Gold-catalyzed domino cyclization enabling construction of diverse fused azaspiro tetracyclic scaffolds: A cascade catalysis mechanism due to substrate and counterion

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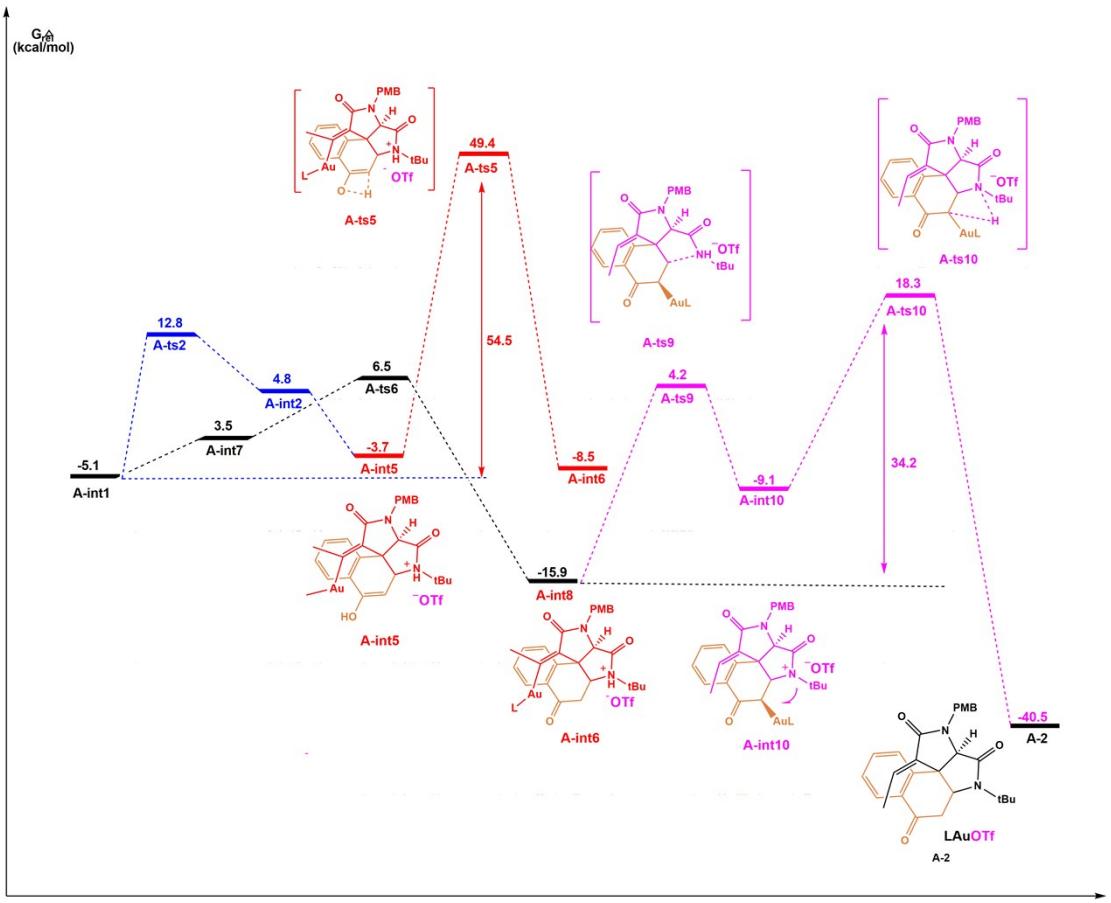

