.2574184
F	4.1462551	4.2829884	1.3107506
S	4.4352811	2.2149994	-0.2470374
O	2.9362051	1.9739434	0.1987636
O	5.3829051	1.6421404	0.6864616
O	4.6030451	2.0108864	-1.6741934
C	6.9394951	-0.3801496	-1.4367674
H	6.0021501	-0.1445266	-1.9456774
H	7.2267731	0.4863364	-0.8332764
H	7.7152011	-0.6010116	-2.1753224
C	4.8140751	-3.8312406	1.3438986

H	5.0807001	-3.9263176	2.4002396
H	3.8393021	-3.3401526	1.2661736
H	4.7533591	-4.8262086	0.8923036
H	-2.5819799	0.7737584	-3.9241214
H	2.6110901	1.0690774	-0.0721044
O	-4.0689779	-1.4773436	0.0909656

Zero-point correction= 0.596542 (Hartree/Particle)

Thermal correction to Energy= 0.642288

Thermal correction to Enthalpy= 0.643233

Thermal correction to Gibbs Free Energy= 0.511303

Sum of electronic and zero-point Energies= -2739.249085

Sum of electronic and thermal Energies= -2739.203339

Sum of electronic and thermal Enthalpies= -2739.202395

Sum of electronic and thermal Free Energies= -2739.334325

D-ts4

H	1.1545229	0.3440166	3.3726171
H	0.8646809	-1.3944724	3.3419831
H	2.3719619	-0.7328934	2.6368861
H	-0.1687291	-3.4471604	-3.0314619
H	-0.4008991	-1.8626674	-2.3125889
H	-0.2455951	-3.3038274	-1.2697889
H	-3.8298381	-2.6680784	-3.6101469
H	-2.5964751	-1.3910954	-3.5179939
H	-2.2665521	-2.8593144	-4.4365549
H	-3.4899751	-4.8876694	-2.4733299
H	-2.0030521	-5.1896764	-1.5344869
H	-1.9326531	-5.0634144	-3.3018749

H	-3.4983081	-3.4666144	-0.6762609
H	-1.4680881	1.4700396	1.8139711
H	-2.7986541	0.8944716	3.8352161
H	-2.0954451	-3.3356334	3.1260301
H	-0.7541991	-2.7805454	1.1017051
H	-2.0619201	-0.3207874	-1.8646799
H	-4.9893141	0.5983686	0.4156871
H	-6.1627831	3.4255266	0.8889601
H	-1.7737791	4.7347506	-1.1682079
H	-3.4160011	6.4725746	-0.4178839
H	-5.5671221	5.8153106	0.5916921
C	1.2986479	-0.5647444	2.7723111
C	-0.6651691	-2.9183914	-2.2088859
C	-2.7533721	-2.4754074	-3.5318819
C	-2.4171111	-4.6649554	-2.4044879
C	-2.1700231	-3.1616344	-2.2985939
N	-2.8969631	-2.7509984	-1.0712519
O	-4.0194571	-1.5230844	0.4308771
C	-3.1795741	-1.5670014	-0.4567899
O	-3.1131451	-1.5351664	4.6991411
C	-1.5961851	0.4386586	2.1472551
C	-2.3056281	0.1319476	3.2367601
C	-2.4971911	-1.2625454	3.6817771
C	-1.9016601	-2.3084144	2.8263531
C	-1.1891381	-2.0104004	1.7375841
C	-0.8847791	-0.5966164	1.3223771
C	0.6317259	-0.4049354	1.4616491

C	1.1935639	-0.1075744	0.2600511
O	0.1946799	0.2872446	-1.9216089
C	0.1063589	-0.0158174	-0.7470179
N	-1.0666981	-0.3899804	-0.1108899
C	-2.3480631	-0.3299034	-0.8026099
C	-4.2581961	1.2944526	0.0323191
C	-3.0662211	0.9501336	-0.5135459
C	-5.2106681	3.7072166	0.4455051
C	-4.2985991	2.7306376	0.0306031
C	-3.0827521	3.1394686	-0.5345919
C	-2.7242031	4.4658896	-0.7158569
C	-3.6465061	5.4167386	-0.2969469
C	-4.8712371	5.0413446	0.2764131
Au	2.9156139	1.1923106	0.1262141
C	6.7504149	2.9359956	-0.2114739
C	6.0348309	4.0853966	-0.1620789
H	7.8128789	2.7641346	-0.3055389
H	6.3434009	5.1200546	-0.1990969
C	4.5858119	2.3718876	-0.0078939
N	4.7080159	3.7178926	-0.0376829
N	5.8472479	1.8974196	-0.1128609
C	2.8452609	-3.8859224	0.6707361
F	3.5091169	-4.6108554	1.5543311
F	2.5076589	-4.6453964	-0.3587049
F	1.7262189	-3.4298274	1.2431701
S	3.8612769	-2.4625614	0.1147271
O	4.0816389	-1.6766544	1.3335871

O	2.8899539	-1.7832004	-0.8300449
O	5.0180689	-3.0218144	-0.5597269
C	3.6049729	4.6571056	0.0502521
H	2.6730699	4.0902746	0.1116831
H	3.7086849	5.2810956	0.9428721
H	3.5805349	5.2931626	-0.8393089
C	6.1928829	0.4789436	-0.1670439
H	7.2678969	0.3746196	-0.0064429
H	5.6536959	-0.0713104	0.6104181
H	5.9292339	0.0607466	-1.1432919
H	2.1492599	-0.8580184	-0.2018019
O	-2.3318631	2.0571526	-0.8705049

Zero-point correction= 0.591791 (Hartree/Particle)

Thermal correction to Energy= 0.636966

Thermal correction to Enthalpy= 0.637910

Thermal correction to Gibbs Free Energy= 0.507314

Sum of electronic and zero-point Energies= -2739.238823

Sum of electronic and thermal Energies= -2739.193648

Sum of electronic and thermal Enthalpies= -2739.192704

Sum of electronic and thermal Free Energies= -2739.323300

D-2

H	2.5461696	-0.1862972	2.9955650
H	1.1520816	-0.1553642	4.0861900
H	2.1411786	-1.6267272	3.9553860
H	-7.0909244	-0.5133952	-0.0693980
H	-6.0373394	-1.1241102	-1.3641410
H	-5.7095484	-1.5639322	0.3291630

H	-5.0183344	2.4625468	-1.0500420
H	-5.6190404	1.2163078	-2.1763070
H	-6.6747164	1.8493168	-0.8997070
H	-4.5640524	1.8841718	1.3489540
H	-4.8382864	0.2292848	1.9478490
H	-6.2226964	1.2686228	1.5353080
H	-3.3678964	0.7076308	-1.3084840
H	1.7310446	0.4579878	0.6001110
H	1.5021106	1.8524778	2.5022920
H	-2.2574684	1.7311508	3.2892480
H	-1.8438224	-0.6430742	2.7456040
H	-1.5841144	-1.6530352	-1.2420130
H	2.0619416	3.3080548	-0.9095020
H	-1.4514634	2.5595718	-4.4166500
H	0.2151646	4.4181208	-4.6336710
H	1.9364026	4.7650328	-2.9015480
C	1.7160676	-0.7906412	3.3911060
C	-6.0544724	-0.7618642	-0.3290830
C	-5.6435684	1.5643868	-1.1355450
C	-5.1987314	0.9943608	1.2532920
C	-5.1737454	0.4744128	-0.1815680
N	-3.7833044	0.1560248	-0.5672460
O	-3.3571674	-1.4703752	0.9806800
C	-3.0015524	-0.7452742	0.0660260
O	-0.7857074	3.6813798	2.3936480
C	0.7045316	0.8024438	0.7894560
C	0.8171136	2.0545848	1.6667450

C	-0.4993444	2.5088938	2.2437590
C	-1.3982794	1.4279988	2.6932100
C	-1.1733104	0.1432628	2.3983680
C	-0.0594454	-0.3496342	1.5033590
C	0.8512286	-1.2813792	2.2908970
C	0.7234866	-2.5350252	1.8309760
O	-0.5526044	-3.5169762	-0.0077710
C	-0.2186374	-2.5746772	0.6957470
N	-0.6376924	-1.2773682	0.5324560
C	-1.5555184	-0.8510472	-0.4857320
C	0.0559756	1.1049718	-0.5295680
C	-0.9662604	0.3881168	-1.0502330
C	1.2759456	3.1631338	-1.6457810
C	0.3330076	2.1386308	-1.5037160
C	-0.6115914	1.9536498	-2.5236400
C	-0.6981494	2.7435048	-3.6560750
C	0.2353156	3.7672318	-3.7631300
C	1.2101186	3.9660378	-2.7757910
Au	3.2528776	-0.8468982	-0.9540420
C	1.9184296	-4.8326282	-1.2616510
C	2.8881966	-4.9547322	-0.3249260
H	1.2155716	-5.5495722	-1.6588010
H	3.2246746	-5.8086502	0.2445730
C	2.8419496	-2.8104352	-0.9848320
N	3.4500696	-3.7012642	-0.1696100
N	1.9120716	-3.5122552	-1.6616930
C	5.0866856	3.1141308	0.4435690

F	3.9837146	3.8532988	0.5228450
F	5.6894216	3.3566508	-0.7069850
F	5.8935406	3.4390308	1.4395780
S	4.6556746	1.3364628	0.5782710
O	3.9027306	1.2183118	1.8269050
O	5.9033366	0.5957688	0.4605470
O	3.7636696	1.2112258	-0.6535550
C	4.4652816	-3.3509012	0.8129580
H	4.9626276	-4.2632342	1.1496280
H	5.2037356	-2.6788202	0.3674810
H	4.0033466	-2.8452992	1.6685730
C	0.9633506	-2.9645972	-2.6159380
H	1.0735436	-1.8765752	-2.6334880
H	1.1559826	-3.3641892	-3.6158340
H	-0.0449444	-3.2257512	-2.2798860
H	1.2627946	2.8864848	1.1117240
O	-1.4130404	0.8743178	-2.2488690
H	1.2246106	-3.4229882	2.2044020

Zero-point correction= 0.599758 (Hartree/Particle)

Thermal correction to Energy= 0.644275

Thermal correction to Enthalpy= 0.645219

Thermal correction to Gibbs Free Energy= 0.520140

Sum of electronic and zero-point Energies= -2739.287897

Sum of electronic and thermal Energies= -2739.243380

Sum of electronic and thermal Enthalpies= -2739.242436

Sum of electronic and thermal Free Energies= -2739.367514

D-int5

H	0.7264751	3.6952161	-1.5279812
H	1.0389501	3.7489631	0.2039868
H	2.3123111	3.1784141	-0.9065802
H	-1.7321889	-5.1348859	-0.4563842
H	-0.9652609	-3.5258589	-0.4870082
H	-0.6155229	-4.6328339	0.8337408
H	-4.5841049	-2.9529419	0.6717398
H	-3.5329819	-2.7436489	-0.7414272
H	-4.1735019	-4.3395739	-0.3634122
H	-3.8899189	-4.4837049	2.5620688
H	-2.2178919	-5.0976249	2.6498148
H	-3.3336299	-5.7369789	1.4323768
H	-2.0082189	-2.8222599	2.7890788
H	-1.5718789	1.6623861	-2.2298292
H	-3.0316429	3.6283851	-1.7639272
H	-1.8206739	3.5475311	2.4096758
H	-0.4000709	1.5434191	1.9636238
H	-1.8210769	-1.6566429	-0.6182342
H	-3.7670629	0.5717631	1.9311348
H	-6.4345929	2.0610841	1.4433978
H	-5.4984649	0.5805321	-3.2627862
H	-7.5394429	1.9227171	-2.7147822
H	-7.9853199	2.6466531	-0.4008802
C	1.2344711	3.1699211	-0.7087852
C	-1.4105959	-4.2873079	0.1621998
C	-3.7834399	-3.4171839	0.0837468
C	-3.0350669	-4.8291369	1.9676958

C	-2.5900149	-3.7570609	0.9754738
N	-2.1796989	-2.6080979	1.8127278
O	-1.2045369	-0.6687579	2.3986008
C	-1.6945499	-1.3692699	1.5256478
O	-3.1845139	4.7712571	0.5635438
C	-1.6235859	2.1228841	-1.2426312
C	-2.4035329	3.1803421	-0.9965052
C	-2.4904659	3.7887151	0.3473078
C	-1.7103849	3.1305881	1.4109528
C	-0.9433189	2.0600921	1.1739778
C	-0.7294769	1.5092591	-0.2070312
C	0.7427391	1.7736241	-0.5791992
C	1.4339921	0.6224611	-0.7107602
O	0.7032981	-1.6986729	-0.4678162
C	0.4867661	-0.4945689	-0.4739282
N	-0.7614559	0.0522211	-0.2539212
C	-1.8586799	-0.8263399	0.0979748
C	-3.9789529	0.4636561	0.8749308
C	-3.1807249	-0.1570079	-0.0254322
C	-6.2350799	1.7308321	0.4271178
C	-5.0945709	0.9770261	0.1307188
C	-4.8665259	0.5887571	-1.1977982
C	-5.7148579	0.9017591	-2.2480272
C	-6.8423429	1.6466851	-1.9273212
C	-7.0963359	2.0564141	-0.6092752
Au	3.3966411	0.2151351	-1.1697042
C	7.3204931	-1.4375989	-1.5884752

C	7.6230071	-0.1373139	-1.8138912
H	7.9467981	-2.3169969	-1.5432632
H	8.5674901	0.3508981	-2.0068252
C	5.3935601	-0.2680749	-1.5074522
N	6.4314221	0.5617241	-1.7603412
N	5.9515061	-1.4976289	-1.4044192
C	4.9089531	0.4952471	2.6765948
F	6.2022841	0.7019241	2.8619338
F	4.7436441	-0.4379879	1.7502558
F	4.3523761	0.1023201	3.8026388
S	4.1538501	2.0818191	2.1252448
O	4.1997061	2.9682821	3.2583408
O	2.6547211	1.6182471	1.9277978
O	4.7731871	2.4091321	0.8558508
C	6.3208551	2.0012611	-1.9254152
H	5.2710841	2.2815091	-1.8133432
H	6.8985601	2.5135871	-1.1511032
H	6.6802081	2.2949131	-2.9161692
C	5.2196341	-2.7115989	-1.0851992
H	5.5198281	-3.0860519	-0.1015922
H	4.1502341	-2.4825109	-1.0668872
H	5.4128851	-3.4774009	-1.8420552
O	-3.7040869	-0.1133739	-1.2941402
H	2.4683131	1.2773391	1.0100238

Zero-point correction= 0.595291 (Hartree/Particle)

Thermal correction to Energy= 0.641368

Thermal correction to Enthalpy= 0.642312

Thermal correction to Gibbs Free Energy= 0.511243

Sum of electronic and zero-point Energies= -2739.217755

Sum of electronic and thermal Energies= -2739.171678

Sum of electronic and thermal Enthalpies= -2739.170734

Sum of electronic and thermal Free Energies= -2739.301803

D-ts5

H	1.1545229	0.3440166	3.3726171
H	0.8646809	-1.3944724	3.3419831
H	2.3719619	-0.7328934	2.6368861
H	-0.1687291	-3.4471604	-3.0314619
H	-0.4008991	-1.8626674	-2.3125889
H	-0.2455951	-3.3038274	-1.2697889
H	-3.8298381	-2.6680784	-3.6101469
H	-2.5964751	-1.3910954	-3.5179939
H	-2.2665521	-2.8593144	-4.4365549
H	-3.4899751	-4.8876694	-2.4733299
H	-2.0030521	-5.1896764	-1.5344869
H	-1.9326531	-5.0634144	-3.3018749
H	-3.4983081	-3.4666144	-0.6762609
H	-1.4680881	1.4700396	1.8139711
H	-2.7986541	0.8944716	3.8352161
H	-2.0954451	-3.3356334	3.1260301
H	-0.7541991	-2.7805454	1.1017051
H	-2.0619201	-0.3207874	-1.8646799
H	-4.9893141	0.5983686	0.4156871
H	-6.1627831	3.4255266	0.8889601
H	-1.7737791	4.7347506	-1.1682079

H	-3.4160011	6.4725746	-0.4178839
H	-5.5671221	5.8153106	0.5916921
C	1.2986479	-0.5647444	2.7723111
C	-0.6651691	-2.9183914	-2.2088859
C	-2.7533721	-2.4754074	-3.5318819
C	-2.4171111	-4.6649554	-2.4044879
C	-2.1700231	-3.1616344	-2.2985939
N	-2.8969631	-2.7509984	-1.0712519
O	-4.0194571	-1.5230844	0.4308771
C	-3.1795741	-1.5670014	-0.4567899
O	-3.1131451	-1.5351664	4.6991411
C	-1.5961851	0.4386586	2.1472551
C	-2.3056281	0.1319476	3.2367601
C	-2.4971911	-1.2625454	3.6817771
C	-1.9016601	-2.3084144	2.8263531
C	-1.1891381	-2.0104004	1.7375841
C	-0.8847791	-0.5966164	1.3223771
C	0.6317259	-0.4049354	1.4616491
C	1.1935639	-0.1075744	0.2600511
O	0.1946799	0.2872446	-1.9216089
C	0.1063589	-0.0158174	-0.7470179
N	-1.0666981	-0.3899804	-0.1108899
C	-2.3480631	-0.3299034	-0.8026099
C	-4.2581961	1.2944526	0.0323191
C	-3.0662211	0.9501336	-0.5135459
C	-5.2106681	3.7072166	0.4455051
C	-4.2985991	2.7306376	0.0306031

C	-3.0827521	3.1394686	-0.5345919
C	-2.7242031	4.4658896	-0.7158569
C	-3.6465061	5.4167386	-0.2969469
C	-4.8712371	5.0413446	0.2764131
Au	2.9156139	1.1923106	0.1262141
C	6.7504149	2.9359956	-0.2114739
C	6.0348309	4.0853966	-0.1620789
H	7.8128789	2.7641346	-0.3055389
H	6.3434009	5.1200546	-0.1990969
C	4.5858119	2.3718876	-0.0078939
N	4.7080159	3.7178926	-0.0376829
N	5.8472479	1.8974196	-0.1128609
C	2.8452609	-3.8859224	0.6707361
F	3.5091169	-4.6108554	1.5543311
F	2.5076589	-4.6453964	-0.3587049
F	1.7262189	-3.4298274	1.2431701
S	3.8612769	-2.4625614	0.1147271
O	4.0816389	-1.6766544	1.3335871
O	2.8899539	-1.7832004	-0.8300449
O	5.0180689	-3.0218144	-0.5597269
C	3.6049729	4.6571056	0.0502521
H	2.6730699	4.0902746	0.1116831
H	3.7086849	5.2810956	0.9428721
H	3.5805349	5.2931626	-0.8393089
C	6.1928829	0.4789436	-0.1670439
H	7.2678969	0.3746196	-0.0064429
H	5.6536959	-0.0713104	0.6104181

H	5.9292339	0.0607466	-1.1432919
H	2.1492599	-0.8580184	-0.2018019
O	-2.3318631	2.0571526	-0.8705049

Zero-point correction= 0.590977 (Hartree/Particle)

Thermal correction to Energy= 0.636293

Thermal correction to Enthalpy= 0.637238

Thermal correction to Gibbs Free Energy= 0.507275

Sum of electronic and zero-point Energies= -2739.201302

Sum of electronic and thermal Energies= -2739.155985

Sum of electronic and thermal Enthalpies= -2739.155041

Sum of electronic and thermal Free Energies= -2739.285004

D-int6

H	1.9974171	-2.8499233	0.8584172
H	0.9963931	-4.1215303	0.1204972
H	2.3292111	-3.3358013	-0.8004978
H	-4.8349429	-1.6753263	-3.4070418
H	-3.3765549	-1.0228493	-2.6659468
H	-3.9838049	-2.6239923	-2.1721048
H	-6.1793999	0.8818757	-0.9569288
H	-4.6290049	1.0973077	-1.7937788
H	-6.0308039	0.5110977	-2.6888998
H	-7.1456779	-1.3901163	-0.5538268
H	-6.2648249	-2.8481353	-1.0818428
H	-6.9922189	-1.7610213	-2.2799118
H	-5.1756779	-1.5340713	0.6605022
H	0.3582181	-0.1032103	1.3826252
H	0.1186561	-1.1007613	3.6341142