Fig. S1. alternative pathway in cooperative catalysis and cascade catalysis**.**

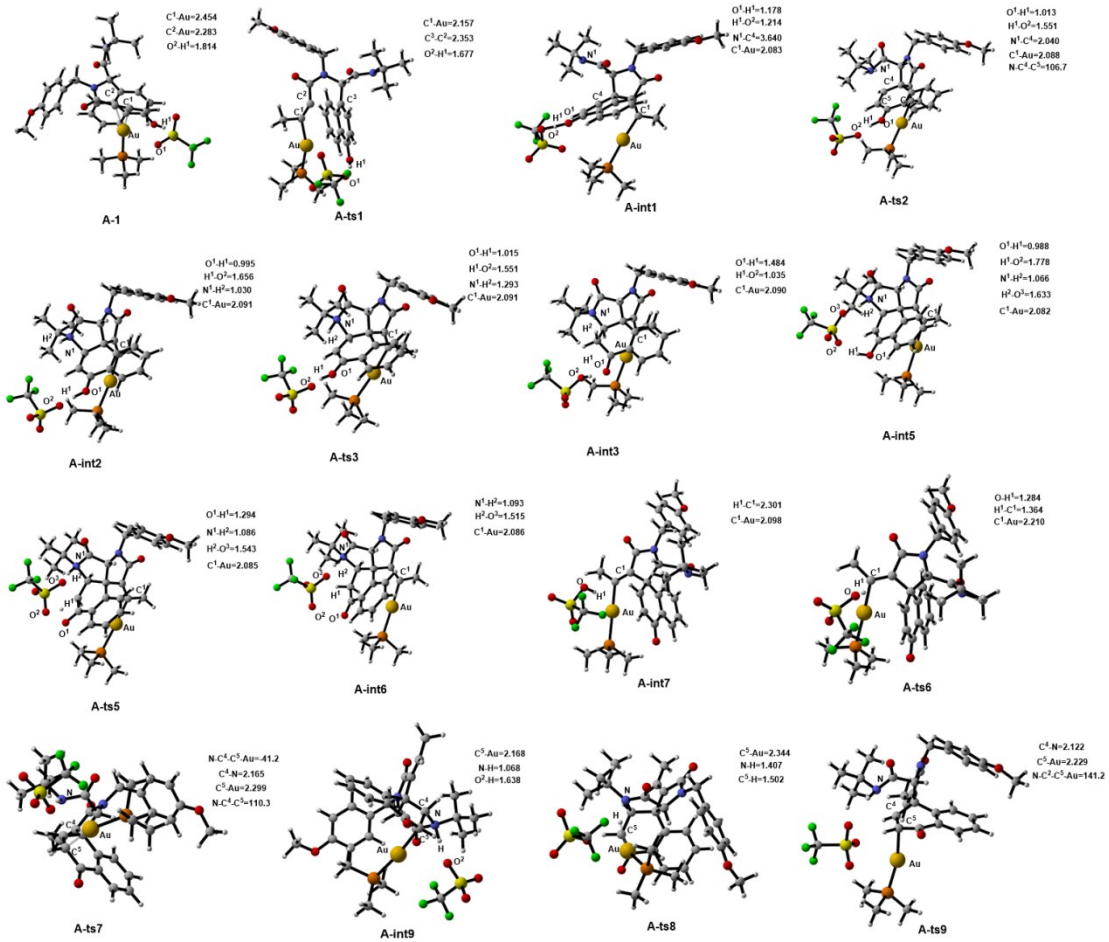

Fig. S2. Optimized geometries of transition states and intermediates shown in Fig. 1. Color scheme: C, gray; N, blue; O, red; Cl, green; P, orange; Au, yellow.

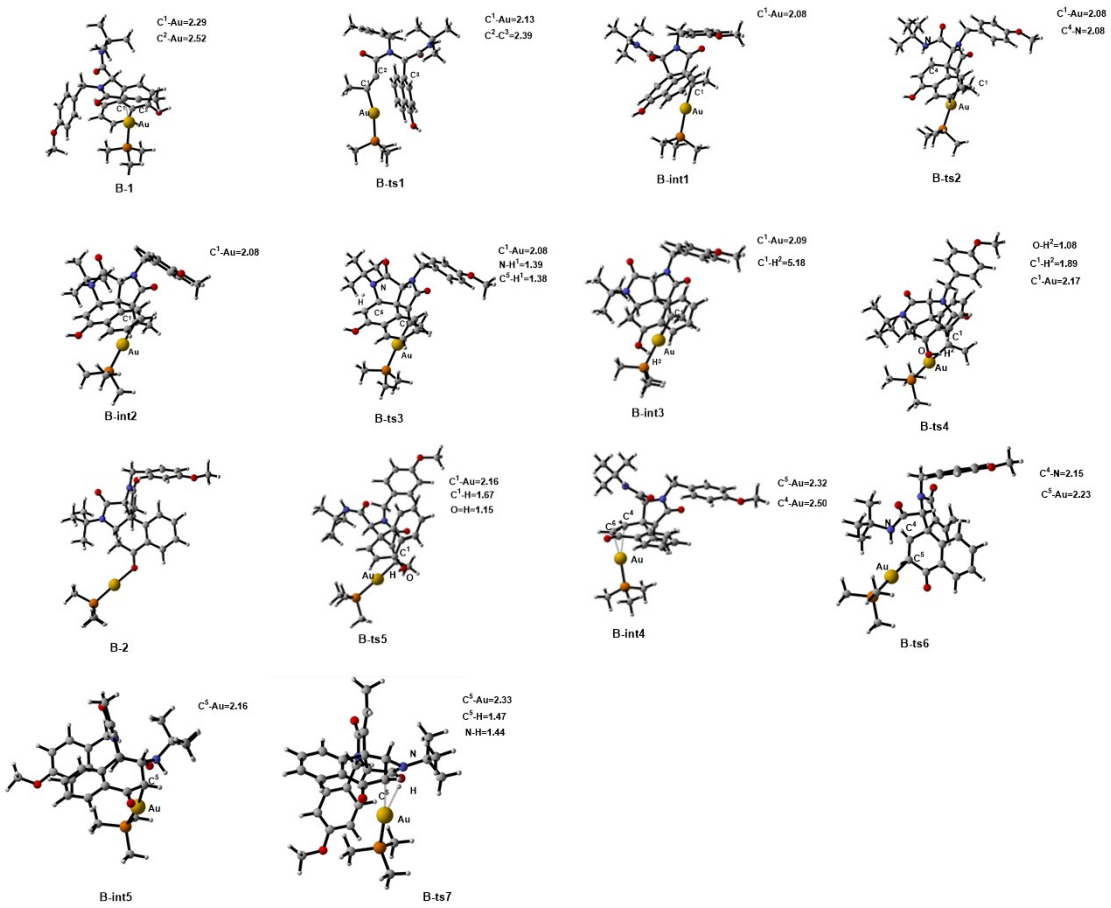

Fig. S3. Optimized geometries of transition states and intermediates shown in Fig. 2. Color scheme: C, gray; N, blue; O, red; Cl, green; P, orange; Au, yellow.

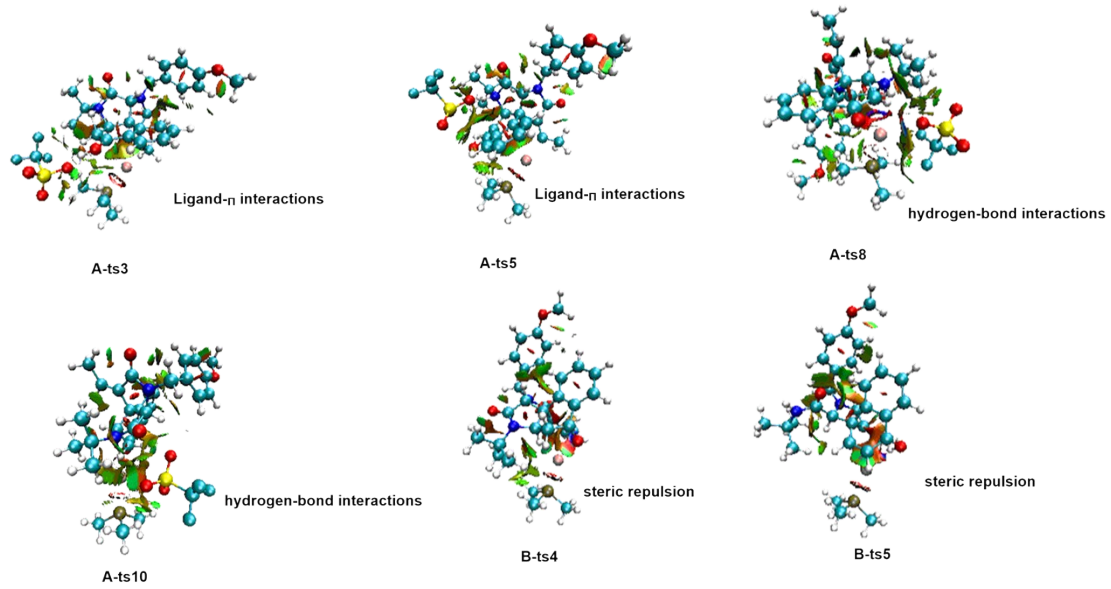

Fig. S4. Noncovalent interaction (NCI) plot for the rate-determining transition states. The green, blue and red regions respectively represent attractive, strongly and repulsive interactions.