H	-2.1583919	-4.4081853	1.9638672
H	-1.8878619	-3.4459793	-0.3195048
H	-2.8057479	0.4222767	-1.2588778
H	-2.5291379	1.5305037	2.4098312
H	-0.9986139	4.0009127	3.5006162
H	1.0341411	3.7790847	-1.0894998
H	1.7720271	5.5088917	0.5664592
H	0.7604991	5.6092277	2.8160612
C	1.5256471	-3.1806043	-0.0759748
C	-4.2792329	-1.6085533	-2.4637948
C	-5.5168869	0.4597157	-1.7215108
C	-6.4705959	-1.7967293	-1.3178438
C	-5.1750679	-0.9922763	-1.3932618
N	-4.5787659	-1.1081813	-0.0410568
O	-3.3515169	-0.6477193	1.7813822
C	-3.4963569	-0.5567863	0.5706222
O	-1.0944919	-3.3584873	4.0861992
C	-0.1616339	-1.0489523	1.5347392
C	-0.2815919	-1.5892013	2.7490842
C	-0.9926589	-2.8615333	2.9780012
C	-1.5857239	-3.5014323	1.7837732
C	-1.4432209	-2.9832173	0.5633112
C	-0.6432269	-1.7337313	0.2872422
C	0.5642561	-2.1659303	-0.5622768
C	0.4562761	-1.6123483	-1.8121638
O	-1.2392059	-0.2140713	-2.8614808
C	-0.7953499	-0.8113593	-1.9021318

N	-1.3782649	-0.8674683	-0.6441538
C	-2.4138559	0.1018227	-0.2852978
C	-1.9073549	1.8822967	1.5989472
C	-1.8129589	1.2990487	0.3789212
C	-0.5623439	3.9524017	2.5058452
C	-0.9793799	2.9812737	1.5873762
C	-0.3875219	2.9594327	0.3151982
C	0.5990701	3.8429507	-0.0951788
C	0.9975131	4.7944077	0.8360642
C	0.4238841	4.8475117	2.1166842
Au	1.8810691	-0.0310163	-0.9665938
C	4.3718391	3.0272447	0.5844082
C	4.8074571	3.0189417	-0.6986938
H	4.6958501	3.5952837	1.4439812
H	5.6010251	3.5662367	-1.1853908
C	3.1409281	1.5340667	-0.5375978
N	4.0298331	2.1028807	-1.3754038
N	3.3464321	2.1088787	0.6622762
C	5.7415611	-2.8225103	0.3694162
F	6.3753321	-2.6013853	1.5136062
F	6.6380641	-3.0731153	-0.5760478
F	4.9653711	-3.8958523	0.5135792
S	4.7093151	-1.3791743	-0.0876318
O	3.7749131	-1.2723423	1.0562302
O	4.0712641	-1.8277733	-1.3472558
O	5.6449011	-0.2594163	-0.2374798
C	4.3199531	1.5982487	-2.7075718

H	4.8688261	2.3593337	-3.2672328
H	4.9183481	0.6853157	-2.6150258
H	3.3831281	1.3745487	-3.2247088
C	2.6721211	1.7086827	1.8862702
H	1.5914431	1.8545877	1.7778212
H	2.9095341	0.6578637	2.0878992
H	3.0269411	2.3399667	2.7039732
H	1.0251411	-1.9150563	-2.6891648
O	-0.9039299	1.9430087	-0.4252558

Zero-point correction= 0.595574 (Hartree/Particle)

Thermal correction to Energy= 0.641359

Thermal correction to Enthalpy= 0.642303

Thermal correction to Gibbs Free Energy= 0.513114

Sum of electronic and zero-point Energies= -2739.238861

Sum of electronic and thermal Energies= -2739.193076

Sum of electronic and thermal Enthalpies= -2739.192131

Sum of electronic and thermal Free Energies= -2739.321320

E-1

Au	-3.9640578	-1.1908283	0.7136303
C	-6.6707888	-3.0408153	-1.9383147
C	-7.5451008	-2.8075863	-0.9308977
H	-6.8058738	-3.5046073	-2.9048837
H	-8.5989888	-3.0261113	-0.8361667
C	-5.5400458	-2.0311703	-0.2865037
N	-6.8317588	-2.1846133	0.0763063
N	-5.4442338	-2.5577293	-1.5262797
C	7.9899562	-2.2460273	-0.0845437

F	8.4464882	-1.6298663	1.0035043
F	8.8030912	-1.9664583	-1.0975787
F	8.0207622	-3.5570793	0.1326193
S	6.2835592	-1.6889383	-0.4532227
O	5.5225312	-2.0782863	0.7405063
O	5.9501772	-2.4775893	-1.6706907
O	6.4154352	-0.2488003	-0.6940447
C	-7.4054728	-1.7732333	1.3457653
H	-6.6316418	-1.2727133	1.9320863
H	-8.2336568	-1.0794663	1.1763023
H	-7.7666108	-2.6455323	1.8977723
C	-4.2323678	-2.6242613	-2.3395147
H	-4.3815118	-2.0600083	-3.2643067
H	-3.3839348	-2.2001083	-1.7918197
H	-4.0122488	-3.6675183	-2.5804877
C	1.0634772	4.4118757	-1.3455147
N	-0.5841908	3.1084557	-1.0997177
C	0.3324562	2.7004337	-0.1604067
C	1.4102502	3.5474827	-0.2882297
C	0.0670802	1.4764697	0.6545063
N	-0.0456548	0.2913107	-0.2309887
C	-1.1000138	-0.5590293	-0.1480407
C	1.0596772	-0.0670633	-1.0828517
O	-1.3672278	-1.4561553	-0.9350807
C	-1.9353718	-0.3911933	1.0654333
C	-2.2766628	-0.3237763	2.2491603
C	1.3784872	0.6569777	-2.2321507

C	2.5080962	0.3263797	-2.9622157
C	3.3399192	-0.7309773	-2.5618437
C	2.9925232	-1.4772663	-1.4206027
C	1.8677862	-1.1373173	-0.6933537
O	4.4173292	-0.9866203	-3.2921657
H	-0.9046528	1.5949967	1.1395173
C	1.0064852	1.1778797	1.8340603
O	0.4948492	0.9213387	2.9234433
N	2.3196932	1.1821117	1.5595383
C	3.4129502	0.7643387	2.4794603
C	3.3056982	-0.7310533	2.7555783
C	4.7060422	1.0760617	1.7421413
C	3.3319942	1.5748747	3.7673263
C	-2.4795468	-0.1172713	3.6680083
H	2.3252032	3.5285507	0.2881023
H	0.7611592	1.4961117	-2.5448807
H	2.7892882	0.8903557	-3.8475437
H	3.6324562	-2.2946873	-1.0983777
H	1.6152872	-1.6932763	0.2096363
H	5.0389392	-1.5771013	-2.7909287
H	2.5815112	1.2331377	0.5795963
H	3.4682302	-1.3069363	1.8372073
H	4.0935702	-1.0330083	3.4559793
H	2.3323062	-0.9763593	3.1966703
H	5.5658132	0.7331517	2.3277713
H	4.8090942	2.1571847	1.5750163
H	4.7717012	0.5536927	0.7792943

H	4.1961022	1.3304247	4.3964173
H	2.4161652	1.3573817	4.3236233
H	3.3643462	2.6496807	3.5480663
H	-1.5431148	0.3316497	4.0300473
H	-2.6622288	-1.0575933	4.1963863
H	-3.3069258	0.5718637	3.8650083
H	1.6466562	5.2227537	-1.7644987
N	-0.1332758	4.1409137	-1.8455997
C	-1.8544958	2.5384497	-1.3841187
C	-2.8378558	2.5021667	-0.3988077
C	-2.1014858	2.0100767	-2.6496037
C	-4.0600048	1.8935477	-0.6695907
H	-2.6471508	2.9678137	0.5661183
C	-3.3262168	1.4104257	-2.9148227
H	-1.3280818	2.0749577	-3.4103857
C	-4.3021238	1.3369147	-1.9231877
H	-4.8331488	1.8722387	0.0968363
H	-3.5158998	0.9968027	-3.9022577
H	-5.2609988	0.8647977	-2.1314177

Zero-point correction= 0.628804 (Hartree/Particle)

Thermal correction to Energy= 0.677840

Thermal correction to Enthalpy= 0.678784

Thermal correction to Gibbs Free Energy= 0.540348

Sum of electronic and zero-point Energies= -2812.663097

Sum of electronic and thermal Energies= -2812.614061

Sum of electronic and thermal Enthalpies= -2812.613117

Sum of electronic and thermal Free Energies= -2812.751554

E-ts1

H	0.5434306	-4.1992783	-1.6760583
H	2.1681366	-4.3498753	-2.3948413
H	1.9047656	-4.7864713	-0.6881693
H	-1.1532964	5.2446777	1.1071347
H	-1.3962164	3.5074347	0.9595417
H	0.2077186	4.2287777	0.5972467
H	-3.1205384	4.8505037	-2.0768923
H	-3.2907734	3.7561277	-0.6873263
H	-3.1942674	5.5126767	-0.4307953
H	-0.9581374	6.1195797	-2.4491733
H	0.4113486	5.8811267	-1.3364893
H	-1.0491084	6.7439027	-0.7967553
H	-0.6064464	3.9160267	-2.7927603
H	-4.1120374	-3.9593903	-2.1131483
H	-1.3021754	-1.7260253	0.6310877
H	-2.8851024	-3.4238093	-0.2672463
H	-2.0514424	-2.1188283	-4.2575753
H	-0.4582164	-0.3907273	-3.3567823
H	0.1539866	1.8823157	0.2097787
H	-3.2057384	1.3919317	-1.7924363
C	1.6195566	-4.0920723	-1.4839613
C	-0.8790614	4.3638087	0.5153687
C	-2.8175394	4.6792937	-1.0368183
C	-0.6825384	5.9108367	-1.4069453
C	-1.2974204	4.5952857	-0.9292623
N	-0.7700304	3.5651987	-1.8543913

O	0.1627376	1.7734397	-2.8087403
C	-0.3619254	2.2641407	-1.8201603
O	-3.4636724	-3.7098963	-2.8233533
C	-1.4579714	-1.8229353	-0.4441033
C	-2.3274104	-2.7770533	-0.9367023
C	-2.5778304	-2.8580033	-2.3168043
C	-1.8586864	-2.0307653	-3.1913013
C	-0.9799724	-1.0788713	-2.6964673
C	-0.7951724	-0.9614663	-1.3189813
C	1.8442266	-2.7089163	-1.0992993
C	1.7556906	-1.5086753	-0.8329393
O	2.1697756	0.7180757	-0.1660263
C	1.3569196	-0.1121073	-0.5657343
N	0.0443926	0.0809307	-0.7805093
C	-0.5060564	1.4260727	-0.5358253
C	-3.0777244	1.2070877	-0.7328483
C	-1.9000044	1.2811507	-0.0266843
N	-2.1986404	0.8981667	1.2649857
C	-4.0405454	0.7719957	0.2003617
Au	3.9151266	-1.8408263	-0.3811983
C	7.5961646	-0.1450713	0.7943937
C	7.9804806	-1.4434713	0.8131727
H	8.1403726	0.7613417	1.0172527
H	8.9265766	-1.9039553	1.0585557
C	5.8245216	-1.3799593	0.1938077
N	6.8772586	-2.1884233	0.4410627
N	6.2690136	-0.1244733	0.4134687

C	-5.4355084	-2.5893043	1.3569547
F	-5.9271444	-1.4346073	1.7966287
F	-4.1014744	-2.5524773	1.5190207
F	-5.9030054	-3.5666763	2.1253697
S	-5.8909594	-2.8485743	-0.4073783
O	-7.3392874	-3.0083933	-0.3566433
O	-5.1285334	-4.0857213	-0.7394973
O	-5.3687534	-1.6440403	-1.0642273
C	6.8688986	-3.6382553	0.3469287
H	7.6065456	-3.9716393	-0.3882653
H	7.0966806	-4.0801253	1.3209507
H	5.8751806	-3.9626613	0.0302977
C	5.4881046	1.0983447	0.2466827
H	5.8198886	1.6301807	-0.6493733
H	4.4236766	0.8576037	0.1495827
H	5.6305526	1.7352877	1.1233427
C	-1.3338784	0.5540217	2.3374587
C	-1.6253184	-0.6037253	3.0642587
C	-0.2310754	1.3347887	2.6817957
C	-0.7984664	-0.9820533	4.1131977
H	-2.5060994	-1.1803903	2.7933947
C	0.5991806	0.9346457	3.7241687
H	-0.0345584	2.2723617	2.1700237
C	0.3224736	-0.2233703	4.4417047
H	-1.0333484	-1.8821473	4.6763017
H	1.4553036	1.5514087	3.9879267
H	0.9679796	-0.5260953	5.2627827

H	-5.0838864	0.5373557	0.0294367
N	-3.5096734	0.5837027	1.3954627

Zero-point correction= 0.628380 (Hartree/Particle)

Thermal correction to Energy= 0.676821

Thermal correction to Enthalpy= 0.677765

Thermal correction to Gibbs Free Energy= 0.540064

Sum of electronic and zero-point Energies= -2812.652172

Sum of electronic and thermal Energies= -2812.603730

Sum of electronic and thermal Enthalpies= -2812.602786

Sum of electronic and thermal Free Energies= -2812.740487

E-int1

H	0.3614188	-3.8491507	-1.2255360
H	0.7818838	-3.3020007	-2.8460540
H	2.0705388	-3.6235507	-1.6638280
H	-0.3456012	5.1766443	1.3094180
H	-0.8488452	3.4954953	1.2632790
H	0.6456958	4.0054663	0.4154850
H	-3.2668952	5.0528673	-1.0929310
H	-3.0776022	3.8153763	0.1669690
H	-2.8131292	5.5305963	0.5565610
H	-1.2374062	6.2334953	-2.0501170
H	0.3781588	5.8838243	-1.3893860
H	-0.8264542	6.7560503	-0.4106740
H	-1.2275522	4.0491673	-2.5943720
H	-4.5260582	-3.3754497	-1.8228090
H	-0.9478962	-1.7084027	0.6259040
H	-2.9995702	-2.8724167	-0.1424110

H	-2.1888192	-1.6314437	-4.2190950
H	-0.1670252	-0.3832087	-3.4475450
H	-0.0550242	2.0260253	0.1127460
H	-3.4750762	1.4794193	-1.5256510
C	1.0619778	-3.2169937	-1.7875450
C	-0.3845332	4.2893223	0.6670340
C	-2.6775102	4.7618773	-0.2146120
C	-0.6875832	5.9521533	-1.1421890
C	-1.1997142	4.6283853	-0.5764650
N	-1.0370012	3.6529643	-1.6790240
O	-0.9537642	1.7927743	-2.9228090
C	-0.9059192	2.3025803	-1.8119320
O	-3.7066292	-2.9732957	-2.6770620
C	-1.2468262	-1.7028067	-0.4230910
C	-2.3473882	-2.3496097	-0.8362000
C	-2.7041382	-2.3532307	-2.2457770
C	-1.8668422	-1.6333357	-3.1814640
C	-0.7817962	-0.9595507	-2.7631380
C	-0.3031552	-1.0098077	-1.3515210
C	1.0310358	-1.8066247	-1.3214040
C	2.0311178	-1.0542687	-0.8330200
O	2.0553458	1.2573283	-0.0457770
C	1.4832958	0.2839033	-0.5186160
N	0.1320398	0.2782193	-0.8411490
C	-0.6814802	1.4437853	-0.5627670
C	-3.2488862	1.1822723	-0.5093790
C	-2.0002752	1.1236363	0.0670800

N	-2.1889322	0.6710973	1.3588890
C	-4.1357992	0.7479033	0.4927880
Au	4.0134058	-1.3866337	-0.4361480
C	8.0871718	-0.8788677	0.7470340
C	8.1632458	-2.1828357	0.3920010
H	8.8360038	-0.2015567	1.1320580
H	8.9910648	-2.8772857	0.4041420
C	6.0370168	-1.5087257	0.0442760
N	6.8996148	-2.5491687	-0.0348790
N	6.7803028	-0.4843037	0.5281480
C	-5.9339852	-2.5218817	1.1842600
F	-6.5473952	-1.4700397	1.7066120
F	-4.6319542	-2.4273777	1.4453920
F	-6.4003172	-3.6257227	1.7417050
S	-6.2315102	-2.5375647	-0.6291350
O	-7.6327482	-2.8662327	-0.7783850
O	-5.3036582	-3.6962497	-1.0362170
O	-5.7159242	-1.2660657	-1.1176110
C	6.5485268	-3.8764377	-0.5043230
H	5.4894558	-3.8749107	-0.7731480
H	7.1438528	-4.1378667	-1.3843080
H	6.7196128	-4.6157987	0.2838510
C	6.2802238	0.8581893	0.7803200
H	6.8003368	1.5792773	0.1428430
H	5.2097588	0.8871443	0.5549250
H	6.4343408	1.1232633	1.8304650
C	-1.2516992	0.2005083	2.3232680

C	-1.6263232	-0.8883007	3.1170120
C	0.0146908	0.7622783	2.4717410
C	-0.7308562	-1.4102367	4.0402690
H	-2.6192512	-1.3087617	2.9881770
C	0.9115798	0.2120233	3.3815240
H	0.3360538	1.6136993	1.8825310
C	0.5460508	-0.8707907	4.1717870
H	-1.0325862	-2.2571407	4.6520230
H	1.9040768	0.6483563	3.4657430
H	1.2498878	-1.2930167	4.8846770
H	-5.2100432	0.6298913	0.4305660
N	-3.4994002	0.4316633	1.6060020

Zero-point correction= 0.629304 (Hartree/Particle)

Thermal correction to Energy= 0.676736

Thermal correction to Enthalpy= 0.677680

Thermal correction to Gibbs Free Energy= 0.543251

Sum of electronic and zero-point Energies= -2812.698834

Sum of electronic and thermal Energies= -2812.651403

Sum of electronic and thermal Enthalpies= -2812.650458

Sum of electronic and thermal Free Energies= -2812.784887

E-ts2

H	-0.7707622	-3.5328557	-1.2222836
H	-0.4142632	-2.8753627	-2.8140556
H	0.9149618	-3.4693837	-1.7876376
H	2.6598828	2.6005793	-2.9760056
H	1.4508578	1.4714843	-2.3350206
H	1.2220518	2.1992743	-3.9387836

H	0.7917088	4.6693593	-0.4288056
H	1.5740108	3.0620843	-0.2836526
H	2.4141908	4.3841823	-1.0814896
H	0.4902808	5.6602403	-2.7909976
H	0.5517498	4.5817853	-4.2091796
H	2.0450208	5.0212013	-3.3664376
H	-1.1540112	3.7704853	-2.9696326
H	-4.8905812	-2.9792027	-1.9958606
H	-1.6343362	-1.2882967	0.7442924
H	-3.6046822	-2.5757187	-0.1138426
H	-2.9870542	-0.8633767	-4.0046996
H	-0.9523822	0.3535463	-3.2173006
H	-0.1710162	2.3937203	0.3230494
H	-3.6685202	0.6497273	-0.5990236
C	-0.0414752	-2.9362107	-1.7841006
C	1.5854478	2.3864643	-2.9204426
C	1.4266718	3.9301333	-0.9353626
C	0.9862828	4.7814503	-3.2207236
C	0.8449788	3.5694363	-2.3011156
N	-0.6132012	3.3066483	-2.2470936
O	-2.6825592	2.7688113	-1.5687416
C	-1.4752782	2.6784993	-1.4000456
O	-4.2878942	-2.5547237	-2.6855606
C	-2.0654232	-1.0298257	-0.2289616
C	-3.0053962	-1.9552357	-0.7720176
C	-3.3333152	-1.8700677	-2.1078126
C	-2.6041422	-0.9695597	-2.9929606

C	-1.5195902	-0.3089637	-2.5651046
C	-0.9815472	-0.5268757	-1.1863016
C	0.1491398	-1.5913777	-1.1824536
C	1.2436168	-1.1332587	-0.5438436
O	1.6385078	0.9920323	0.5864624
C	0.9652088	0.2466003	-0.1088336
N	-0.2635562	0.6240883	-0.6674736
C	-0.9304892	1.8390403	-0.2379746
C	-3.0754292	0.5034503	0.2988754
C	-2.0312912	1.3991173	0.6650374
N	-1.9581752	1.3921103	1.9987854
C	-3.6398982	0.1414173	1.5821424
Au	3.0416118	-1.9887897	-0.0549656
C	6.9298278	-2.8457547	1.5105344
C	6.7063678	-4.0314987	0.8972204
H	7.7733068	-2.4893937	2.0843654
H	7.3140868	-4.9221717	0.8260794
C	4.8954778	-2.7322067	0.5395024
N	5.4577028	-3.9422237	0.3094074
N	5.8122688	-2.0647947	1.2809244
C	-6.1955812	-3.0027007	1.7088044
F	-6.6911642	-2.1409677	2.5926484
F	-4.8734292	-3.0863517	1.9276084
F	-6.7275382	-4.1943507	1.9258544
S	-6.5215292	-2.4153127	0.0011234
O	-7.9710662	-2.4085977	-0.1104136
O	-5.8198672	-3.4641697	-0.7970176