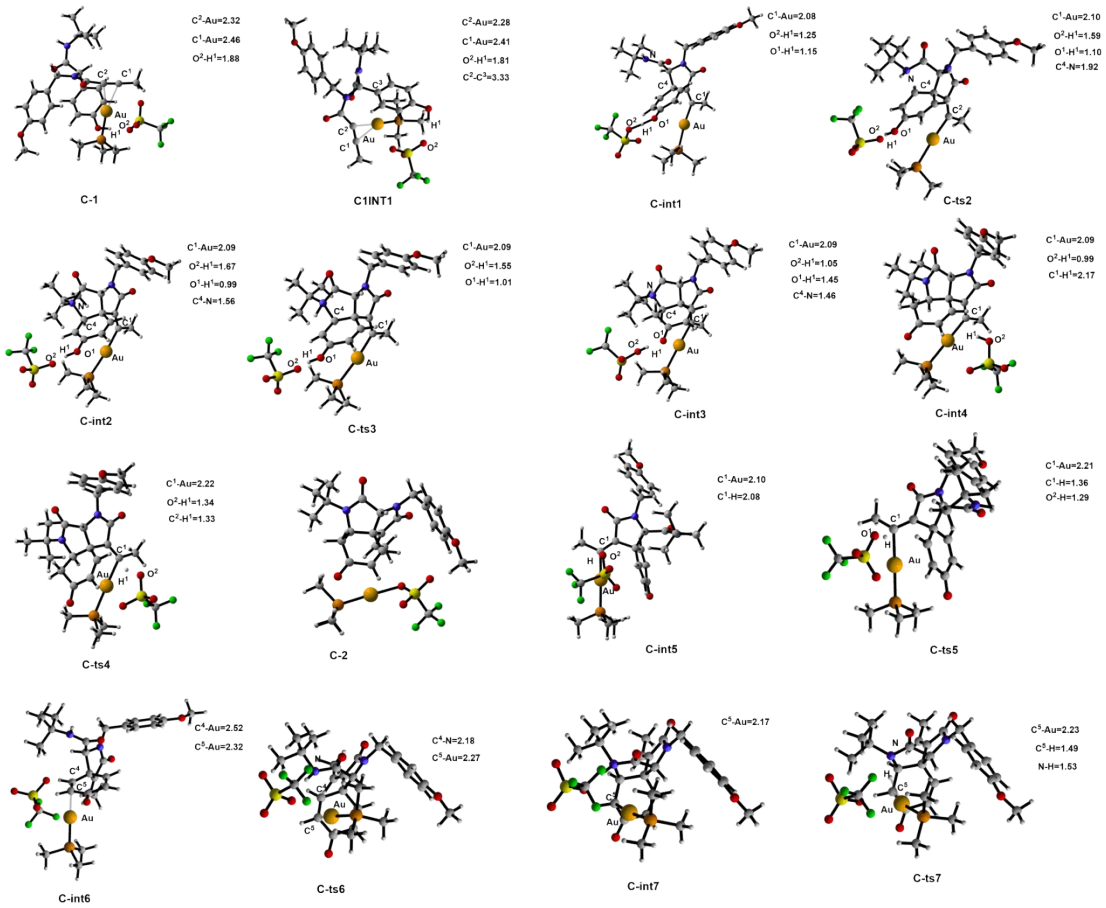

Fig. S5. Optimized geometries of transition states and intermediates shown in Fig. 3a.

Color scheme: C, gray; N, blue; O, red; Cl, green; P, orange; Au, yellow.

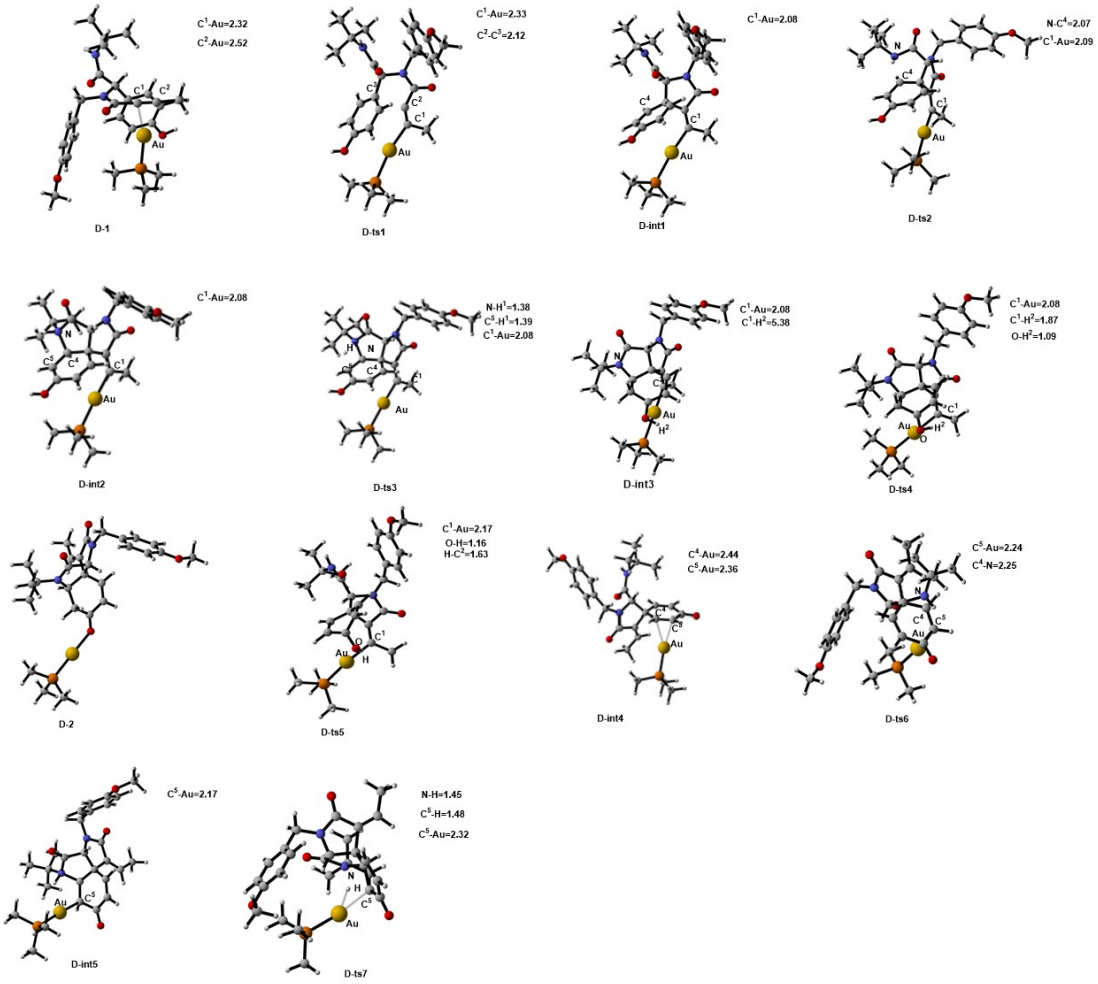

Fig. S6. Optimized geometries of transition states and intermediates shown in Fig. 3b. Color scheme: C, gray; N, blue; O, red; Cl, green; P, orange; Au, yellow.