O	-5.8317192	-1.1150407	-0.0301256
C	4.8347268	-5.0113927	-0.4493396
H	3.8557288	-4.6653027	-0.7898866
H	5.4487808	-5.2682427	-1.3176306
H	4.7046098	-5.8968697	0.1798644
C	5.6501118	-0.7078177	1.7767424
H	6.4293878	-0.0602527	1.3640174
H	4.6698638	-0.3337297	1.4671014
H	5.7093208	-0.6979277	2.8690874
H	-4.5119982	-0.4844747	1.7372184
C	-1.0135012	2.0449403	2.8380414
C	-0.6518382	3.3645083	2.5778524
C	-0.4718842	1.3461713	3.9114344
C	0.3034838	3.9751423	3.3805654
H	-1.1368382	3.9131333	1.7721434
C	0.4688108	1.9745673	4.7167234
H	-0.7968732	0.3271193	4.1000074
C	0.8660898	3.2813863	4.4472164
H	0.5931588	5.0036713	3.1812254
H	0.8979378	1.4364233	5.5578994
H	1.6075378	3.7649253	5.0781594
N	-2.9536742	0.6216763	2.5829984

Zero-point correction= 0.629891 (Hartree/Particle)

Thermal correction to Energy= 0.676957

Thermal correction to Enthalpy= 0.677901

Thermal correction to Gibbs Free Energy= 0.541886

Sum of electronic and zero-point Energies= -2812.664525

Sum of electronic and thermal Energies= -2812.617458

Sum of electronic and thermal Enthalpies= -2812.616514

Sum of electronic and thermal Free Energies= -2812.752529

E-int2

H	-0.2036615	-3.6880459	-0.8578774
H	0.1598645	-3.1180109	-2.4772734
H	1.4971965	-3.5227089	-1.3672054
H	2.5610085	2.1472261	-3.3714324
H	1.4392445	1.0958921	-2.4885714
H	1.0524365	1.6184581	-4.1430204
H	0.8875365	4.5126381	-0.9492784
H	1.6033135	2.9054461	-0.6245024
H	2.4644685	4.0674261	-1.6261454
H	0.4025375	5.2011511	-3.3570134
H	0.3695145	3.9652621	-4.6430204
H	1.9150165	4.4956651	-3.9614934
H	-1.2525175	3.4146801	-3.1216514
H	-4.2457405	-3.6655099	-1.9191404
H	-1.3363855	-1.4511919	0.8608066
H	-3.1189495	-3.0004339	0.0295416
H	-2.5181245	-1.4328209	-3.9138174
H	-0.6738385	0.0435991	-3.1398554
H	-0.1866885	2.3194351	0.3609066
H	-3.3560195	0.1733941	-0.7762684
C	0.4996955	-3.0749709	-1.4351624
C	1.5007635	1.9317261	-3.1917094
C	1.4663125	3.6850231	-1.3814114

C	0.8703315	4.2764451	-3.7169054
C	0.8026405	3.1779601	-2.6576474
N	-0.6513475	2.9354971	-2.4583174
O	-2.6187255	2.7458521	-1.3824314
C	-1.4141525	2.5015331	-1.4275524
O	-3.6464675	-3.2432589	-2.5923414
C	-1.7980745	-1.2117849	-0.1086884
C	-2.5805495	-2.3484719	-0.6511724
C	-2.8268895	-2.3955979	-1.9834084
C	-2.1680585	-1.4473309	-2.8838754
C	-1.1819485	-0.6422529	-2.4644934
C	-0.6663775	-0.7393149	-1.0542964
C	0.5438375	-1.6791979	-0.9288794
C	1.5722965	-1.0881449	-0.2837104
O	1.7324495	1.1389791	0.7052126
C	1.1615505	0.2840281	0.0436766
N	-0.0795225	0.5119841	-0.5737744
C	-0.8447365	1.6887741	-0.2590234
C	-2.7879575	0.0291411	0.1538196
C	-2.0257265	1.2207291	0.5282836
N	-2.3905015	1.5768881	1.7313536
C	-3.6378815	-0.1344109	1.3546936
Au	3.4002795	-1.7952249	0.3182236
C	7.2712725	-2.4710489	2.0284706
C	7.1008245	-3.6774939	1.4390096
H	8.0863605	-2.0754609	2.6174076
H	7.7360405	-4.5511239	1.4078936

C	5.2636285	-2.4418649	0.9960176
N	5.8680055	-3.6399169	0.8131116
N	6.1385105	-1.7299559	1.7464876
C	-5.7718875	-3.4860349	1.7877696
F	-6.4385385	-2.6331319	2.5619466
F	-4.4635105	-3.3286219	2.0609696
F	-6.1144845	-4.7208219	2.1163796
S	-6.0972985	-3.1304599	0.0163886
O	-7.5296015	-3.3387639	-0.1327324
O	-5.2253625	-4.1369249	-0.6452404
O	-5.6035905	-1.7475979	-0.1171454
C	5.3001185	-4.7467059	0.0647706
H	4.3230665	-4.4389879	-0.3162104
H	5.9490945	-5.0085599	-0.7761994
H	5.1747135	-5.6184629	0.7137786
C	5.9205295	-0.3677219	2.2029576
H	6.6973965	0.2922861	1.8056066
H	4.9436785	-0.0307439	1.8448686
H	5.9349765	-0.3301239	3.2962576
H	-4.4063875	-0.8961779	1.4678716
C	-1.9570205	2.6981651	2.4937116
C	-1.7953035	3.9253491	1.8554556
C	-1.7343495	2.5423391	3.8574626
C	-1.3582645	5.0124311	2.6024846
H	-2.0559325	4.0257621	0.8030046
C	-1.3057595	3.6411001	4.5897596
H	-1.9032715	1.5750291	4.3215696

C	-1.1098805	4.8701621	3.9641376
H	-1.2319285	5.9783101	2.1208066
H	-1.1241595	3.5367521	5.6560056
H	-0.7749915	5.7254791	4.5453436
N	-3.3981455	0.7373891	2.2756726

Zero-point correction= 0.631212 (Hartree/Particle)

Thermal correction to Energy= 0.678369

Thermal correction to Enthalpy= 0.679313

Thermal correction to Gibbs Free Energy= 0.544575

Sum of electronic and zero-point Energies= -2812.667134

Sum of electronic and thermal Energies= -2812.619977

Sum of electronic and thermal Enthalpies= -2812.619033

Sum of electronic and thermal Free Energies= -2812.753771

E-ts3

H	-2.5784064	1.6839304	-1.3941031
H	-2.0979824	0.9116004	-2.8977571
H	-3.2403854	0.0949024	-1.8097121
H	1.8478946	-3.4722836	-3.0770621
H	1.1829536	-1.9918696	-2.3593061
H	2.0204086	-1.9232556	-3.9264781
H	4.3177806	-2.6294676	-0.3440161
H	2.5340766	-2.7961106	-0.2877521
H	3.5049186	-3.9985396	-1.1228511
H	5.4615936	-2.5339796	-2.6481591
H	4.4989726	-2.1194616	-4.0911511
H	4.3516196	-3.7239946	-3.3603261
H	4.2183046	-0.3086606	-2.7707991

H	-1.5780784	4.8302594	-1.7973511
H	-0.9069744	1.4717394	0.7441909
H	-0.9001084	3.8994374	0.2093039
H	0.6696986	2.9462114	-3.6691591
H	1.1057236	0.6004224	-2.9818011
H	2.6130586	-0.9476416	0.5592809
H	1.1782176	3.1167584	0.1045139
C	-2.3359994	0.7106134	-1.8446611
C	2.0196686	-2.3982846	-2.9369471
C	3.4251266	-2.9257456	-0.9113731
C	4.4873256	-2.6608116	-3.1356501
C	3.3555966	-2.1700946	-2.2344951
N	3.6154216	-0.7175726	-2.0638601
O	3.7526786	1.3710254	-1.2487601
C	3.2869486	0.2372184	-1.1616201
O	-0.7766004	4.5802644	-2.3203191
C	-0.0923294	1.8203614	0.1010989
C	-0.3496764	3.2147854	-0.4337441
C	-0.2805524	3.4858974	-1.7817981
C	0.4064496	2.5749654	-2.6823341
C	0.6336586	1.3109434	-2.3037401
C	0.1277306	0.7487914	-1.0083761
C	-1.2090694	0.0254464	-1.1601321
C	-1.2104954	-1.1386706	-0.4717871
O	0.6220716	-2.2410846	0.7332659
C	0.1630626	-1.3624266	0.0250369
N	0.9701876	-0.3203916	-0.4943321

C	2.3075056	-0.0606446	-0.0174951
C	1.1777536	2.0546604	0.8921799
C	2.2522386	1.1283054	0.8968549
N	2.9840446	1.3835834	1.9764329
C	1.3471676	2.7428894	2.1572809
Au	-2.9994944	-1.9453306	0.1515889
C	-6.8910504	-3.1998156	1.5114819
C	-7.1103614	-1.8888376	1.2509339
H	-7.5477724	-3.9730616	1.8834449
H	-8.0013994	-1.2845646	1.3435459
C	-4.9499604	-2.3147156	0.7774079
N	-5.9140024	-1.3626566	0.8068009
N	-5.5615774	-3.4406596	1.2146749
C	-3.6091804	3.1873434	1.3315899
F	-2.6844864	3.9778674	1.8863259
F	-3.0206494	1.9974064	1.1024949
F	-4.5748424	2.9858114	2.2176009
S	-4.2787154	3.8958274	-0.2311751
O	-5.0166324	5.0683224	0.2180739
O	-5.0460364	2.7643374	-0.7601011
O	-3.0350964	4.1849794	-0.9876171
C	-5.7364314	0.0240264	0.3801559
H	-4.6899134	0.3122534	0.4950869
H	-6.0194394	0.1531414	-0.6680631
H	-6.3480714	0.6841454	0.9997069
C	-4.9081854	-4.7262886	1.3624969
H	-5.3950254	-5.4753146	0.7303379

H	-3.8652384	-4.6178486	1.0550449
H	-4.9436824	-5.0541096	2.4060049
H	0.7216286	3.5340044	2.5591519
C	4.1619826	0.7205924	2.4306289
C	5.1915796	0.4417574	1.5370709
C	4.2434286	0.3686264	3.7752639
C	6.3126886	-0.2374256	2.0027299
H	5.1259296	0.7949214	0.5106129
C	5.3730676	-0.3005756	4.2242309
H	3.4265356	0.6222484	4.4447089
C	6.4032696	-0.6112386	3.3392619
H	7.1269796	-0.4572386	1.3171669
H	5.4471976	-0.5855316	5.2703159
H	7.2841696	-1.1381656	3.6970569
N	2.4455876	2.3917474	2.7637259

Zero-point correction= 0.628079 (Hartree/Particle)

Thermal correction to Energy= 0.674071

Thermal correction to Enthalpy= 0.675015

Thermal correction to Gibbs Free Energy= 0.546632

Sum of electronic and zero-point Energies= -2812.617657

Sum of electronic and thermal Energies= -2812.571666

Sum of electronic and thermal Enthalpies= -2812.570721

Sum of electronic and thermal Free Energies= -2812.699105

E-int3

H	0.2552838	-4.1237257	0.1264391
H	0.3170368	-3.5010127	1.7813571
H	-1.2351352	-4.0028407	1.0705931

H	-0.8247672	5.8588033	2.0679101
H	0.5521048	4.8747973	1.5039211
H	-0.5855792	5.5633643	0.3277261
H	-1.9174122	2.3518543	2.8736291
H	-0.2654052	2.9923263	3.0716701
H	-1.6688642	3.9714533	3.5640261
H	-3.4468482	3.3080153	1.1198991
H	-2.8867322	4.6349283	0.0724101
H	-3.2089672	4.9351123	1.7930401
H	-1.6200332	2.4508103	-0.1838879
H	5.5289098	-2.9435867	1.4473121
H	1.3930768	-1.9856297	-1.5298569
H	2.2915788	-3.4007187	0.2481801
H	2.4964098	-0.8175847	3.1848331
H	0.3199408	-0.1513027	2.2206861
H	-0.1175972	1.6283073	-1.6006649
C	-0.2821182	-3.5060977	0.8607021
C	-0.5006682	5.1174623	1.3267161
C	-1.2969152	3.2558703	2.8199681
C	-2.8132492	4.2040503	1.0788841
C	-1.3686522	3.8654513	1.4218131
N	-0.9202262	2.8916463	0.4128081
O	1.2123228	2.5556613	1.1913851
C	0.3084978	2.3265583	0.4016111
O	4.2629808	-2.1832837	1.9339951
C	1.7922028	-1.4749477	-0.6393309
C	2.7558318	-2.4184187	0.0798841

C	3.1730158	-1.9055047	1.4298211
C	2.2061938	-1.1106127	2.1789771
C	1.0333808	-0.7409167	1.6422151
C	0.5862088	-1.0940387	0.2496031
C	-0.5336892	-2.1332527	0.3432641
C	-1.7141122	-1.6295507	-0.0718499
O	-2.2777752	0.5953073	-0.9256329
C	-1.4750282	-0.2332887	-0.4970619
N	-0.1338932	0.0284353	-0.3333089
C	0.4654968	1.2884963	-0.7307719
C	2.4968578	-0.2083707	-1.0301099
C	1.8859118	1.0229223	-1.0723129
N	2.8468028	1.9371393	-1.3793169
C	3.8532278	0.0647293	-1.3185189
Au	-3.6157522	-2.3690627	-0.2530749
C	-7.7842432	-2.7418587	-1.1173239
C	-7.5897572	-3.9918357	-0.6355139
H	-8.6709142	-2.2568497	-1.4998639
H	-8.2710482	-4.8212637	-0.5108019
C	-5.6100452	-2.9108567	-0.5350569
N	-6.2541872	-4.0751507	-0.2849379
N	-6.5639372	-2.0962487	-1.0477549
C	5.8370698	-5.2448977	-0.5273639
F	5.8933248	-5.5584317	-1.8089019
F	4.5642008	-5.1504167	-0.1541989
F	6.4316698	-6.1795397	0.1873181
S	6.6595958	-3.6235067	-0.2689009

O	8.0661158	-3.8309617	-0.4967439
O	6.3969328	-3.4435927	1.2618291
O	5.8818098	-2.6703037	-1.0404379
C	-5.6288122	-5.2579157	0.2760641
H	-4.5725092	-5.0370917	0.4474131
H	-6.1010592	-5.5232087	1.2267621
H	-5.7134572	-6.0983247	-0.4194289
C	-6.3423002	-0.7241737	-1.4773549
H	-6.9871222	-0.0458197	-0.9109169
H	-5.2957942	-0.4596867	-1.2977979
H	-6.5586772	-0.6254857	-2.5451949
H	3.6510448	-2.5988327	-0.5244459
H	4.6859428	-0.6295757	-1.3817789
N	4.0602588	1.3576513	-1.5238029
C	2.7284908	3.3487983	-1.4184519
C	1.6234218	3.9449733	-2.0195769
C	3.7231608	4.1268343	-0.8320349
C	1.4990558	5.3302313	-2.0046089
H	0.8775478	3.3315223	-2.5194559
C	3.5958218	5.5088333	-0.8359849
H	4.5748348	3.6307643	-0.3766959
C	2.4815838	6.1152713	-1.4118409
H	0.6349838	5.7951263	-2.4739139
H	4.3691798	6.1179543	-0.3741949
H	2.3839638	7.1981113	-1.4036899

Zero-point correction= 0.632458 (Hartree/Particle)

Thermal correction to Energy= 0.679619

Thermal correction to Enthalpy= 0.680563

Thermal correction to Gibbs Free Energy= 0.544830

Sum of electronic and zero-point Energies= -2812.735983

Sum of electronic and thermal Energies= -2812.688822

Sum of electronic and thermal Enthalpies= -2812.687878

Sum of electronic and thermal Free Energies= -2812.823611

E-int4

H	-1.9723545	1.2236543	3.5422290
H	-1.7900795	2.4773843	2.3067090
H	-3.2126455	1.4071333	2.2986260
H	4.7488785	1.2168683	-3.8358080
H	5.0694395	0.0546823	-2.5236850
H	3.6030255	-0.1109027	-3.5201400
H	3.9752435	3.1005863	-0.6658290
H	5.2866865	1.9106113	-0.8754720
H	4.9667975	3.1168953	-2.1380220
H	1.9085175	2.9537383	-2.0874140
H	1.6999425	1.6128843	-3.2433080
H	2.8642135	2.9169823	-3.5854460
H	3.2131525	0.8987073	-0.0570470
H	0.3062825	-0.4884887	3.3312460
H	0.0393815	1.8548573	3.9656150
H	1.4609295	3.7045463	0.8872230
H	0.1793335	1.9168013	-0.2458330
H	1.4260895	-2.1016387	-0.2432300
C	-2.1331855	1.4480473	2.4782130
C	4.2811505	0.6085473	-3.0515120

C	4.4937725	2.4642753	-1.3959140
C	2.4289505	2.2938893	-2.7943450
C	3.5242335	1.5090263	-2.0789580
N	2.9304625	0.6908553	-1.0065040
O	1.5940055	-0.6575207	-2.2781960
C	2.0549885	-0.3250747	-1.1996320
O	2.3401195	3.5100613	3.3281390
C	0.8813935	0.2570763	2.7588060
C	1.0214215	1.5293673	3.5963760
C	1.6052445	2.6867033	2.8162970
C	1.1788245	2.7905603	1.4078450
C	0.4947445	1.8146933	0.7960090
C	0.0996175	0.5126673	1.4421510
C	-1.4210335	0.4690873	1.6120130
C	-1.9710965	-0.5314327	0.8903180
O	-0.9219085	-2.3044477	-0.4176340
C	-0.8647805	-1.2736807	0.2289370
N	0.3069775	-0.5886777	0.5117150
C	1.6038665	-1.0669027	0.0831350
C	2.2309925	-0.3072097	2.4222800
C	2.5354975	-0.9446957	1.2394190
N	3.8665115	-1.2609247	1.2870640
C	3.4528165	-0.2866407	3.1305820
Au	-3.8682185	-1.2885767	0.6101240
C	-7.1369735	-3.6743367	-0.7321440
C	-7.8528135	-2.6242077	-0.2645240
H	-7.4476915	-4.5907347	-1.2129350

H	-8.9159685	-2.4315307	-0.2627300
C	-5.6796125	-2.1887237	0.1330200
N	-6.9436845	-1.7285617	0.2650480
N	-5.8083925	-3.3888187	-0.4814870
C	-4.6942355	3.7077383	-1.2728870
F	-3.9367825	4.4866443	-0.5268100
F	-5.9418945	4.1448043	-1.2517780
F	-4.2469235	3.6915053	-2.5113490
S	-4.7138705	2.0015493	-0.5852330
O	-3.1575605	1.7565193	-0.7494340
O	-5.4944575	1.1849043	-1.4912090
O	-5.0865375	2.1022703	0.8135080
C	-7.2966995	-0.4234337	0.7999150
H	-6.4721435	-0.0564057	1.4151290
H	-7.4588485	0.2884023	-0.0153300
H	-8.1996105	-0.5127887	1.4101730
C	-4.7029125	-4.2690047	-0.8261590
H	-4.7993345	-4.5891957	-1.8673610
H	-3.7610885	-3.7248117	-0.7077490
H	-4.6961075	-5.1474087	-0.1735970
H	1.6451815	1.3618493	4.4811460
H	-2.8597585	0.9496743	-0.2426200
C	4.6951385	-1.7590167	0.2472490
C	5.9892225	-1.2545267	0.1253030
C	4.2188655	-2.7125867	-0.6486280
C	6.7997705	-1.7003037	-0.9103570
H	6.3376005	-0.5244557	0.8502210