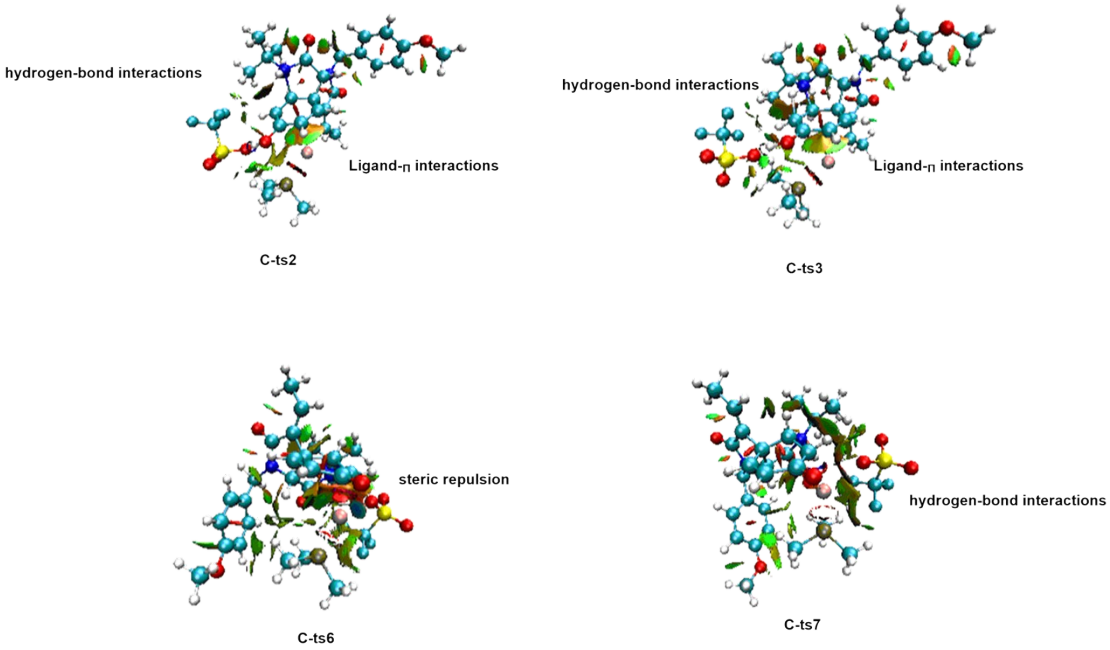

Fig. S7. Noncovalent interaction (NCI) plot for the rate-determining transition states. The green, blue and red regions respectively represent attractive, strongly and repulsive interactions.

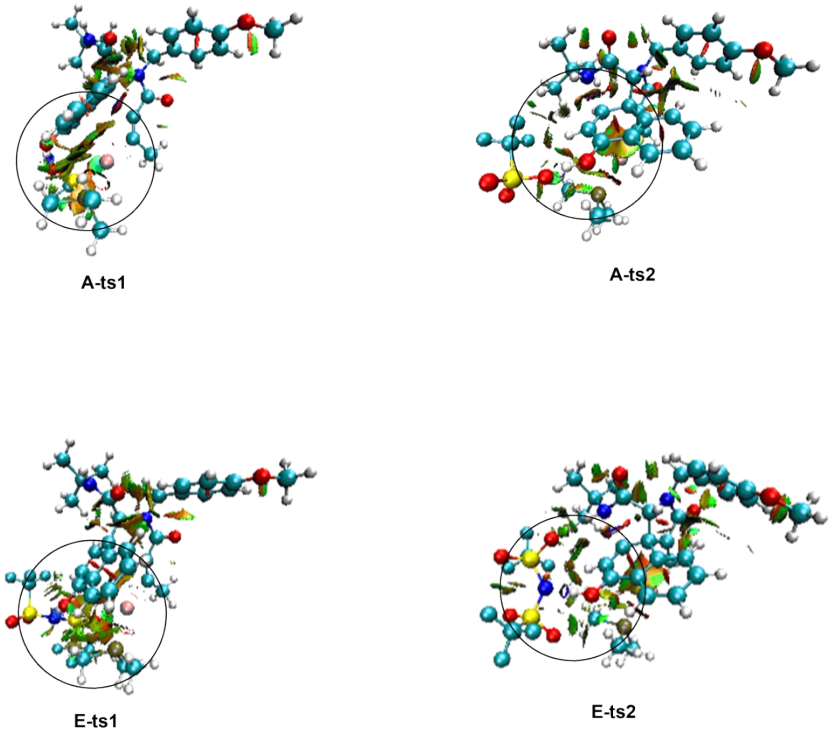

Fig. S8. Noncovalent interaction (NCI) plot for the rate-determining transition states. The green, blue and red regions respectively represent attractive, strongly and repulsive interactions.