C	5.0338745	-3.1365337	-1.6924880
H	3.2255915	-3.1353317	-0.5268230
C	6.3231045	-2.6334737	-1.8283850
H	7.8095225	-1.3080867	-1.0051880
H	4.6559675	-3.8737177	-2.3960230
H	6.9573355	-2.9706397	-2.6442720
H	3.6605515	0.1220303	4.1134950
N	4.4339775	-0.8536327	2.4461540

Zero-point correction= 0.630929 (Hartree/Particle)

Thermal correction to Energy= 0.678595

Thermal correction to Enthalpy= 0.679539

Thermal correction to Gibbs Free Energy= 0.543752

Sum of electronic and zero-point Energies= -2812.726750

Sum of electronic and thermal Energies= -2812.679083

Sum of electronic and thermal Enthalpies= -2812.678139

Sum of electronic and thermal Free Energies= -2812.813927

E-ts4

H	-2.3789219	0.9675874	3.0663660
H	-1.7315429	2.4699384	2.3914560
H	-3.2709569	1.7813104	1.7787690
H	5.4793931	2.0636474	-3.0786310
H	5.4470361	0.5542434	-2.1323980
H	4.1726651	0.8812584	-3.3328770
H	4.3445701	3.1182134	0.3503330
H	5.5579501	1.8609604	-0.0079450
H	5.5703531	3.3937374	-0.9030310
H	2.5546211	3.6496344	-1.3267680

H	2.4110591	2.7002274	-2.8288910
H	3.7382171	3.8716674	-2.6328470
H	3.3151451	0.9377864	0.1879990
H	-0.2315959	-0.9515026	2.6161370
H	-0.3572779	1.0975844	3.9444810
H	1.7850331	3.5444874	1.8411890
H	0.5288981	2.4228394	0.0303990
H	1.2559701	-1.5894246	-1.0883850
C	-2.2620849	1.5445174	2.1373890
C	4.8226891	1.3388554	-2.5814300
C	4.9195921	2.6365384	-0.4521540
C	3.1181561	3.1306304	-2.1136180
C	3.9969911	2.0414414	-1.5072190
N	3.1526751	1.0574424	-0.8038520
O	1.9236871	0.2970984	-2.5751080
C	2.2306751	0.2611114	-1.3966700
O	2.1859121	2.4854694	4.1813200
C	0.5072031	-0.1624056	2.3995490
C	0.6330641	0.7525884	3.6175640
C	1.4665141	1.9842604	3.3394320
C	1.3104661	2.5766964	1.9955850
C	0.6386211	1.9617884	1.0140610
C	-0.0056579	0.6055214	1.1471800
C	-1.5250409	0.7414834	1.1337530
C	-2.0686759	0.0645084	0.0886670
O	-1.0370169	-1.4297066	-1.5411780
C	-0.9646249	-0.6125016	-0.6445180

N	0.2170361	-0.1863216	-0.0563340
C	1.5025561	-0.7273806	-0.4520060
C	1.8273731	-0.7922226	2.0657080
C	2.2480031	-1.0846836	0.7866580
N	3.5143791	-1.5920806	0.8899640
C	2.9166611	-1.1621656	2.8846810
Au	-3.8647209	-1.1319136	0.1352140
C	-6.7409269	-4.2045336	-0.3562070
C	-7.5559039	-3.2193216	0.0920540
H	-6.9502809	-5.2190426	-0.6629240
H	-8.6251939	-3.1950416	0.2443590
C	-5.4670429	-2.4012506	0.0652220
N	-6.7567739	-2.1237406	0.3495560
N	-5.4617899	-3.6826846	-0.3684480
C	-5.4219249	3.6681524	-1.1168900
F	-4.6142799	4.4485314	-0.4141950
F	-6.6788329	3.9621244	-0.8145630
F	-5.2224279	3.8785974	-2.4062770
S	-5.1128869	1.9072634	-0.7017410
O	-3.6575499	1.7858414	-1.1119570
O	-6.0327189	1.1387324	-1.5332630
O	-5.2926739	1.8152874	0.7516030
C	-7.2548579	-0.8143316	0.7574310
H	-6.4911089	-0.3015516	1.3465450
H	-7.4612499	-0.1973716	-0.1229510
H	-8.1576939	-0.9531146	1.3571110
C	-4.2768799	-4.4171406	-0.7801480

H	-4.4949359	-4.9784116	-1.6926120
H	-3.4715149	-3.7059846	-0.9849350
H	-3.9593969	-5.1082726	0.0066750
H	1.0733401	0.2249064	4.4704500
H	-2.9735419	0.8229184	-0.5312750
C	4.4400851	-1.8815676	-0.1484170
C	5.7825881	-1.5598056	0.0461240
C	4.0127571	-2.4517716	-1.3445130
C	6.6951221	-1.8018886	-0.9723610
H	6.0876521	-1.1314696	0.9965470
C	4.9332261	-2.6705096	-2.3636450
H	2.9737021	-2.7389576	-1.4791240
C	6.2735351	-2.3475446	-2.1828140
H	7.7428371	-1.5534796	-0.8211990
H	4.5956341	-3.1062336	-3.3002530
H	6.9896251	-2.5241446	-2.9812580
H	3.0078161	-1.0988606	3.9635070
N	3.9294201	-1.6370956	2.1767940

Zero-point correction= 0.626053 (Hartree/Particle)

Thermal correction to Energy= 0.673042

Thermal correction to Enthalpy= 0.673986

Thermal correction to Gibbs Free Energy= 0.540726

Sum of electronic and zero-point Energies= -2812.716693

Sum of electronic and thermal Energies= -2812.669704

Sum of electronic and thermal Enthalpies= -2812.668760

Sum of electronic and thermal Free Energies= -2812.802020

E-2

H	3.4546773	-3.2088464	-0.0997807
H	2.2152513	-4.3351414	-0.6747167
H	3.3265403	-3.5530404	-1.8290327
H	-4.6630627	-2.7747954	-3.2618337
H	-2.8879257	-2.7432614	-3.1894357
H	-3.8413227	-2.8329814	-1.6846867
H	-3.7525017	0.8032636	-3.9974667
H	-2.8013177	-0.6097324	-4.5164667
H	-4.5720597	-0.6345054	-4.6393487
H	-5.1227337	0.7057836	-1.8949647
H	-5.1978057	-0.7864174	-0.9338927
H	-5.9914307	-0.7136414	-2.5278777
H	-1.9381697	0.1065706	-2.3940387
H	2.1412003	-0.9335444	1.1997793
H	2.4982273	-3.2410014	1.7914153
H	-1.0807177	-4.7331434	1.1107293
H	-0.8889527	-3.2436924	-0.8482777
H	-0.9864347	0.9221466	-0.5551767
C	2.7454393	-3.4044484	-0.9142267
C	-3.8040337	-2.4023774	-2.6900807
C	-3.7309517	-0.2935724	-4.0254547
C	-5.1167057	-0.3900844	-1.9501557
C	-3.8369137	-0.8777794	-2.6231177
N	-2.6689677	-0.3778354	-1.8755187
O	-3.0928097	-1.3728974	0.1488873
C	-2.3985617	-0.6899574	-0.5850367
O	0.3380793	-4.4861494	3.2607753

C	1.2320973	-1.5392064	1.3470683
C	1.6020383	-2.7537314	2.1984723
C	0.4990543	-3.7811374	2.2830543
C	-0.3507857	-3.9271494	1.0826133
C	-0.2523157	-3.1106044	0.0293723
C	0.7147833	-1.9546334	-0.0553597
C	1.7971613	-2.2770444	-1.0776267
C	1.7080993	-1.4312484	-2.1165357
O	0.2075833	0.4384406	-2.6163167
C	0.6115913	-0.4816734	-1.9041747
N	0.0591323	-0.8136064	-0.6935457
C	-1.0536707	-0.0862994	-0.1216267
C	0.1618673	-0.7179524	2.0101603
C	-0.8636257	-0.0778254	1.3510453
C	-0.1088997	-0.4781544	3.3752913
Au	3.4763613	1.3160196	-0.1867447
C	1.8258753	5.1843546	-0.0188497
C	3.1074233	5.4502046	0.3315453
H	0.9655843	5.8304346	-0.1146987
H	3.5963443	6.3774346	0.5923483
C	2.9511863	3.2444236	-0.0533557
N	3.7836263	4.2460526	0.3098123
N	1.7512123	3.8257746	-0.2552027
C	6.5532423	-1.7153124	-0.2152717
F	6.0882563	-2.7386274	-0.9191427
F	7.5528773	-2.1276334	0.5460153
F	6.9950283	-0.7822674	-1.0472187

S	5.2202513	-1.0269314	0.8410613
O	4.1957073	-0.6804744	-0.2359487
O	5.7908553	0.1553646	1.4779603
O	4.7689023	-2.1371174	1.6703893
C	5.2006543	4.0843116	0.6059113
H	5.4886353	4.8051366	1.3749043
H	5.3804433	3.0715396	0.9781663
H	5.8006253	4.2488266	-0.2939607
C	0.5347493	3.0911886	-0.5673557
H	0.7071713	2.3901516	-1.3922787
H	0.2068813	2.5372706	0.3210463
H	-0.2418687	3.8028916	-0.8584517
H	1.8781853	-2.4533904	3.2148933
H	2.3409193	-1.4129724	-2.9966787
N	-1.6632507	0.4953096	2.2990063
N	-1.2025337	0.2469966	3.5464583
H	0.4513483	-0.8074824	4.2432613
C	-2.9114437	1.1502716	2.1455553
C	-3.1718047	1.9565276	1.0393853
C	-3.8835397	0.9735666	3.1282743
C	-4.4180357	2.5582936	0.9027003
H	-2.4052127	2.1307446	0.2885063
C	-5.1173497	1.5933206	2.9899353
H	-3.6521257	0.3469736	3.9836753
C	-5.3952897	2.3795086	1.8749223
H	-4.6175427	3.1809196	0.0334233
H	-5.8745657	1.4486466	3.7567083

H	-6.3679277	2.8526566	1.7664003

Zero-point correction= 0.632876 (Hartree/Particle)

Thermal correction to Energy= 0.680003

Thermal correction to Enthalpy= 0.680947

Thermal correction to Gibbs Free Energy= 0.546441

Sum of electronic and zero-point Energies= -2812.760822

Sum of electronic and thermal Energies= -2812.713695

Sum of electronic and thermal Enthalpies= -2812.712751

Sum of electronic and thermal Free Energies= -2812.847257

F-1

Au	-4.8512743	-0.2665514	0.1415812
C	-7.8657073	1.0347106	-2.5104438
C	-8.6483093	0.8394096	-1.4224028
H	-8.1045243	1.3793346	-3.5062768
H	-9.7092293	0.9783016	-1.2725748
C	-6.5433053	0.3102156	-0.8524288
N	-7.8172763	0.3949216	-0.4117828
N	-6.5765943	0.7055296	-2.1427728
C	6.4340837	-0.5975004	-1.0022688
F	6.4764807	-1.5337504	-0.0540908
F	6.8748577	0.5412386	-0.4821398
F	7.2510427	-0.9614024	-1.9835498
S	4.7228557	-0.3954964	-1.6328538
O	4.3821047	-1.7142274	-2.1889118
O	4.9009887	0.6758216	-2.6330428
O	3.9572297	-0.0224254	-0.4270068
C	-8.2705053	0.0705966	0.9296972

H	-7.4034783	-0.2030784	1.5350102
H	-8.7616393	0.9381346	1.3790172
H	-8.9687003	-0.7706644	0.8996272
C	-5.4322883	0.7654226	-3.0492458
H	-5.4218893	1.7368866	-3.5495928
H	-4.5007253	0.6450456	-2.4871098
H	-5.5102503	-0.0297814	-3.7956418
C	3.9431467	4.0515496	3.3089762
C	2.9991267	4.9317116	2.7517582
C	1.8967937	4.4599656	2.0582892
C	1.7588827	3.0774506	1.9386992
C	2.7016647	2.1748636	2.4807642
C	3.8057407	2.6809986	3.1784352
N	0.7721207	2.3340226	1.3312252
C	1.1037437	0.9897476	1.4215172
C	2.2572137	0.8576916	2.1462932
C	0.1134837	-0.0363044	0.9824832
N	-0.5423493	0.3132056	-0.3057188
C	-1.8696903	0.1547896	-0.5210588
C	0.2669087	0.6990986	-1.4211258
O	-2.4614503	0.4375486	-1.5569258
C	-2.6284463	-0.4522324	0.5854492
C	-3.1525473	-1.2043534	1.4115062
C	0.3177987	2.0266716	-1.8339118
C	1.2103677	2.4719206	-2.7833658
C	2.0908277	1.5454576	-3.3514588
C	1.9552237	0.1834376	-3.0564278

C	1.0699907	-0.2280484	-2.0795018
O	3.0666807	1.9873396	-4.1546008
H	-0.6997553	-0.0396774	1.7226582
C	0.5420307	-1.5192674	0.9676642
O	-0.3611273	-2.3384164	1.1609972
N	1.8285857	-1.8192844	0.7499442
C	2.3619967	-3.2062324	0.8001792
C	1.8904717	-3.9724684	-0.4316598
C	3.8802877	-3.1005644	0.7897152
C	1.9239887	-3.8940834	2.0907852
C	-3.3668433	-2.1572184	2.4887772
H	4.7988847	4.4589256	3.8424302
H	3.1388937	6.0045746	2.8648032
H	1.1674487	5.1399746	1.6229262
H	4.5470517	2.0043496	3.5978552
H	0.0905987	2.7087506	0.6856362
H	2.7438937	-0.0714984	2.4126512
H	1.2885007	3.5274566	-3.0229708
H	2.6167647	-0.5367304	-3.5288278
H	3.8657397	1.4689886	-3.9101128
H	2.4790377	-1.0923174	0.4215342
H	2.2788197	-3.4912124	-1.3385048
H	2.2753957	-4.9998524	-0.4049398
H	0.7961147	-4.0126084	-0.4722048
H	4.3115507	-4.0958974	0.9493442
H	4.2386367	-2.4389624	1.5894952
H	4.2433717	-2.7216394	-0.1690588

H	2.4103987	-4.8751074	2.1519402
H	0.8420277	-4.0330454	2.1364772
H	2.2433557	-3.3044724	2.9602382
H	-2.3940963	-2.6398634	2.6527772
H	-4.1083123	-2.9157884	2.2232632
H	-3.6868783	-1.6564534	3.4079082
H	1.0228467	-1.2771974	-1.7928248
F	-0.4988563	2.9196136	-1.2309948

Zero-point correction= 0.598761 (Hartree/Particle)

Thermal correction to Energy= 0.647084

Thermal correction to Enthalpy= 0.648028

Thermal correction to Gibbs Free Energy= 0.509779

Sum of electronic and zero-point Energies= -2818.537871

Sum of electronic and thermal Energies= -2818.489547

Sum of electronic and thermal Enthalpies= -2818.488603

Sum of electronic and thermal Free Energies= -2818.626852

F-ts1

H	1.1956579	-4.6022855	-0.4310883
H	2.9000969	-4.8227025	-0.9040773
H	2.4458579	-4.8826155	0.8107147
H	0.4255959	5.3004265	0.5560357
H	-0.0516751	3.6420975	0.8861217
H	1.4287879	3.9718705	-0.0654433
H	-2.4839171	4.6108185	-1.7711743
H	-2.3110621	3.7034865	-0.2585303
H	-2.0414561	5.4626795	-0.2769683
H	-0.4657451	5.5402715	-2.9653723

H	1.1510669	5.3672825	-2.2410273
H	-0.0626281	6.4348015	-1.4936153
H	-0.3604231	3.2888755	-2.9865543
H	-3.7509771	-4.3037155	-1.5196033
H	-1.5571091	-1.2888125	1.0726687
H	-3.0973061	-3.0748575	0.3153757
H	0.6019929	1.8115515	0.2039837
H	-2.9118081	0.6379225	-1.2134553
H	-0.8030151	1.8001825	2.2600037
H	-5.5468501	0.3632875	0.1653927
H	-2.9110871	1.9213235	4.1490877
H	-5.3474731	1.4655875	4.3258967
H	-6.6364781	0.6731135	2.3716417
C	2.2348369	-4.3971055	-0.1468403
C	0.3969639	4.2916745	0.1276377
C	-1.9022741	4.5338695	-0.8447993
C	0.0839659	5.4832875	-2.0167883
C	-0.4221521	4.3243125	-1.1590713
N	-0.2248261	3.1202875	-1.9946503
O	-0.2317701	1.0032615	-2.7428053
C	-0.2044201	1.7665145	-1.7948703
O	-2.9052381	-4.2779635	-2.0521623
C	-1.4147581	-1.7532885	0.0992127
C	-2.2647321	-2.7605155	-0.3074173
C	-2.1017631	-3.3407415	-1.5808293
C	-1.0192551	-2.9452965	-2.3836923
C	-0.2025461	-1.9190775	-1.9638663

C	-0.3879931	-1.2858725	-0.7298643
C	2.3969589	-2.9474915	-0.0553983
C	2.0900209	-1.7507265	-0.0924553
O	2.5683229	0.5517255	0.0476667
C	1.7241719	-0.3243685	-0.1359343
N	0.4094029	-0.1559445	-0.3601263
C	-0.1307661	1.2276405	-0.3624163
C	-2.6973971	0.9617155	-0.2007263
C	-1.4629961	1.2847465	0.2936197
N	-1.5707121	1.5664795	1.6503167
C	-4.9887111	0.7495685	1.0154807
C	-3.6206861	1.0303725	0.8892897
C	-2.8876521	1.4274825	2.0338567
C	-3.4872071	1.6062365	3.2811677
C	-4.8447581	1.3478245	3.3682327
C	-5.5832671	0.9130585	2.2531207
Au	4.3835279	-1.9186965	0.2742487
C	8.4991789	-1.0917265	0.9543137
C	8.0615229	0.1357285	0.5859017
H	9.4795309	-1.4428065	1.2423627
H	8.5834459	1.0762655	0.4838597
C	6.3002819	-1.2507295	0.5329507
N	6.7090529	0.0201175	0.3325177
N	7.4019459	-1.9311775	0.9164767
C	-6.3774271	-2.5762505	0.9681007
F	-7.1387361	-1.4813345	1.0477367
F	-5.2916221	-2.3805525	1.7201517

F	-7.0605171	-3.5915705	1.4826177
S	-5.9119351	-2.8962845	-0.7763623
O	-7.1897571	-3.0782575	-1.4535493
O	-5.0972511	-4.1364945	-0.6163333
O	-5.1176241	-1.7145825	-1.1376353
C	5.8677369	1.1217665	-0.1254993
H	4.8109699	0.8569425	-0.0149233
H	6.0794279	2.0072665	0.4790707
H	6.0783269	1.3381985	-1.1765953
C	7.4489569	-3.3448985	1.2486507
H	6.4400689	-3.7563665	1.1719217
H	8.1065659	-3.8740145	0.5533067
H	7.8133099	-3.4780635	2.2710067
H	-0.8680461	-3.4030365	-3.3564093
F	0.8302569	-1.5616965	-2.7327893

Zero-point correction= 0.598506 (Hartree/Particle)

Thermal correction to Energy= 0.647043

Thermal correction to Enthalpy= 0.647987

Thermal correction to Gibbs Free Energy= 0.508972

Sum of electronic and zero-point Energies= -2818.518114

Sum of electronic and thermal Energies= -2818.469577

Sum of electronic and thermal Enthalpies= -2818.468633

Sum of electronic and thermal Free Energies= -2818.607648

F-int1

H	0.7493333	-3.4512205	-1.9579458
H	1.5684493	-2.7004555	-3.3289228
H	2.5213213	-3.2715595	-1.9436668

H	-0.7176567	5.4722335	1.0559552
H	-0.5892757	3.7187665	1.1101212
H	0.3085043	4.6486195	-0.1292318
H	-3.9914887	4.2990225	-0.3609218
H	-3.0837637	3.3368545	0.8242202
H	-3.2483927	5.0960145	1.0409352
H	-2.7812597	5.8685365	-1.9348478
H	-1.0144247	6.0479695	-1.8217868
H	-2.0686277	6.6803905	-0.5339748
H	-2.3292827	3.6797115	-2.3560278
H	-4.0041987	-3.0126725	-2.3752738
H	-0.5829327	-1.4372085	0.2700492
H	-2.5583157	-2.6184155	-0.6187978
H	-1.5496087	-1.2895885	-4.6394798
H	0.3416683	2.4197965	-0.2188938
H	-3.1999337	0.7586825	-0.2089338
H	0.4167283	1.0839475	1.9429942
H	-4.7100077	-0.5846775	1.9590342
H	-0.3747577	-0.1061645	4.4443422
H	-2.3274447	-1.2247095	5.4936452
H	-4.4615697	-1.4764105	4.2685932
C	1.5819723	-2.7908375	-2.2338708
C	-0.6320207	4.5762995	0.4302482
C	-3.1157317	4.2980585	0.2996452
C	-1.9271257	5.8586785	-1.2449808
C	-1.8361207	4.5273355	-0.5010928
N	-1.7204197	3.4996765	-1.5629308