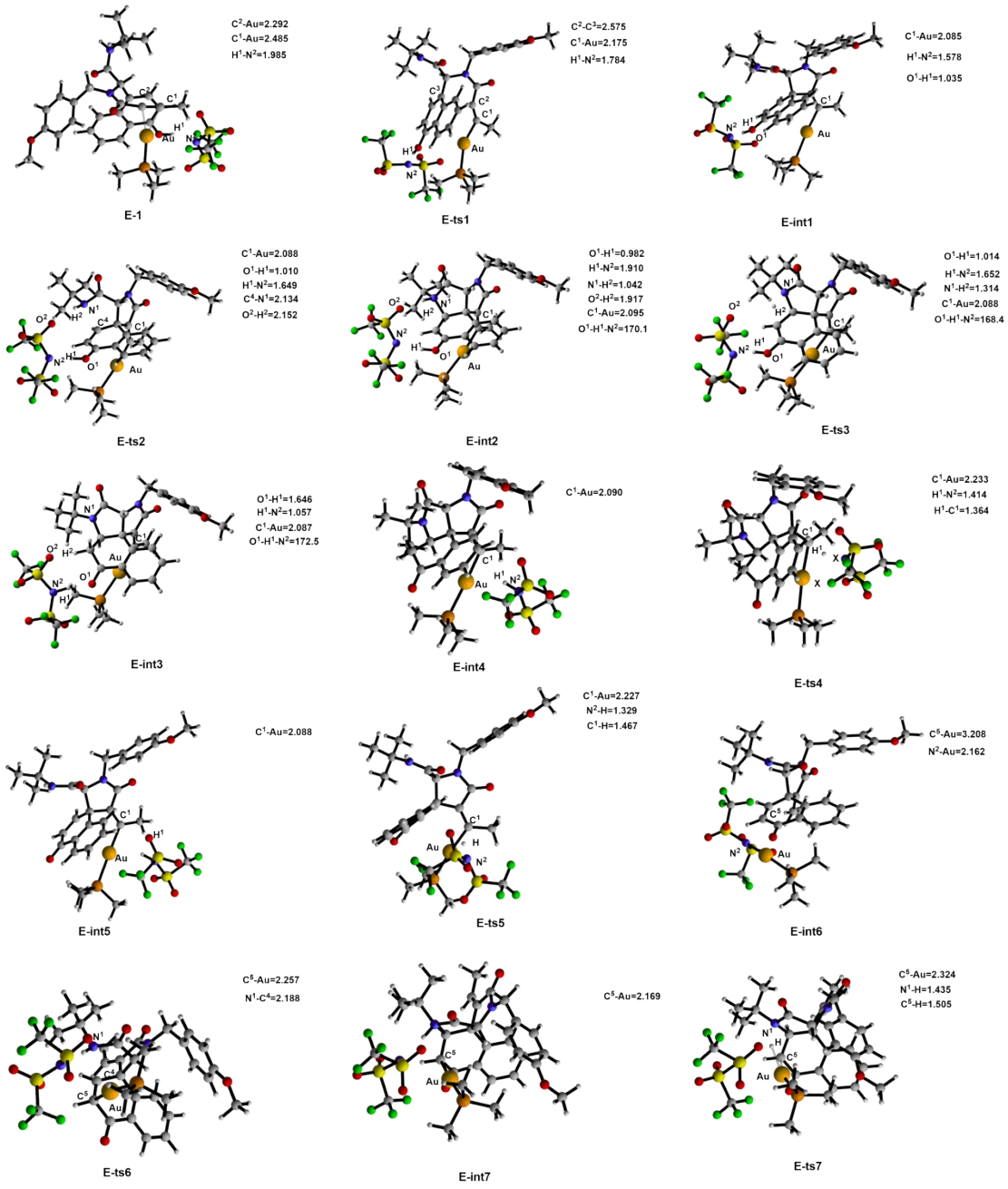

Fig. S9. Optimized geometries of transition states and intermediates shown in Fig. 4.