O	-1.4958367	1.5657585	-2.6689198
C	-1.2319607	2.2349015	-1.6769198
O	-3.2328767	-2.5633785	-3.1681428
C	-0.8288597	-1.4090705	-0.7907518
C	-1.8854227	-2.0762335	-1.2761768
C	-2.2009237	-2.0135545	-2.6924188
C	-1.3110607	-1.3250425	-3.5818318
C	-0.2873157	-0.6143285	-3.0735468
C	0.1461663	-0.6652465	-1.6487548
C	1.4779773	-1.4610335	-1.5811908
C	2.4032543	-0.7790105	-0.8877628
O	2.2223033	1.3183775	0.3342472
C	1.7853913	0.4921645	-0.4592778
N	0.5406513	0.6134065	-1.0773798
C	-0.3579187	1.6569535	-0.5784688
C	-2.4857937	0.7418535	0.6077302
C	-1.1865777	1.1703595	0.5637382
N	-0.5651467	0.9043905	1.7726722
C	-3.7784987	-0.4711425	2.5079322
C	-2.6881667	0.1636785	1.8998492
C	-1.4657957	0.2778585	2.6076732
C	-1.3164167	-0.2051625	3.9085152
C	-2.4124577	-0.8275075	4.4844422
C	-3.6283307	-0.9657845	3.7907802
Au	4.3296403	-1.1810005	-0.3150628
C	8.2188803	-1.0144625	1.4527892
C	8.3542673	-2.2014735	0.8166372

H	8.9054473	-0.4581965	2.0748142
H	9.1824163	-2.8940085	0.7695952
C	6.2805353	-1.4279355	0.3733662
N	7.1586413	-2.4365315	0.1624452
N	6.9451633	-0.5569075	1.1704112
C	-5.3167617	-3.3814815	0.9048392
F	-5.9429217	-2.6997095	1.8579062
F	-4.0233287	-3.4465025	1.2081872
F	-5.8095517	-4.6069785	0.8588932
S	-5.5540287	-2.5266275	-0.7026378
O	-6.9838617	-2.5428205	-0.9337198
O	-4.7818537	-3.4921745	-1.6012698
O	-4.8573037	-1.2500405	-0.5668738
C	6.8860093	-3.6133465	-0.6417008
H	5.8713063	-3.5295645	-1.0383268
H	7.5941703	-3.6769255	-1.4732478
H	6.9606403	-4.5171425	-0.0296128
C	6.4010753	0.6972585	1.6662782
H	6.9999673	1.5371585	1.3020352
H	5.3743093	0.8051955	1.3045312
H	6.3989073	0.6985625	2.7602502
F	0.5282303	0.0457775	-3.8647658

Zero-point correction= 0.598814 (Hartree/Particle)

Thermal correction to Energy= 0.645371

Thermal correction to Enthalpy= 0.646315

Thermal correction to Gibbs Free Energy= 0.513484

Sum of electronic and zero-point Energies= -2818.576718

Sum of electronic and thermal Energies= -2818.530162

Sum of electronic and thermal Enthalpies= -2818.529217

Sum of electronic and thermal Free Energies= -2818.662049

F-ts2

H	-0.5787549	-2.4011903	-2.0855615
H	0.0900601	-1.3435793	-3.3219145
H	1.1711191	-2.4300803	-2.4189255
H	3.2878111	3.9612387	-1.3722995
H	2.0426191	2.7002587	-1.2313415
H	1.8659981	3.9801717	-2.4422625
H	1.3684241	4.8794917	1.7470785
H	2.1519681	3.3469097	1.2388055
H	3.0058851	4.8717557	1.0714185
H	1.1594501	6.7576117	-0.0441715
H	1.2730861	6.3282037	-1.7698695
H	2.7323441	6.3569087	-0.7696955
H	-0.4595979	5.0505507	-1.1502555
H	-4.4381909	-1.4905253	-2.8355695
H	-1.3378739	-0.9642093	0.5247545
H	-3.3782229	-1.6531993	-0.7378235
H	-2.3334149	1.1449377	-3.8616555
H	0.3939451	2.5813397	1.3888495
H	-3.1951869	1.4846127	0.0837205
H	-0.3571699	1.1295027	3.1215265
H	-5.0864959	-0.6112923	1.2109815
H	-1.7482749	-0.5217903	4.9702245
H	-3.8275589	-1.8860593	5.1379355

H	-5.4611329	-1.9313143	3.2835515
C	0.2919531	-1.7828803	-2.3364665
C	2.2096691	3.7648827	-1.4235255
C	2.0155841	4.4069127	0.9976295
C	1.6656751	6.1081917	-0.7683225
C	1.4716471	4.6359197	-0.4107845
N	0.0070221	4.4195627	-0.5057635
O	-2.0078829	3.4340537	-0.6041285
C	-0.8557369	3.4152187	-0.1951185
O	-3.8314219	-0.7782783	-3.2289545
C	-1.6960969	-0.3346423	-0.2966325
C	-2.6962309	-0.9049693	-1.1326675
C	-2.9140149	-0.3785563	-2.3943155
C	-2.0659089	0.6820847	-2.9173215
C	-0.9668419	1.0341757	-2.2491075
C	-0.5141869	0.3537847	-0.9965385
C	0.5425881	-0.7404273	-1.3088635
C	1.6240241	-0.6085843	-0.5159445
O	2.0437971	0.9733027	1.3005335
C	1.4027401	0.5698407	0.3399555
N	0.2542131	1.2207667	-0.1256665
C	-0.3752809	2.2563317	0.6808425
C	-2.6194959	0.9622797	0.8404345
C	-1.4651879	1.5592817	1.4103515
N	-1.2314159	1.0224067	2.6205385
C	-4.3627279	-0.5963093	2.0254845
C	-3.1972599	0.1573577	1.9195745

C	-2.2817929	0.1693617	2.9855255
C	-2.4710289	-0.5480063	4.1582955
C	-3.6353239	-1.3028223	4.2406845
C	-4.5639509	-1.3245393	3.1933805
Au	3.3210821	-1.7415973	-0.3114125
C	7.0612231	-3.5018123	0.8095385
C	6.7114541	-4.3807453	-0.1585245
H	7.9309431	-3.4564003	1.4492185
H	7.2125451	-5.2601223	-0.5370125
C	5.0698581	-2.8375563	-0.0201095
N	5.4913521	-3.9574883	-0.6535765
N	6.0456471	-2.5662933	0.8795365
C	-6.0683679	-3.2282743	0.1589245
F	-6.7818439	-2.8366443	1.2164405
F	-4.7797589	-3.2365403	0.5216085
F	-6.4186839	-4.4661713	-0.1529405
S	-6.3399329	-2.0791823	-1.2473295
O	-7.7388379	-2.2693293	-1.5952225
O	-5.3503099	-2.6033393	-2.2360395
O	-5.9413179	-0.7732593	-0.7022095
C	4.7623091	-4.6344653	-1.7109655
H	3.8384341	-4.0822583	-1.9001645
H	5.3603901	-4.6610253	-2.6266175
H	4.5149471	-5.6558623	-1.4070175
C	6.0348761	-1.4429443	1.8013295
H	6.8915691	-0.7898263	1.6103695
H	5.1108191	-0.8772193	1.6532075

H	6.0743631	-1.8031473	2.8335675
F	-0.1307199	1.9555457	-2.7152065

Zero-point correction= 0.602614 (Hartree/Particle)

Thermal correction to Energy= 0.648037

Thermal correction to Enthalpy= 0.648981

Thermal correction to Gibbs Free Energy= 0.519930

Sum of electronic and zero-point Energies= -2818.545513

Sum of electronic and thermal Energies= -2818.500090

Sum of electronic and thermal Enthalpies= -2818.499146

Sum of electronic and thermal Free Energies= -2818.628197

F-int2

H	-0.5856978	-2.4637538	-1.8357205
H	0.0012822	-1.4479848	-3.1411055
H	1.1479962	-2.4841388	-2.2532055
H	3.5302982	3.4852632	-1.6847115
H	2.1606092	2.3823352	-1.4238725
H	2.0791972	3.5958782	-2.7076095
H	1.8881062	4.8766592	1.4063645
H	2.4012282	3.1994382	1.0263095
H	3.4700332	4.5491602	0.6798005
H	1.7918212	6.5905632	-0.5063645
H	1.7711852	6.0223492	-2.1963025
H	3.2710602	5.9566102	-1.2599255
H	-0.0782928	5.0666942	-1.3252505
H	-4.2519908	-1.6699678	-2.7882335
H	-1.3399538	-0.8091948	0.6386445
H	-3.2966868	-1.6696618	-0.6326605

H	-2.2931658	1.0723152	-3.8116165
H	0.5249592	2.6319442	1.4135255
H	-2.9311748	1.6742532	-0.2209465
H	-0.9284058	1.9443632	3.2939735
H	-5.0497518	-0.4095428	0.7033995
H	-2.7979688	0.7650082	5.0472465
H	-4.9182608	-0.5531978	5.0103295
H	-6.0017768	-1.1327268	2.8632435
C	0.2636172	-1.8459758	-2.1528435
C	2.4361402	3.4073862	-1.6887135
C	2.4179292	4.2404092	0.6858085
C	2.1845932	5.8342302	-1.1966935
C	1.8452922	4.4242452	-0.7165305
N	0.3620392	4.3754932	-0.7262995
O	-1.7876268	3.8005892	-0.4168975
C	-0.6006128	3.5728372	-0.2149495
O	-3.7109588	-0.9357688	-3.1959625
C	-1.7116998	-0.1659798	-0.1732225
C	-2.6723268	-0.8813458	-1.0422015
C	-2.8533988	-0.4479318	-2.3176535
C	-2.0252358	0.6361752	-2.8538705
C	-0.9320778	1.0269372	-2.1978865
C	-0.4684338	0.3742352	-0.9264855
C	0.5414472	-0.7619638	-1.1764445
C	1.6227862	-0.6475088	-0.3769405
O	2.1014712	0.9928092	1.3704425
C	1.4495332	0.5690742	0.4271555

N	0.3260142	1.2504632	-0.0739755
C	-0.2294938	2.3671762	0.6596185
C	-2.4750318	1.0674002	0.5678395
C	-1.4469078	1.8089452	1.3049285
N	-1.5929318	1.6231892	2.5974235
C	-4.5464208	-0.1565968	1.6386955
C	-3.3617458	0.5627242	1.6568395
C	-2.7658238	0.8761862	2.8821225
C	-3.2834508	0.5042972	4.1101475
C	-4.4677618	-0.2287368	4.0759045
C	-5.0837048	-0.5507808	2.8646755
Au	3.2553532	-1.8595018	-0.1094425
C	6.8765632	-3.8113158	1.0909385
C	6.4734712	-4.6978918	0.1510115
H	7.7457882	-3.8004038	1.7328285
H	6.9181272	-5.6196628	-0.1958135
C	4.9334752	-3.0490288	0.2305615
N	5.2842172	-4.2143728	-0.3633365
N	5.9227992	-2.8110048	1.1250685
C	-5.8225998	-3.4409168	0.3667685
F	-6.7321308	-3.1218668	1.2898175
F	-4.6231828	-3.0843048	0.8498785
F	-5.8263488	-4.7559958	0.2088715
S	-6.1803148	-2.5703088	-1.2111155
O	-7.4480868	-3.1398578	-1.6425575
O	-4.9916888	-2.9416828	-2.0272755
O	-6.1791948	-1.1545838	-0.8122555

C	4.5159682	-4.8786178	-1.4011035
H	3.6281952	-4.2769058	-1.6112425
H	5.1126132	-4.9716568	-2.3133595
H	4.2052672	-5.8723568	-1.0653635
C	5.9808832	-1.6597518	2.0093825
H	6.8793182	-1.0703118	1.8034355
H	5.0962552	-1.0408558	1.8357465
H	5.9914482	-1.9870378	3.0532685
F	-0.1160648	1.9653162	-2.6840585

Zero-point correction= 0.602352 (Hartree/Particle)

Thermal correction to Energy= 0.648621

Thermal correction to Enthalpy= 0.649565

Thermal correction to Gibbs Free Energy= 0.516345

Sum of electronic and zero-point Energies= -2818.548726

Sum of electronic and thermal Energies= -2818.502457

Sum of electronic and thermal Enthalpies= -2818.501513

Sum of electronic and thermal Free Energies= -2818.634733

F-ts3

H	0.3794145	-3.3776206	0.9997133
H	-0.3842985	-3.0101166	2.5407473
H	-1.3642805	-3.6734416	1.2143853
H	-3.0638815	4.8552154	0.5068033
H	-2.3947015	3.2177924	0.4796873
H	-2.4867905	4.1129354	2.0119013
H	0.3870755	5.4441814	-0.9101817
H	-0.6938725	4.0825704	-1.3420577
H	-1.3385505	5.7105324	-1.2186797

H	0.0933525	6.6959584	1.2430433
H	-1.0998395	6.1411154	2.4461203
H	-1.6446765	6.8659174	0.9249943
H	0.5626085	4.5161994	2.2063983
H	4.6778655	-1.6977516	2.2650443
H	1.1146725	-1.6814306	-0.5324397
H	3.4947285	-1.6926606	0.3134283
H	1.8746255	-0.6736676	4.1733883
H	-0.7109315	2.3574614	-0.4278517
H	2.8151625	0.3311714	0.3740853
H	1.5818675	3.3443694	-1.6847637
H	3.9348375	-1.5311306	-1.8426087
H	3.6322585	3.1660484	-3.6035317
H	5.3035295	1.5527104	-4.5057797
H	5.4473025	-0.7496436	-3.6044297
C	-0.5435355	-2.9899766	1.4536643
C	-2.2891595	4.2088564	0.9379053
C	-0.6155055	5.0170984	-0.7734657
C	-0.8851835	6.2166534	1.3729223
C	-0.9171705	4.8394494	0.7148543
N	0.1521115	4.0680524	1.3931323
O	1.2738005	2.2806614	2.1879783
C	0.5134205	2.7580104	1.3619753
O	3.9402355	-1.4714456	2.9065463
C	1.4230685	-0.8830906	0.1571623
C	2.7128335	-1.2096406	0.8961583
C	2.8302335	-1.1871306	2.2691473

C	1.7306535	-0.7565566	3.1011173
C	0.5825565	-0.3868266	2.5296663
C	0.2097915	-0.5313036	1.0765783
C	-0.8646925	-1.6179056	0.9833653
C	-2.0169805	-1.1466516	0.4736053
O	-2.5738615	1.0840274	-0.3488127
C	-1.8151835	0.2867704	0.1865023
N	-0.5331265	0.6361204	0.6164473
C	0.0595085	1.8745324	0.1856503
C	1.9461185	0.3330354	-0.5890407
C	1.2539745	1.5658924	-0.6410117
N	1.8264325	2.3722074	-1.5439067
C	3.8342295	-0.5162876	-2.2281087
C	2.8919165	0.3768174	-1.7263877
C	2.8397935	1.6864844	-2.2329807
C	3.6858305	2.1451494	-3.2328017
C	4.6134425	1.2368414	-3.7276357
C	4.6876995	-0.0691456	-3.2299767
Au	-3.8169795	-2.0184676	0.0331923
C	-7.8154905	-2.8633866	-1.2384507
C	-7.4868345	-4.1037206	-0.8077057
H	-8.7272025	-2.4795936	-1.6734447
H	-8.0520425	-5.0245306	-0.7899357
C	-5.6941435	-2.7729006	-0.4713467
N	-6.1865705	-4.0277436	-0.3424987
N	-6.7076245	-2.0641546	-1.0250197
C	7.0853335	-3.9612626	0.3048503

F	7.2849495	-4.7206706	-0.7666577
F	6.5088585	-4.7023626	1.2467203
F	8.2621055	-3.5442256	0.7559803
S	6.0187785	-2.5338946	-0.1219337
O	6.7622955	-1.8064156	-1.1471207
O	5.8970325	-1.8246726	1.1794383
O	4.7615565	-3.1657606	-0.5630627
C	-5.4496185	-5.1503276	0.2080733
H	-4.4554335	-4.7995206	0.4956553
H	-5.9622295	-5.5445556	1.0905863
H	-5.3498065	-5.9425976	-0.5398577
C	-6.6467695	-0.6495186	-1.3536357
H	-5.6538085	-0.2705026	-1.0945697
H	-6.8187585	-0.5048306	-2.4243377
H	-7.4017835	-0.0979876	-0.7854537
F	-0.4265405	0.0461914	3.2728703

Zero-point correction= 0.597316 (Hartree/Particle)

Thermal correction to Energy= 0.643588

Thermal correction to Enthalpy= 0.644533

Thermal correction to Gibbs Free Energy= 0.510586

Sum of electronic and zero-point Energies= -2818.508951

Sum of electronic and thermal Energies= -2818.462679

Sum of electronic and thermal Enthalpies= -2818.461735

Sum of electronic and thermal Free Energies= -2818.595681

F-int3

H	0.1720696	-3.6339824	-0.0346794
H	0.1753676	-3.3536644	1.7118236

H	-1.3302714	-3.8097784	0.8825886
H	-3.1713074	4.8683526	0.0667436
H	-2.5342984	3.2161536	0.2014346
H	-2.7897924	4.1886466	1.6611946
H	0.3858076	5.4320226	-0.9745394
H	-0.5656664	4.0097826	-1.4632144
H	-1.3052624	5.6087596	-1.4662784
H	-0.0572174	6.6535106	1.1379836
H	-1.4077544	6.1710056	2.1971176
H	-1.7366884	6.8749416	0.6055466
H	0.1158956	4.4482226	2.2381746
H	5.4543556	-1.7982554	0.8852696
H	0.9932016	-1.2562394	-1.2787464
H	2.1145926	-2.7685464	0.2880836
H	2.3848896	-0.7753694	3.4848766
H	-0.7234734	2.2872736	-0.5470714
H	1.9033636	3.7456546	-0.5019534
H	4.4462446	-0.8506984	-1.7876024
H	4.4364196	4.1554136	-1.6412874
H	6.4256636	2.8920496	-2.4434434
H	6.3970896	0.4162896	-2.5066224
C	-0.4150724	-3.2150294	0.7952316
C	-2.4659684	4.2301016	0.6140066
C	-0.6052984	4.9618866	-0.9242014
C	-1.0613774	6.2114586	1.1565136
C	-1.0615204	4.8208386	0.5263996
N	-0.0931064	4.0325906	1.3348456

O	0.5623486	2.1818986	2.4493136
C	0.1161826	2.6770896	1.4304226
O	4.2608596	-1.3941404	1.7619476
C	1.4354106	-0.8107414	-0.3732504
C	2.5219786	-1.7585104	0.1418336
C	3.0633026	-1.3167784	1.4712446
C	2.0855096	-0.8885534	2.4474266
C	0.8198116	-0.6438584	2.0692146
C	0.2832916	-0.6769784	0.6603796
C	-0.7689444	-1.7879364	0.5615926
C	-1.9845684	-1.2924054	0.2709536
O	-2.6927014	0.9934796	-0.1968054
C	-1.8449914	0.1727306	0.1303246
N	-0.5285734	0.5036256	0.4088286
C	-0.0188464	1.8270326	0.1584416
C	2.0111196	0.5432926	-0.6881364
C	1.3439906	1.7072916	-0.4319634
N	2.1212756	2.7934626	-0.7571004
C	4.4209406	0.2337106	-1.7170144
C	3.2974706	0.9212826	-1.2283634
C	3.3340456	2.3387556	-1.2294754
C	4.4406476	3.0674086	-1.6592124
C	5.5412046	2.3563166	-2.1069494
C	5.5254336	0.9536776	-2.1401114
Au	-3.8362104	-2.1101224	-0.0378114
C	-7.9851014	-2.6142434	-0.9323424
C	-7.6956574	-3.9131734	-0.6848584

H	-8.9102694	-2.1330444	-1.2156994
H	-8.3154434	-4.7980674	-0.7077994
C	-5.7936124	-2.7292024	-0.4032644
N	-6.3511544	-3.9624144	-0.3632014
N	-6.8109814	-1.9061184	-0.7552554
C	5.7287546	-4.6385784	0.6092546
F	5.5337906	-5.7424314	-0.0900124
F	4.5988686	-4.3006554	1.2220076
F	6.6702746	-4.8429134	1.5092416
S	6.2117576	-3.2840124	-0.5338244
O	7.5183866	-3.6020584	-1.0517684
O	6.3446496	-2.1007044	0.4742816
O	5.0645826	-3.1148864	-1.4093324
C	-5.6349144	-5.1785844	-0.0276564
H	-4.5943354	-4.9161494	0.1780736
H	-6.0720574	-5.6444334	0.8606936
H	-5.6707484	-5.8837114	-0.8635774
C	-6.6925674	-0.4665014	-0.9267364
H	-7.3551124	0.0504136	-0.2262164
H	-5.6582934	-0.1687884	-0.7289424
H	-6.9566394	-0.1880184	-1.9512484
H	3.3374896	-1.8658974	-0.5742804
F	-0.1025374	-0.4102434	2.9785376

Zero-point correction= 0.602632 (Hartree/Particle)

Thermal correction to Energy= 0.648923

Thermal correction to Enthalpy= 0.649868

Thermal correction to Gibbs Free Energy= 0.516793

Sum of electronic and zero-point Energies= -2818.594824

Sum of electronic and thermal Energies= -2818.548533

Sum of electronic and thermal Enthalpies= -2818.547589

Sum of electronic and thermal Free Energies= -2818.680664

F-int4

H	0.9274740	-0.1958417	-3.4017602
H	1.0581350	1.4175243	-2.6899302
H	2.4509360	0.3148073	-2.6572532
H	-4.1962070	3.0246703	4.3005258
H	-4.7099320	1.3866693	3.8395108
H	-3.0576620	1.6624943	4.4461958
H	-4.2203530	3.0541363	0.5307028
H	-5.3837080	2.1994103	1.5722998
H	-4.8722080	3.8496603	1.9764138
H	-1.8818230	3.5398473	1.3947098
H	-1.3709950	2.9209283	2.9779258
H	-2.5274980	4.2727103	2.8804238
H	-3.4084410	0.8385883	0.9002258
H	-1.0294600	-1.5838187	-2.2160092
H	-1.1864300	0.4235823	-3.5468252
H	-1.9121690	3.1894163	-1.0526202
H	-1.3614550	-1.7400067	2.0102318
H	-4.1912790	-2.0806987	1.7859478
H	-3.9717850	-1.9105087	-3.6048972
H	-6.4946090	-3.1096407	0.5529908
H	-7.4524430	-3.5479937	-1.6996782
H	-6.1888410	-2.9592947	-3.7410532

C	1.3615890	0.3680583	-2.5639192
C	-3.8643840	2.0856163	3.8406738
C	-4.5308270	2.8903313	1.5719578
C	-2.2171990	3.3280953	2.4169348
C	-3.3852360	2.3454813	2.4155908
N	-2.9832320	1.0699233	1.7903198
O	-1.3012460	0.4728213	3.2205978
C	-1.9677550	0.2790273	2.2191708
O	-3.5014770	2.0946193	-2.8560732
C	-1.5614470	-0.7382457	-1.7492022
C	-2.0245260	0.2039373	-2.8699782
C	-2.5387110	1.5339513	-2.3677172
C	-1.7448850	2.1424563	-1.2948322
C	-0.8492880	1.4170333	-0.6183502
C	-0.5378950	-0.0463897	-0.7992152
C	0.9191060	-0.1842637	-1.2548362
C	1.6655020	-0.8164567	-0.3261022
O	1.0203080	-1.8616757	1.7844548
C	0.7641100	-1.1983967	0.7964528
N	-0.4897260	-0.6893777	0.5004898
C	-1.6566900	-0.9397177	1.3136878
C	-2.7254320	-1.2811207	-0.9650392
C	-2.7486310	-1.3638437	0.4013278
N	-3.9357030	-1.9168657	0.8245918
C	-4.5132470	-2.1423227	-2.6904752
C	-3.9595160	-1.8628847	-1.4319432
C	-4.6950830	-2.2388197	-0.2795222

C	-5.9512100	-2.8370157	-0.3492912
C	-6.4749210	-3.0807617	-1.6079022
C	-5.7582610	-2.7427597	-2.7664252
Au	3.6315700	-1.4097747	-0.1524182
C	7.2703310	-3.0336077	1.3625948
C	7.7982010	-2.3107837	0.3463768
H	7.7380420	-3.6526487	2.1146308
H	8.8221690	-2.1618847	0.0352878
C	5.5634280	-2.0454067	0.2721298
N	6.7376820	-1.7175847	-0.3113602
N	5.9011090	-2.8576567	1.3021218
C	4.4490560	3.8802133	-0.7857742
F	3.4705450	4.2716023	-1.5773702
F	5.6122180	4.2351813	-1.3056772
F	4.3103420	4.4177373	0.4081118
S	4.4570850	2.0454723	-0.6556752
O	3.0047630	1.9361543	-0.0363872
O	5.4876750	1.6878883	0.2967718
O	4.4972080	1.5171253	-2.0070502
C	6.8797190	-0.7908167	-1.4224312
H	5.9121000	-0.6776967	-1.9163912
H	7.1934390	0.1916243	-1.0568722
H	7.6129480	-1.1825737	-2.1328882
C	4.9559440	-3.4720467	2.2213228
H	5.2761350	-3.2935357	3.2516498
H	3.9689670	-3.0235627	2.0734208
H	4.8928890	-4.5494237	2.0404308

H	-2.8131030	-0.2503047	-3.4749282
H	2.6514290	1.0050493	-0.0862042
F	-0.1152240	1.9841833	0.3330708

Zero-point correction= 0.601816 (Hartree/Particle)

Thermal correction to Energy= 0.648537

Thermal correction to Enthalpy= 0.649481

Thermal correction to Gibbs Free Energy= 0.517064

Sum of electronic and zero-point Energies= -2818.596489

Sum of electronic and thermal Energies= -2818.549768

Sum of electronic and thermal Enthalpies= -2818.548824

Sum of electronic and thermal Free Energies= -2818.681242

F-ts4

H	-1.2205047	-0.8537911	3.1362716
H	-0.7333977	0.8407469	3.2681616
H	-2.3505147	0.4049349	2.6260846
H	3.8488043	4.9840469	-1.7972974
H	3.3259693	3.9570579	-0.4410054
H	4.3578333	3.2806229	-1.7257474
H	0.2306163	4.2471389	-2.5178594
H	0.9227853	4.5219929	-0.8988314
H	1.4109773	5.5480889	-2.2620724
H	1.6498433	3.2780809	-4.3494254
H	3.3553173	2.8683369	-4.0506394
H	2.8470403	4.5737649	-4.1271044
H	0.9929283	2.1933259	-1.3072874
H	0.7882583	-2.0397701	1.4338646
H	0.9034973	-0.9204511	3.6115726

H	2.6553723	2.3805039	2.8140976
H	1.5712303	-0.7299501	-2.1781394
H	4.5199463	-0.7947651	-1.8407824
H	3.7726373	-3.1407801	2.9804956
H	6.7110063	-2.4338861	-1.0102644
H	7.4879483	-3.7744741	0.9389526
H	6.0107713	-4.1158401	2.8933846
C	-1.2898877	0.1283109	2.6469016
C	3.5344873	3.9708249	-1.5187664
C	1.1422193	4.5257159	-1.9746694
C	2.5534733	3.5684679	-3.8007114
C	2.2855383	3.5739569	-2.3002964
N	1.8395473	2.2370829	-1.8590104
O	3.6392263	0.9905369	-2.5182424
C	2.5580923	1.1080469	-1.9450164
O	3.5297213	0.2578429	4.1211576
C	1.4921163	-1.1958471	1.5348186
C	1.8229653	-1.0148481	3.0183996
C	2.6521323	0.2216529	3.2837086
C	2.2483323	1.4165869	2.5214206
C	1.3716723	1.3217659	1.5210366
C	0.7543873	0.0596179	0.9739626
C	-0.7455017	0.0491769	1.2714506
C	-1.4741447	0.0006899	0.1263316
O	-0.7567997	-0.2089101	-2.1972954
C	-0.5248407	-0.0515301	-1.0136354
N	0.7537413	0.0806619	-0.4860014

C	1.9217643	-0.1434441	-1.3112484
C	2.7330503	-1.4446251	0.7227586
C	2.9150863	-0.9260221	-0.5308264
N	4.1382993	-1.2752561	-1.0328284
C	4.3945193	-2.9573491	2.1080926
C	3.9382013	-2.1781291	1.0324216
C	4.7995923	-2.0228791	-0.0862114
C	6.0757663	-2.5797041	-0.1394574
C	6.4975583	-3.3256371	0.9472696
C	5.6594363	-3.5167661	2.0566586
Au	-3.2068977	-1.2480021	-0.2070164
C	-6.0455247	-3.9613321	-1.7977454
C	-6.7831817	-3.4503791	-0.7826914
H	-6.2839657	-4.6957531	-2.5533084
H	-7.8027687	-3.6390081	-0.4793304
C	-4.7612637	-2.4828421	-0.6953554
N	-5.9778907	-2.5495051	-0.1153864
N	-4.8069287	-3.3531751	-1.7298514
C	-5.0518407	3.2786129	1.5640086
F	-4.1461847	3.6519659	2.4552736
F	-6.2395127	3.2230809	2.1496606
F	-5.0897897	4.1618519	0.5812436
S	-4.6381397	1.6153679	0.9072676
O	-3.2845847	1.9027749	0.2840656
O	-5.6834607	1.3010819	-0.0601184
O	-4.5344967	0.7462159	2.0849006
C	-6.4211377	-1.7036221	0.9877806

H	-7.1849477	-2.2393591	1.5565186
H	-5.5715307	-1.4695901	1.6332896
H	-6.8137667	-0.7572811	0.6032846
C	-3.7058807	-3.6266881	-2.6384474
H	-3.2331867	-4.5827621	-2.3937444
H	-4.0792787	-3.6563241	-3.6655164
H	-2.9675777	-2.8245221	-2.5521344
H	2.3602883	-1.8777101	3.4157406
H	-2.4860577	0.8664009	0.1628316
F	0.9213873	2.4255729	0.9161756

Zero-point correction= 0.597226 (Hartree/Particle)

Thermal correction to Energy= 0.643096

Thermal correction to Enthalpy= 0.644040

Thermal correction to Gibbs Free Energy= 0.512935

Sum of electronic and zero-point Energies= -2818.596637

Sum of electronic and thermal Energies= -2818.550767

Sum of electronic and thermal Enthalpies= -2818.549823

Sum of electronic and thermal Free Energies= -2818.680927

F-2

H	-0.5948559	3.9776891	2.6269152
H	-2.0663669	3.2313921	3.3044632
H	-0.5323939	3.2185921	4.2113282
H	-2.8375959	-5.5365649	0.6251322
H	-3.5101809	-3.9146929	0.3473072
H	-2.1559459	-4.4966309	-0.6495478
H	-1.5326609	-3.4984499	3.4982982
H	-3.1372909	-3.2785209	2.7552672

H	-2.5129839	-4.9117499	3.0632422
H	0.4036231	-4.3006579	2.1055082
H	0.1515031	-4.7740579	0.4057472
H	-0.5176679	-5.7754219	1.7164012
H	-1.4081709	-1.8307559	1.7517832
H	-0.3273129	2.6744431	0.0256152
H	-2.1252019	3.9257381	1.1089862
H	-4.7312819	1.0860301	1.7151242
H	0.7845201	-0.6596589	-0.4281778
H	-1.1267639	-1.4664099	-2.6301078
H	-3.1242649	3.5693121	-2.3952038
H	-2.4680419	-0.6600119	-4.9927868
H	-3.7276819	1.2610031	-5.9552108
H	-4.0351609	3.3373651	-4.6459028
C	-0.9776819	3.1327501	3.2162972
C	-2.5853409	-4.5035129	0.3560832
C	-2.2321839	-3.8992749	2.7532862
C	-0.3084829	-4.7464579	1.3991742
C	-1.5991859	-3.9321929	1.3686982
N	-1.2805229	-2.5320319	1.0313572
O	-0.3958199	-2.8319809	-1.0598968
C	-0.6680049	-2.1236019	-0.0871048
O	-4.7763659	3.2237171	0.1903392
C	-1.3088469	2.1881141	0.0994082
C	-2.3804679	3.2600141	0.2749442
C	-3.7499729	2.6879291	0.5595452
C	-3.7685609	1.4647471	1.3831262

C	-2.6376059	0.8408881	1.7194362
C	-1.2365239	1.2591501	1.3414542
C	-0.5658469	1.8569861	2.5805592
C	0.4425311	1.0731121	2.9759972
O	1.4935041	-0.8837909	1.9869502
C	0.6224761	-0.0251959	2.0298482
N	-0.3988359	0.0813561	1.1001212
C	-0.2871919	-0.6412499	-0.1474228
C	-1.5475379	1.3379861	-1.1207158
C	-1.0615669	0.0631811	-1.1984708
N	-1.3572929	-0.5064509	-2.4072008
C	-2.9457339	2.6478131	-2.9420948
C	-2.2212989	1.5846891	-2.3752448
C	-2.0743179	0.4013641	-3.1495998
C	-2.6024339	0.2623701	-4.4317678
C	-3.3010919	1.3343981	-4.9576218
C	-3.4717759	2.5131411	-4.2150978
Au	3.1564401	0.6134141	-0.1929598
C	5.1040201	-2.9579789	-1.2739328
C	6.0643001	-2.0580199	-1.5967018
H	5.0853181	-4.0354119	-1.3481548
H	7.0576301	-2.1897429	-2.0000818
C	4.2981611	-0.9193579	-0.8041168
N	5.5501151	-0.8106979	-1.3045658
N	4.0290101	-2.2424039	-0.7854618
C	1.9811641	4.8030241	0.1214292
F	0.6557421	4.8766491	0.2647082

F	2.2613801	4.6264931	-1.1601158
F	2.5153041	5.9404761	0.5328842
S	2.6447691	3.4145441	1.1225242
O	2.1513511	3.6652621	2.4694212
O	4.0811941	3.4067421	0.8748572
O	1.9324851	2.2464881	0.4468142
C	6.2651611	0.4495201	-1.4471048
H	7.1569791	0.2826451	-2.0551628
H	5.6225901	1.1846611	-1.9376808
H	6.5544891	0.8379331	-0.4662158
C	2.7718791	-2.8387439	-0.3426088
H	2.0225031	-2.8189199	-1.1416508
H	2.9641081	-3.8755829	-0.0554188
H	2.3894081	-2.2887129	0.5243872
H	-2.4378769	3.9036621	-0.6061008
F	-2.6809139	-0.2339139	2.5181912
H	1.1174501	1.2520261	3.8042522

Zero-point correction= 0.603374 (Hartree/Particle)

Thermal correction to Energy= 0.648654

Thermal correction to Enthalpy= 0.649598

Thermal correction to Gibbs Free Energy= 0.520652

Sum of electronic and zero-point Energies= -2818.642128

Sum of electronic and thermal Energies= -2818.596849

Sum of electronic and thermal Enthalpies= -2818.595905

Sum of electronic and thermal Free Energies= -2818.724851

G-1

Au	3.2599891	-1.1451399	-0.8297414

C	4.6193541	2.8366041	-1.1098964
C	5.4950751	2.3800931	-0.1821594
H	4.4680371	3.8227641	-1.5240294
H	6.2721911	2.8838451	0.3738736
C	4.2286871	0.6496821	-0.8398854
N	5.2455231	1.0294611	-0.0339914
N	3.8569671	1.7589751	-1.5083274
C	-1.1911449	4.4911041	0.8989176
F	-0.2535079	4.1883111	1.7989326
F	-2.3691489	4.4921631	1.5067766
F	-0.9464409	5.7085091	0.4329506
S	-1.1736319	3.2632481	-0.4632634
O	0.1829771	3.3994101	-1.0281294
O	-2.2674319	3.7252791	-1.3315854
O	-1.4018759	1.9848741	0.2400976
C	5.8861321	0.1802011	0.9538006
H	5.8507801	-0.8572489	0.6112546
H	6.9297491	0.4820061	1.0714026
H	5.3695921	0.2605851	1.9167656
C	2.7243001	1.8654241	-2.4240854
H	2.9991661	2.5228671	-3.2525874
H	2.4981891	0.8726161	-2.8245354
H	1.8527851	2.2835231	-1.8977364
C	-6.5533759	-1.2513319	1.2102166
C	-6.6447419	-2.6225209	0.9088196
C	-5.5301509	-3.3553789	0.5390346
C	-4.3118749	-2.6777009	0.4783186

C	-4.1928209	-1.3030049	0.7931046
C	-5.3423539	-0.5869019	1.1559076
N	-3.0575069	-3.1267009	0.1326556
C	-2.1545519	-2.0799129	0.2511066
C	-2.8149909	-0.9501449	0.6499106
C	-0.7254769	-2.2883089	-0.1113524
N	-0.4001699	-1.8812279	-1.5102144
C	0.7960571	-2.2309159	-2.0681794
C	-1.1776699	-0.8897899	-2.1975624
O	1.1601561	-1.9984209	-3.2077614
C	1.7458981	-2.8438799	-1.1095504
C	2.4493421	-3.3562019	-0.2421034
C	-2.5135809	-1.1031199	-2.5314714
C	-3.2670769	-0.0361609	-2.9855514
C	-2.7160279	1.2408661	-3.1444904
C	-1.3427899	1.3842631	-2.9554364
C	-0.5909349	0.3445591	-2.4414634
O	-3.5103749	2.2844421	-3.4312074
H	-0.5165729	-3.3638019	-0.0346224
C	0.1477681	-1.6948029	1.0132416
O	0.4634521	-2.4547429	1.9200846
N	0.5156761	-0.3918339	0.9140506
C	1.1091931	0.3736711	2.0459716
C	2.2211721	-0.4117829	2.7389586
C	1.7189101	1.6452231	1.4639946
C	-0.0021089	0.7218011	3.0330786
C	3.1049691	-4.0597099	0.8479926

H	-7.4537849	-0.7084769	1.4876546
H	-7.6125389	-3.1160339	0.9621776
H	-5.6026899	-4.4143849	0.2998886
H	-5.2743749	0.4738271	1.3857686
H	-2.8075509	-4.0882649	-0.0370964
H	-2.3925679	0.0458291	0.7443136
H	-0.8926319	2.3609981	-3.1079444
H	-3.1677479	3.0331411	-2.9034614
H	-0.0229679	0.2015661	0.2763746
H	2.9363441	-0.8015619	1.9962216
H	2.7632101	0.2744231	3.4039246
H	1.8419371	-1.2534069	3.3201156
H	1.9543011	2.3428241	2.2767816
H	1.0436831	2.1573581	0.7725036
H	2.6525851	1.4174241	0.9332186
H	0.4124401	1.2502001	3.9010356
H	-0.4989739	-0.1892209	3.3873076
H	-0.7435439	1.3706661	2.5526116
H	2.3285231	-4.5082809	1.4780446
H	3.6673091	-3.3634939	1.4791606
H	3.7844271	-4.8347299	0.4807466
H	0.4501551	0.5056461	-2.1752144
H	-3.0040149	-2.0588839	-2.3669374
F	-4.5652779	-0.2128489	-3.2274954

Zero-point correction= 0.599824 (Hartree/Particle)

Thermal correction to Energy= 0.647296

Thermal correction to Enthalpy= 0.648240

Thermal correction to Gibbs Free Energy= 0.517274

Sum of electronic and zero-point Energies= -2818.546043

Sum of electronic and thermal Energies= -2818.498571

Sum of electronic and thermal Enthalpies= -2818.497627

Sum of electronic and thermal Free Energies= -2818.628593

G-ts1

H	-1.0119032	-4.3734018	0.7282250
H	-2.6817712	-4.6401238	1.2826620
H	-2.2729202	-4.8382398	-0.4424440
H	0.2465098	5.5058442	-0.4243940
H	0.4092118	3.7935812	-0.7862860
H	-1.0366472	4.3894232	0.0864840
H	2.7905268	4.2378232	2.0711430
H	2.6142408	3.5289422	0.4573610
H	2.5947898	5.2960842	0.6576270
H	0.8608788	5.4241242	3.1840160
H	-0.7113352	5.5400032	2.3523450
H	0.6936448	6.4524682	1.7546010
H	0.1688368	3.2814422	3.0254090
H	3.5258668	-4.3542138	1.4154550
H	1.2579618	-1.3884968	-1.2291390
H	2.7608238	-3.2218938	-0.4558600
H	-0.4220492	-1.1291488	2.7247420
H	-0.6565152	1.9164362	-0.3273070
H	2.7658868	0.5561772	1.2247190
H	0.8251498	1.9843822	-2.2466080
H	5.4247858	0.2191642	-0.0895320

H	2.9900998	2.0956882	-4.0639700
H	5.4052678	1.5230262	-4.1967840
H	6.5954148	0.5820472	-2.2476910
C	-2.0712342	-4.2545518	0.4606030
C	0.0484128	4.5007032	-0.0337540
C	2.2818238	4.3447182	1.1059780
C	0.3748898	5.5052102	2.2029660
C	0.7683018	4.3357342	1.3001730
N	0.3218608	3.1277242	2.0344670
O	-0.6471782	1.1906302	2.5945130
C	-0.1147592	1.8722322	1.7315850
O	2.7328618	-4.2313078	2.0104600
C	1.1910628	-1.7611418	-0.2083230
C	2.0178398	-2.7923328	0.2115820
C	1.9700868	-3.2616748	1.5335630
C	1.0351078	-2.6666308	2.3983360
C	0.2305758	-1.6173058	2.0070430
C	0.3101318	-1.1620638	0.6886950
C	-2.2915712	-2.8368328	0.2489460
C	-2.2623642	-1.6097278	0.1307990
O	-2.6405322	0.7009102	-0.1603490
C	-1.8339282	-0.1961138	0.0748300
N	-0.5081712	-0.0543988	0.2678240
C	0.0283128	1.3255422	0.2973070
C	2.5944988	0.9372402	0.2232090
C	1.3957958	1.3582992	-0.2846000
N	1.5634698	1.6989452	-1.6227140

C	4.9123818	0.6716892	-0.9356040
C	3.5549468	1.0102472	-0.8348030
C	2.8795498	1.5023192	-1.9774420
C	3.5239598	1.7093352	-3.1977920
C	4.8684738	1.3859842	-3.2604200
C	5.5510218	0.8640772	-2.1468280
Au	-4.4239122	-1.8557578	-0.2390720
C	-8.5617122	-1.3130348	-1.0780240
C	-8.1619592	-0.0272808	-0.9332740
H	-9.5289292	-1.7381018	-1.3042350
H	-8.7105142	0.9008022	-1.0054050
C	-6.3656182	-1.3305098	-0.6180370
N	-6.8102472	-0.0563148	-0.6522010
N	-7.4429232	-2.1004578	-0.8811050
C	6.1308198	-2.7697938	-1.1856050
F	6.9733598	-1.7362698	-1.2527960
F	5.0443988	-2.4668488	-1.8987130
F	6.7193508	-3.8184778	-1.7492410
S	5.6897128	-3.1127718	0.5606560
O	6.9706478	-3.3907798	1.1984510
O	4.7953378	-4.2962558	0.3901170
O	4.9759348	-1.8988988	0.9800050
C	-6.0048362	1.1364462	-0.4047120
H	-4.9422822	0.8730652	-0.3604070
H	-6.1611202	1.8504542	-1.2174430
H	-6.3011132	1.5919232	0.5441800
C	-7.4463872	-3.5517038	-0.9531390

H	-7.7820762	-3.8777478	-1.9414190
H	-6.4297702	-3.9129898	-0.7832340
H	-8.1073522	-3.9655358	-0.1865500
F	0.9588108	-3.1117578	3.6561790

Zero-point correction= 0.597494 (Hartree/Particle)

Thermal correction to Energy= 0.645392

Thermal correction to Enthalpy= 0.646337

Thermal correction to Gibbs Free Energy= 0.509464

Sum of electronic and zero-point Energies= -2818.516389

Sum of electronic and thermal Energies= -2818.468491

Sum of electronic and thermal Enthalpies= -2818.467546

Sum of electronic and thermal Free Energies= -2818.604419

G-int1

H	0.6947203	-3.5565818	-1.7261119
H	1.4780783	-2.9302388	-3.1754809
H	2.4651203	-3.3868578	-1.7706029
H	-0.6202607	5.5127492	0.8568641
H	-0.5109937	3.7597522	0.9471601
H	0.3790933	4.6513952	-0.3247609
H	-3.9266327	4.3428852	-0.4913009
H	-3.0137907	3.3987732	0.7040971
H	-3.1579987	5.1637532	0.8829611
H	-2.7236897	5.8721342	-2.1086519
H	-0.9536037	6.0358212	-2.0233899
H	-1.9833457	6.7019692	-0.7329239
H	-2.2705357	3.6881622	-2.5133299
H	-4.0664087	-3.2044098	-2.0985469

H	-0.5542687	-1.3820548	0.3482571
H	-2.5325167	-2.6482048	-0.4031659
H	0.3743493	2.4117422	-0.3692979
H	-3.1897397	0.7805012	-0.2966659
H	0.4252613	1.2077422	1.8384971
H	-4.7054247	-0.4429618	1.9437791
H	-0.3689307	0.1573592	4.3984181
H	-2.3226997	-0.9027638	5.5056591
H	-4.4577347	-1.2150358	4.2942161
C	1.5215263	-2.9255358	-2.0784209
C	-0.5541037	4.6026512	0.2494161
C	-3.0426977	4.3480342	0.1582121
C	-1.8600187	5.8660972	-1.4306779
C	-1.7717477	4.5470462	-0.6642399
N	-1.6782197	3.5011382	-1.7097229
O	-1.4397207	1.5771042	-2.8277069
C	-1.1933087	2.2323382	-1.8236809
O	-3.2643437	-2.7777118	-2.9464659
C	-0.8292877	-1.4210818	-0.7052869
C	-1.8864257	-2.1425648	-1.1147509
C	-2.2459287	-2.1868598	-2.5146779
C	-1.3726707	-1.5099488	-3.4560129
C	-0.3378977	-0.7567468	-3.0606849
C	0.1130483	-0.7386898	-1.6448549
C	1.4391043	-1.5464598	-1.5325739
C	2.3811753	-0.8318128	-0.8956859
O	2.2376853	1.3353402	0.2006661

C	1.7826143	0.4700362	-0.5402179
N	0.5359033	0.5717112	-1.1586709
C	-0.3420647	1.6532712	-0.7059299
C	-2.4762437	0.8018992	0.5206721
C	-1.1766867	1.2273472	0.4556281
N	-0.5578997	1.0256152	1.6783001
C	-3.7727197	-0.3041718	2.4844091
C	-2.6815417	0.2947582	1.8423521
C	-1.4596827	0.4448362	2.5444001
C	-1.3107997	0.0309292	3.8687971
C	-2.4073107	-0.5590178	4.4770131
C	-3.6232317	-0.7313288	3.7914371
Au	4.3060793	-1.2262928	-0.3111799
C	8.2138973	-1.0189178	1.4131101
C	8.3201193	-2.2483208	0.8570171
H	8.9167643	-0.4363508	1.9913181
H	9.1339303	-2.9591948	0.8504581
C	6.2582873	-1.4640058	0.3781031
N	7.1144343	-2.5021508	0.2287871
N	6.9470683	-0.5553728	1.1099821
C	-5.2929967	-3.3402028	1.1722511
F	-5.8961897	-2.5952758	2.0914131
F	-3.9933057	-3.3893118	1.4466961
F	-5.7897707	-4.5635018	1.2148571
S	-5.5683397	-2.5911958	-0.4822729
O	-7.0014277	-2.6209658	-0.6811159
O	-4.8204357	-3.6271478	-1.3332679

O	-4.8588847	-1.3161398	-0.4605829
C	6.8113273	-3.7247518	-0.4918029
H	5.7970703	-3.6449058	-0.8903979
H	7.5142293	-3.8615858	-1.3189709
H	6.8678963	-4.5859918	0.1806181
C	6.4319213	0.7396782	1.5248851
H	7.0444493	1.5412552	1.1017181
H	5.4046353	0.8439112	1.1635041
H	6.4383643	0.8137382	2.6163331
H	0.2431403	-0.1923238	-3.7837289
F	-1.7268197	-1.5885318	-4.7344479

Zero-point correction= 0.598872 (Hartree/Particle)

Thermal correction to Energy= 0.645402

Thermal correction to Enthalpy= 0.646346

Thermal correction to Gibbs Free Energy= 0.513975

Sum of electronic and zero-point Energies= -2818.564708

Sum of electronic and thermal Energies= -2818.518177

Sum of electronic and thermal Enthalpies= -2818.517233

Sum of electronic and thermal Free Energies= -2818.649605

G-ts2

H	-0.4626693	-2.0881266	-2.2623337
H	0.1317847	-0.8507756	-3.3645067
H	1.2785137	-1.9835416	-2.6109447
H	2.9203557	4.0044224	-1.6113237
H	1.7572877	2.6913104	-1.3436067
H	1.3676567	4.0161054	-2.4691597
H	1.4511447	4.7954854	1.7733163

H	2.0890187	3.2413164	1.1567493
H	2.9748887	4.7319014	0.8733113
H	0.9580897	6.6822284	0.1100803
H	0.8467847	6.3192384	-1.6309037
H	2.4251947	6.3332434	-0.8304597
H	-0.7916313	5.0526464	-0.7373377
H	-4.4631953	-1.1772166	-2.8241587
H	-1.2604153	-0.9934406	0.4953383
H	-3.3154393	-1.5699786	-0.7896117
H	-0.3716713	2.1963984	-2.3631307
H	0.3048547	2.5431044	1.7373993
H	-3.2850493	1.3819284	0.4833733
H	-0.2001693	0.7544644	3.2344393
H	-4.9855293	-0.9402716	1.4324553
H	-1.3721413	-1.2215056	4.9157083
H	-3.3632793	-2.7171866	5.0161563
H	-5.1358113	-2.5769676	3.3026273
C	0.3698807	-1.3961916	-2.4426747
C	1.8531047	3.7689534	-1.5161537
C	1.9659777	4.3071184	0.9362093
C	1.3706147	6.0679674	-0.6992027
C	1.2381187	4.5798964	-0.3769107
N	-0.2232283	4.3450314	-0.2832797
O	-2.2662413	3.5986514	0.2678163
C	-1.0562163	3.4411604	0.3078393
O	-3.8714123	-0.4045966	-3.1420147
C	-1.6415073	-0.2888146	-0.2495477

C	-2.6593723	-0.7660486	-1.1118837
C	-2.9399383	-0.1028826	-2.2931967
C	-2.1025663	1.0349444	-2.6802807
C	-0.9878653	1.3680224	-2.0242357
C	-0.5170303	0.5412494	-0.8745867
C	0.5793977	-0.4762046	-1.2959707
C	1.6442237	-0.4156486	-0.4703897
O	1.9627407	0.9194664	1.5553803
C	1.3666077	0.6359944	0.5237933
N	0.2244887	1.3246444	0.1023863
C	-0.4588063	2.2240964	1.0169503
C	-2.6386883	0.8190214	1.1474353
C	-1.4691083	1.3807104	1.7060333
N	-1.1169623	0.6878544	2.8067243
C	-4.2037603	-1.0067336	2.1876073
C	-3.0874693	-0.1759786	2.1169643
C	-2.0917703	-0.2701626	3.1057153
C	-2.1544323	-1.1681166	4.1624373
C	-3.2704733	-1.9947946	4.2088003
C	-4.2774723	-1.9133166	3.2391533
Au	3.3585377	-1.5388906	-0.3868037
C	7.0777807	-3.4881016	0.4851173
C	6.7390607	-4.1793656	-0.6281257
H	7.9361447	-3.5647796	1.1370223
H	7.2407877	-4.9832446	-1.1474767
C	5.1055157	-2.6686766	-0.2458207
N	5.5308287	-3.6640686	-1.0600047

N	6.0673557	-2.5694576	0.7024753
C	-5.9174493	-3.3507236	-0.0617767
F	-6.5919593	-3.1494366	1.0705723
F	-4.6156403	-3.4001846	0.2441093
F	-6.2704403	-4.5232376	-0.5637957
S	-6.2544793	-1.9883086	-1.2455107
O	-7.6691203	-2.1220006	-1.5500117
O	-5.3177663	-2.3451596	-2.3564457
O	-5.8159283	-0.7858496	-0.5222677
C	4.8180347	-4.1377856	-2.2328497
H	3.8928627	-3.5640726	-2.3289187
H	5.4265247	-3.9934076	-3.1305107
H	4.5737887	-5.1986066	-2.1243907
C	6.0466757	-1.6273036	1.8083123
H	6.9155627	-0.9646156	1.7559293
H	5.1335097	-1.0299056	1.7407833
H	6.0553917	-2.1645716	2.7612443
F	-2.5049883	1.7116764	-3.7452477

Zero-point correction= 0.601245 (Hartree/Particle)

Thermal correction to Energy= 0.646898

Thermal correction to Enthalpy= 0.647842

Thermal correction to Gibbs Free Energy= 0.517698

Sum of electronic and zero-point Energies= -2818.540780

Sum of electronic and thermal Energies= -2818.495127

Sum of electronic and thermal Enthalpies= -2818.494183

Sum of electronic and thermal Free Energies= -2818.624327

G-int2

H	-0.4417123	-2.3850611	-1.7856637
H	0.0553007	-1.2929241	-3.0681157
H	1.2766037	-2.2989461	-2.2472777
H	3.1247707	3.4839479	-2.1320827
H	1.8874557	2.3367039	-1.5900797
H	1.5232157	3.4935199	-2.8939017
H	1.9633447	4.9529649	1.1412963
H	2.3625987	3.2443379	0.7892903
H	3.4092477	4.5312619	0.2083983
H	1.5292007	6.5681059	-0.7753967
H	1.2688857	5.9407849	-2.4246387
H	2.8914787	5.9283469	-1.7171607
H	-0.4049853	5.0959589	-1.1125777
H	-4.1279243	-1.6849661	-2.7526427
H	-1.2541153	-0.8203321	0.7131313
H	-3.1704523	-1.7086791	-0.5862177
H	-0.3117123	1.9739759	-2.4716167
H	0.5101767	2.6353599	1.6162843
H	-2.9201213	1.6378589	-0.0563907
H	-0.9870003	1.8958339	3.4826673
H	-4.9810733	-0.5402171	0.7683133
H	-2.8490943	0.6223569	5.1737813
H	-4.9302113	-0.7545351	5.0728013
H	-5.9548583	-1.3258551	2.8949763
C	0.3640757	-1.7106291	-2.1019887
C	2.0517397	3.3603139	-1.9415267
C	2.3611017	4.2627809	0.3863013

C	1.8284467	5.7931639	-1.4917357
C	1.5884647	4.3962659	-0.9216147
N	0.1188047	4.3281459	-0.7042397
O	-1.8689133	3.9770449	0.2958943
C	-0.7064883	3.6289809	0.1109453
O	-3.6202253	-0.9114961	-3.1314067
C	-1.6476043	-0.1519381	-0.0684817
C	-2.5872843	-0.8751221	-0.9670187
C	-2.7935383	-0.4230191	-2.2280217
C	-1.9874423	0.7161489	-2.6968597
C	-0.9030923	1.1643449	-2.0537337
C	-0.4321483	0.4509869	-0.8180707
C	0.6099447	-0.6460581	-1.0957487
C	1.6937857	-0.5280311	-0.2971817
O	2.1432147	1.0815839	1.4889933
C	1.4924857	0.6577609	0.5437433
N	0.3428557	1.3173999	0.0742783
C	-0.2429653	2.3747169	0.8550653
C	-2.4440603	1.0105989	0.7056983
C	-1.4485823	1.7668659	1.4837153
N	-1.6172533	1.5533699	2.7647593
C	-4.5010133	-0.2908841	1.7165853
C	-3.3366133	0.4579729	1.7704533
C	-2.7762363	0.7678469	3.0124033
C	-3.3075243	0.3625539	4.2229563
C	-4.4702513	-0.4028491	4.1529963
C	-5.0523863	-0.7207191	2.9248843

Au	3.3441797	-1.7271111	-0.0835697
C	6.9858477	-3.7510931	0.9429863
C	6.5270787	-4.6132371	0.0060373
H	7.8810237	-3.7675971	1.5480373
H	6.9391727	-5.5368481	-0.3745337
C	5.0230537	-2.9379311	0.1783943
N	5.3269317	-4.0992431	-0.4493387
N	6.0532827	-2.7342241	1.0342453
C	-5.5920193	-3.6109361	0.3526883
F	-6.5100823	-3.3570121	1.2869873
F	-4.4072813	-3.2112081	0.8389813
F	-5.5355833	-4.9202751	0.1620253
S	-5.9981013	-2.7178251	-1.2009287
O	-7.2377363	-3.3368201	-1.6447737
O	-4.7947463	-3.0087901	-2.0289157
O	-6.0632403	-1.3145831	-0.7651107
C	4.5041907	-4.7326851	-1.4644927
H	3.6149327	-4.1171411	-1.6215487
H	5.0575017	-4.8134571	-2.4048187
H	4.1971277	-5.7296461	-1.1350317
C	6.1692977	-1.6005371	1.9348373
H	7.0648847	-1.0186411	1.6973053
H	5.2857777	-0.9680851	1.8139283
H	6.2244917	-1.9469041	2.9711423
F	-2.3803043	1.2739249	-3.8337557

Zero-point correction= 0.602331 (Hartree/Particle)

Thermal correction to Energy= 0.648489

Thermal correction to Enthalpy= 0.649434

Thermal correction to Gibbs Free Energy= 0.516043

Sum of electronic and zero-point Energies= -2818.546494

Sum of electronic and thermal Energies= -2818.500335

Sum of electronic and thermal Enthalpies= -2818.499391

Sum of electronic and thermal Free Energies= -2818.632781

G-ts3

H	0.3488321	-3.4371832	0.8245104
H	-0.2946639	-3.1310182	2.4320634
H	-1.3776739	-3.7198502	1.1488424
H	-3.0515409	4.8859688	0.4945124
H	-2.4025389	3.2400678	0.5245474
H	-2.4785949	4.1926598	2.0236244
H	0.3902161	5.4056958	-0.9535576
H	-0.6763109	4.0153478	-1.3298796
H	-1.3368729	5.6408558	-1.2684566
H	0.1334931	6.7092958	1.1601014
H	-1.0714599	6.2180628	2.3786054
H	-1.6008209	6.8943608	0.8299634
H	0.5525521	4.5571198	2.2114594
H	4.7079711	-1.8172382	2.1436924
H	1.0787711	-1.6615122	-0.5885776
H	3.4701051	-1.7371362	0.2163524
H	-0.7260919	2.3308638	-0.3413666
H	2.8172791	0.2631578	0.4129864
H	1.6034951	3.4194298	-1.4676906
H	3.9077031	-1.4630622	-1.9069366

H	3.6830791	3.3388928	-3.3681426
H	5.3475911	1.7659038	-4.3493406
H	5.4541991	-0.5916252	-3.5910116
C	-0.5320519	-3.0583562	1.3623454
C	-2.2833159	4.2459078	0.9460764
C	-0.6071469	4.9716858	-0.7978346
C	-0.8527609	6.2502858	1.3040174
C	-0.9039369	4.8504498	0.6967764
N	0.1589821	4.0900258	1.4002024
O	1.1572081	2.3001448	2.3430354
C	0.4622431	2.7617148	1.4556054
O	3.9779931	-1.6181932	2.8085204
C	1.4026921	-0.9009122	0.1354424
C	2.7017061	-1.2752882	0.8343434
C	2.8650021	-1.3084192	2.2012814
C	1.7670301	-0.8726072	3.0498484
C	0.5960381	-0.4763292	2.5510274
C	0.2149351	-0.5838632	1.1005434
C	-0.8606869	-1.6618662	0.9751014
C	-2.0247439	-1.1707632	0.5085614
O	-2.5908229	1.0851168	-0.2328546
C	-1.8239649	0.2705678	0.2655064
N	-0.5371739	0.6055258	0.6923034
C	0.0429911	1.8562348	0.2816554
C	1.9316661	0.3458028	-0.5540316
C	1.2531911	1.5851608	-0.5353946
N	1.8432411	2.4393528	-1.3825856

C	3.8255101	-0.4238492	-2.2253146
C	2.8886791	0.4476188	-1.6771846
C	2.8567171	1.7870208	-2.1015816
C	3.7204661	2.2963048	-3.0613866
C	4.6440181	1.4099168	-3.6012156
C	4.6970621	0.0742078	-3.1863496
Au	-3.8309169	-2.0259952	0.0594744
C	-7.8407399	-2.8318172	-1.2047646
C	-7.5107739	-4.0834642	-0.8091716
H	-8.7550319	-2.4355582	-1.6228556
H	-8.0772449	-5.0036712	-0.8113016
C	-5.7135909	-2.7642552	-0.4511936
N	-6.2069919	-4.0214202	-0.3517486
N	-6.7301399	-2.0398942	-0.9784886
C	7.0371851	-4.0172922	0.1403444
F	7.2064521	-4.7773312	-0.9354056
F	6.4620351	-4.7491682	1.0899654
F	8.2268801	-3.6198982	0.5735054
S	5.9878361	-2.5718442	-0.2676146
O	6.7311671	-1.8475642	-1.2945116
O	5.8881821	-1.8665422	1.0395014
O	4.7154311	-3.1806222	-0.6969996
C	-5.4678469	-5.1590152	0.1639974
H	-4.4704309	-4.8176002	0.4517604
H	-5.9737339	-5.5744442	1.0406614
H	-5.3762779	-5.9323722	-0.6045046
C	-6.6693089	-0.6173272	-1.2707656

H	-5.6749929	-0.2459762	-1.0058306
H	-6.8453209	-0.4447362	-2.3366796
H	-7.4216789	-0.0800902	-0.6856346
H	-0.1747119	-0.1027422	3.2207104
F	2.0150831	-0.8310132	4.3547914

Zero-point correction= 0.596838 (Hartree/Particle)

Thermal correction to Energy= 0.643157

Thermal correction to Enthalpy= 0.644102

Thermal correction to Gibbs Free Energy= 0.509259

Sum of electronic and zero-point Energies= -2818.500112

Sum of electronic and thermal Energies= -2818.453792

Sum of electronic and thermal Enthalpies= -2818.452847

Sum of electronic and thermal Free Energies= -2818.587690

G-int3

H	0.1817757	-3.6236254	-0.1046521
H	0.3353127	-3.3011984	1.6299849
H	-1.2338763	-3.7751074	0.9406849
H	-3.1450793	4.9137576	-0.6429891
H	-2.5807063	3.2685496	-0.2660501
H	-3.0293993	4.3701716	1.0426979
H	0.5350027	5.3529636	-1.1769801
H	-0.3795403	3.9255386	-1.7065391
H	-1.0664263	5.5354336	-1.9072421
H	-0.1676943	6.7187106	0.7759609
H	-1.6742443	6.3417866	1.6508459
H	-1.7430693	6.9419926	-0.0134201
H	-0.3317403	4.5548496	2.0547779

H	5.4745407	-2.1801874	0.9553319
H	1.0552507	-1.0427184	-1.3791771
H	2.0865857	-2.7319584	0.0628029
H	-0.6755773	2.2745086	-0.7249301
H	1.8976417	3.8412306	-0.0982361
H	4.6819877	-0.6027454	-1.4378851
H	4.5490187	4.3718506	-0.8652361
H	6.6499867	3.2019006	-1.5104091
H	6.6795497	0.7428216	-1.7887431
C	-0.3294643	-3.1833804	0.7637959
C	-2.5487923	4.3160246	0.0579799
C	-0.4670803	4.9094386	-1.2356181
C	-1.1774973	6.3023586	0.6728329
C	-1.1299013	4.8729366	0.1389009
N	-0.3175363	4.1170866	1.1369799
O	-0.1008213	2.2923116	2.4565179
C	-0.2190133	2.7537896	1.3368849
O	4.2098927	-1.6857754	1.7511119
C	1.4840637	-0.7020884	-0.4231391
C	2.5273987	-1.7260164	0.0267419
C	3.0566797	-1.4460564	1.4008799
C	2.0848197	-0.9162374	2.3568089
C	0.8498237	-0.5358074	2.0068839
C	0.3229587	-0.6236564	0.6001869
C	-0.7034253	-1.7616454	0.5241319
C	-1.9392343	-1.2988194	0.2523179
O	-2.7112783	0.9694586	-0.2267101

C	-1.8377823	0.1662826	0.0804869
N	-0.5250023	0.5230836	0.3093079
C	-0.0659183	1.8655386	0.0938669
C	2.0872957	0.6722736	-0.5677431
C	1.3743977	1.8073156	-0.2916141
N	2.1686657	2.9209436	-0.4156571
C	4.6224637	0.4716436	-1.2820371
C	3.4275767	1.1036546	-0.8938431
C	3.4386227	2.5169516	-0.7645321
C	4.5777047	3.2900056	-0.9783351
C	5.7403037	2.6313896	-1.3389231
C	5.7567427	1.2365956	-1.4935131
Au	-3.7801083	-2.1622674	0.0132919
C	-7.9538183	-2.7576134	-0.6908261
C	-7.6262023	-4.0494694	-0.4541991
H	-8.9012053	-2.2965244	-0.9309201
H	-8.2280473	-4.9469164	-0.4452571
C	-5.7377523	-2.8257934	-0.2662401
N	-6.2672633	-4.0701024	-0.1967061
N	-6.7874643	-2.0249204	-0.5715521
C	5.3280457	-4.9542174	0.2090239
F	5.0048077	-5.8556954	-0.7004521
F	4.2272847	-4.5376434	0.8270079
F	6.1506787	-5.4847104	1.0909739
S	6.1177627	-3.5208004	-0.6264771
O	7.4008927	-3.9578924	-1.1128361
O	6.3405797	-2.5761604	0.6006899

O	5.0954267	-2.9970994	-1.5150441
C	-5.5109573	-5.2698504	0.1085589
H	-4.4673383	-4.9852624	0.2630939
H	-5.8952903	-5.7403654	1.0185979
H	-5.5723653	-5.9795964	-0.7219511
C	-6.7071543	-0.5835704	-0.7507711
H	-7.3482553	-0.0788854	-0.0219561
H	-5.6715223	-0.2635734	-0.6002461
H	-7.0230623	-0.3134044	-1.7627551
H	3.3610397	-1.7986984	-0.6740141
H	0.1786867	-0.1203084	2.7550159
F	2.5166417	-0.8067864	3.6104009

Zero-point correction= 0.603027 (Hartree/Particle)

Thermal correction to Energy= 0.649248

Thermal correction to Enthalpy= 0.650192

Thermal correction to Gibbs Free Energy= 0.517707

Sum of electronic and zero-point Energies= -2818.586952

Sum of electronic and thermal Energies= -2818.540731

Sum of electronic and thermal Enthalpies= -2818.539787

Sum of electronic and thermal Free Energies= -2818.672273

G-int4

H	0.9381846	-0.2258974	-3.4019995
H	1.0455886	1.4005886	-2.7124005
H	2.4529866	0.3131086	-2.6638605
H	-4.2785134	2.9847226	4.2938895
H	-4.7633134	1.3358976	3.8393245
H	-3.1173444	1.6446276	4.4489315

H	-4.2515374	2.9992616	0.5167645
H	-5.4227624	2.1008076	1.5225985
H	-4.9732664	3.7638716	1.9449965
H	-1.9973724	3.5434966	1.3815265
H	-1.4516174	2.9502756	2.9758465
H	-2.6512454	4.2608176	2.8654015
H	-3.4770044	0.7455396	0.9563005
H	-0.9941894	-1.6348614	-2.1851865
H	-1.1787544	0.3687546	-3.5318655
H	-1.3126974	-1.7132294	2.0502005
H	-4.1286424	-2.1270884	1.8345965
H	-3.9340234	-2.0301384	-3.5591695
H	-6.4191524	-3.2130374	0.6260915
H	-7.3765134	-3.7031174	-1.6159625
H	-6.1321094	-3.1208924	-3.6708595
C	1.3629006	0.3574716	-2.5724585
C	-3.9302304	2.0496976	3.8381225
C	-4.5914774	2.8177006	1.5457535
C	-2.3090204	3.3237726	2.4089735
C	-3.4483794	2.3081446	2.4142795
N	-3.0136264	1.0319986	1.8101665
O	-1.2207784	0.5715636	3.1530165
C	-1.9384944	0.3061556	2.2035765
O	-3.5481914	1.9856346	-2.8560585
C	-1.5359444	-0.7898504	-1.7282465
C	-2.0169024	0.1272276	-2.8623345
C	-2.5776494	1.4393966	-2.3754755

C	-1.7920014	2.0552896	-1.2868565
C	-0.8592414	1.4001146	-0.5938045
C	-0.5255274	-0.0551504	-0.7955095
C	0.9272446	-0.1826074	-1.2564475
C	1.6893186	-0.8012684	-0.3293375
O	1.0709656	-1.8525994	1.7873155
C	0.8002056	-1.1943534	0.7991485
N	-0.4574054	-0.6921944	0.5110185
C	-1.6189944	-0.9357134	1.3325365
C	-2.6897244	-1.3388264	-0.9338265
C	-2.7065984	-1.3994654	0.4337665
N	-3.8826164	-1.9668314	0.8701275
C	-4.4678924	-2.2577214	-2.6391345
C	-3.9146064	-1.9497794	-1.3870025
C	-4.6392404	-2.3212164	-0.2261555
C	-5.8840814	-2.9438654	-0.2821805
C	-6.4076764	-3.2162284	-1.5350045
C	-5.7019224	-2.8819864	-2.7013015
Au	3.6665486	-1.3614994	-0.1811775
C	7.3654136	-2.9158494	1.2633465
C	7.8601776	-2.1642054	0.2513825
H	7.8595476	-3.5331764	1.9997225
H	8.8755696	-1.9833784	-0.0707265
C	5.6183006	-1.9574304	0.2106215
N	6.7754436	-1.5897304	-0.3831815
N	5.9912396	-2.7754684	1.2235375
C	4.3451166	3.9841956	-0.6786755

F	3.3790786	4.3810896	-1.4824425
F	5.5116756	4.3982726	-1.1436085
F	4.1519446	4.4604976	0.5335375
S	4.4068416	2.1461476	-0.6295995
O	2.9455086	1.9679676	-0.0435475
O	5.4282446	1.7761546	0.3277705
O	4.4854266	1.6756136	-2.0000385
C	6.8777406	-0.6433264	-1.4817565
H	5.8990206	-0.5427024	-1.9562475
H	7.1786856	0.3392696	-1.1065645
H	7.6054186	-1.0081884	-2.2119995
C	5.0743816	-3.4274634	2.1453745
H	5.4062586	-3.2600704	3.1738645
H	4.0755736	-2.9985124	2.0203015
H	5.0324196	-4.5026274	1.9461175
H	-2.7857914	-0.3525184	-3.4733785
H	2.6390506	1.0205956	-0.1116545
H	-0.3108994	1.9077546	0.2022205
F	-2.1070514	3.3205726	-1.0050315

Zero-point correction= 0.601503 (Hartree/Particle)

Thermal correction to Energy= 0.648255

Thermal correction to Enthalpy= 0.649199

Thermal correction to Gibbs Free Energy= 0.516462

Sum of electronic and zero-point Energies= -2818.590902

Sum of electronic and thermal Energies= -2818.544151

Sum of electronic and thermal Enthalpies= -2818.543206

Sum of electronic and thermal Free Energies= -2818.675943

G-ts4

H	1.1913528	-0.8304633	-3.0961975
H	0.6215298	0.8423857	-3.2101125
H	2.2668048	0.4769517	-2.5959245
H	-3.7411142	5.0272297	1.6987055
H	-3.2424312	3.9442607	0.3783605
H	-4.3022532	3.3392857	1.6727415
H	-0.1580962	4.2195707	2.4908915
H	-0.8317632	4.4950107	0.8629675
H	-1.3065622	5.5415797	2.2114975
H	-1.6329002	3.3423477	4.3344815
H	-3.3371252	2.9426117	4.0118365
H	-2.8126152	4.6432737	4.0577355
H	-0.8731412	2.1175647	1.4942415
H	-0.7933132	-2.0760953	-1.3564665
H	-0.9490862	-0.9499223	-3.5277945
H	-1.5839562	-0.7119913	2.2848935
H	-4.5327892	-0.8276653	1.9254975
H	-3.7539462	-3.2532463	-2.8418305
H	-6.6933772	-2.5266283	1.1451275
H	-7.4598062	-3.8995013	-0.7851215
H	-5.9832512	-4.2521003	-2.7376525
C	1.2194328	0.1521747	-2.6033245
C	-3.4559952	3.9968447	1.4542495
C	-1.0601382	4.5101177	1.9373665
C	-2.5226302	3.6278897	3.7608655
C	-2.2286472	3.5905287	2.2650945

N	-1.8084522	2.2326587	1.8620885
O	-3.6837852	1.0668377	2.4486045
C	-2.5656342	1.1239457	1.9449325
O	-3.5827312	0.2019477	-4.0301765
C	-1.5094822	-1.2410093	-1.4457125
C	-1.8609062	-1.0628253	-2.9258665
C	-2.7162352	0.1526557	-3.1863455
C	-2.3474042	1.3363037	-2.3706055
C	-1.4554682	1.2983357	-1.3785735
C	-0.7932912	0.0330887	-0.8989985
C	0.6984458	0.0393517	-1.2211935
C	1.4521018	-0.0356513	-0.0908325
O	0.7816168	-0.2750953	2.2469745
C	0.5258548	-0.1161833	1.0673405
N	-0.7582472	0.0226867	0.5631145
C	-1.9276182	-0.1641063	1.3903255
C	-2.7353602	-1.5082623	-0.6163555
C	-2.9162222	-0.9773913	0.6322985
N	-4.1319102	-1.3387473	1.1470405
C	-4.3788442	-3.0631473	-1.9727075
C	-3.9308972	-2.2629263	-0.9092355
C	-4.7893152	-2.1044003	0.2107485
C	-6.0585162	-2.6753843	0.2745265
C	-6.4745732	-3.4397253	-0.8018955
C	-5.6370662	-3.6366753	-1.9107085
Au	3.2199398	-1.2488063	0.1457105
C	6.2129668	-3.9525363	1.4615945

C	6.8876988	-3.3543283	0.4504605
H	6.5087358	-4.7223613	2.1594915
H	7.8986608	-3.4872813	0.0934165
C	4.8318228	-2.4571403	0.5077695
N	6.0239338	-2.4447443	-0.1250875
N	4.9525688	-3.3868953	1.4829575
C	4.8679518	3.4433327	-1.4376705
F	3.9134618	3.8352867	-2.2681355
F	6.0307758	3.4624377	-2.0728395
F	4.9189908	4.2702457	-0.4073515
S	4.5372718	1.7318297	-0.8628855
O	3.1916558	1.9323177	-0.1884895
O	5.6207028	1.4072977	0.0575465
O	4.4320288	0.9250417	-2.0834035
C	6.3898868	-1.5216453	-1.1940035
H	7.1404678	-1.9987493	-1.8287515
H	5.5043248	-1.2757673	-1.7844925
H	6.7741798	-0.5881133	-0.7717555
C	3.9038368	-3.7553303	2.4189245
H	3.4744018	-4.7260673	2.1531805
H	4.3159918	-3.8030263	3.4304605
H	3.1211028	-2.9925053	2.3901365
H	-2.3871982	-1.9323553	-3.3247975
H	2.4375858	0.8643037	-0.1095685
H	-1.2094582	2.2201417	-0.8521935
F	-2.9545312	2.4671207	-2.7011435

Zero-point correction= 0.596480 (Hartree/Particle)

Thermal correction to Energy= 0.642629

Thermal correction to Enthalpy= 0.643573

Thermal correction to Gibbs Free Energy= 0.511615

Sum of electronic and zero-point Energies= -2818.589235

Sum of electronic and thermal Energies= -2818.543087

Sum of electronic and thermal Enthalpies= -2818.542143

Sum of electronic and thermal Free Energies= -2818.674101

G-2

H	-0.8693346	-3.9945697	-2.5886010
H	-2.3488706	-3.2059567	-3.1990870
H	-0.8631196	-3.2527557	-4.1814810
H	-2.5851986	5.7051673	-0.8579100
H	-3.3699036	4.1314633	-0.5973470
H	-2.0375576	4.6447563	0.4635400
H	-1.2575006	3.5591913	-3.6362490
H	-2.9137256	3.4551763	-2.9792990
H	-2.1637246	5.0368093	-3.2656660
H	0.6504434	4.2473583	-2.1407150
H	0.3294964	4.7728543	-0.4658410
H	-0.1959626	5.7844723	-1.8313470
H	-1.2405316	1.9184763	-1.8919680
H	-0.4127336	-2.6543997	-0.0297590
H	-2.3020416	-3.8667847	-0.9928050
H	0.7647634	0.6905343	0.3092740
H	-1.0278016	1.5673003	2.5835480
H	-2.9672986	-3.4966357	2.6006300
H	-2.2014126	0.8015593	5.0496460

H	-3.3743276	-1.1087357	6.1351930
H	-3.7356386	-3.2207517	4.8982920
C	-1.2546196	-3.1423977	-3.1662980
C	-2.4116426	4.6628973	-0.5636080
C	-1.9687376	4.0116883	-2.9326020
C	-0.0713906	4.7513143	-1.4847420
C	-1.4106416	4.0193933	-1.5159130
N	-1.2029346	2.6046423	-1.1484870
O	-0.4159906	2.8801643	0.9820310
C	-0.6656936	2.1734393	0.0029350
O	-4.8803256	-3.0888697	0.0804910
C	-1.3819886	-2.1393417	-0.0547680
C	-2.4870906	-3.1901967	-0.1488030
C	-3.8586256	-2.5973617	-0.3471900
C	-3.8762516	-1.3736037	-1.1884800
C	-2.7761696	-0.7630847	-1.6363430
C	-1.3783926	-1.2326837	-1.3164600
C	-0.7731086	-1.8738547	-2.5651760
C	0.2554114	-1.1436447	-3.0123970
O	1.4220284	0.7868023	-2.0981870
C	0.5153944	-0.0371257	-2.0968290
N	-0.4924696	-0.0678547	-1.1450480
C	-0.3196646	0.6827803	0.0791160
C	-1.5274056	-1.2698187	1.1656750
C	-1.0421986	0.0075323	1.1863470
N	-1.2568266	0.5981593	2.4022820
C	-2.7759976	-2.5557427	3.1087310

C	-2.1093836	-1.4963147	2.4687630
C	-1.9199396	-0.2964727	3.2074110
C	-2.3635266	-0.1340237	4.5186100
C	-3.0138036	-1.2004887	5.1133610
C	-3.2166766	-2.3987307	4.4111340
Au	3.0796404	-0.7279387	0.1070230
C	5.0778854	2.7669003	1.3278980
C	5.9874964	1.8371933	1.7064480
H	5.0888094	3.8445343	1.4024140
H	6.9545814	1.9365623	2.1774630
C	4.2525884	0.7559043	0.7754760
N	5.4652624	0.6073083	1.3568460
N	4.0216704	2.0865283	0.7551060
C	1.8299824	-4.8586117	-0.2038760
F	0.5004244	-4.8992077	-0.3176830
F	2.1413154	-4.6670107	1.0687480
F	2.3255824	-6.0169417	-0.6052060
S	2.5073244	-3.5037847	-1.2408960
O	1.9906464	-3.7665147	-2.5758530
O	3.9465844	-3.5196717	-1.0099940
O	1.8264904	-2.3103767	-0.5775110
C	6.1189414	-0.6682047	1.6069270
H	7.1912084	-0.5674747	1.4203920
H	5.9545184	-0.9863017	2.6407640
H	5.7055764	-1.4211137	0.9301630
C	2.8220614	2.7239633	0.2217550
H	2.0434654	2.8008283	0.9897750

H	3.0857264	3.7264883	-0.1251590
H	2.4409724	2.1396593	-0.6235290
H	-2.5050836	-3.8276267	0.7384570
H	0.8916824	-1.3702757	-3.8597630
H	-2.8801776	0.1066063	-2.2854320
F	-5.0845366	-0.9131537	-1.4883560

Zero-point correction= 0.603775 (Hartree/Particle)

Thermal correction to Energy= 0.649675

Thermal correction to Enthalpy= 0.650619

Thermal correction to Gibbs Free Energy= 0.520510

Sum of electronic and zero-point Energies= -2818.632076

Sum of electronic and thermal Energies= -2818.586177

Sum of electronic and thermal Enthalpies= -2818.585232

Sum of electronic and thermal Free Energies= -2818.715341