Color scheme: C, gray; N, blue; O, red; Cl, green; P, orange; Au, yellow.

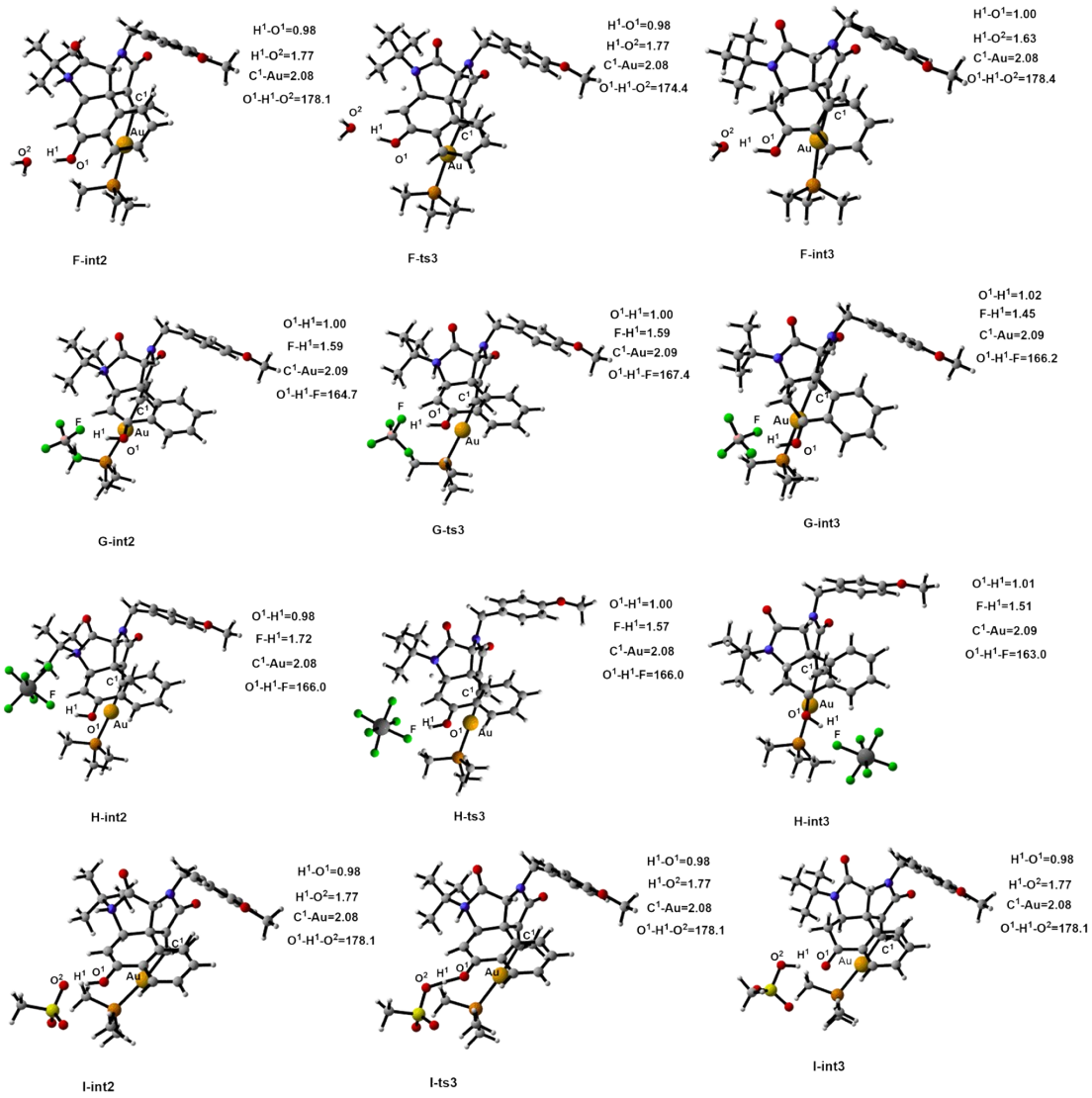

Fig. S10. Optimized transition states and intermediates for different counterions. Color scheme: C, gray; N, blue; O, red; Cl, green; P, orange; Au, yellow.

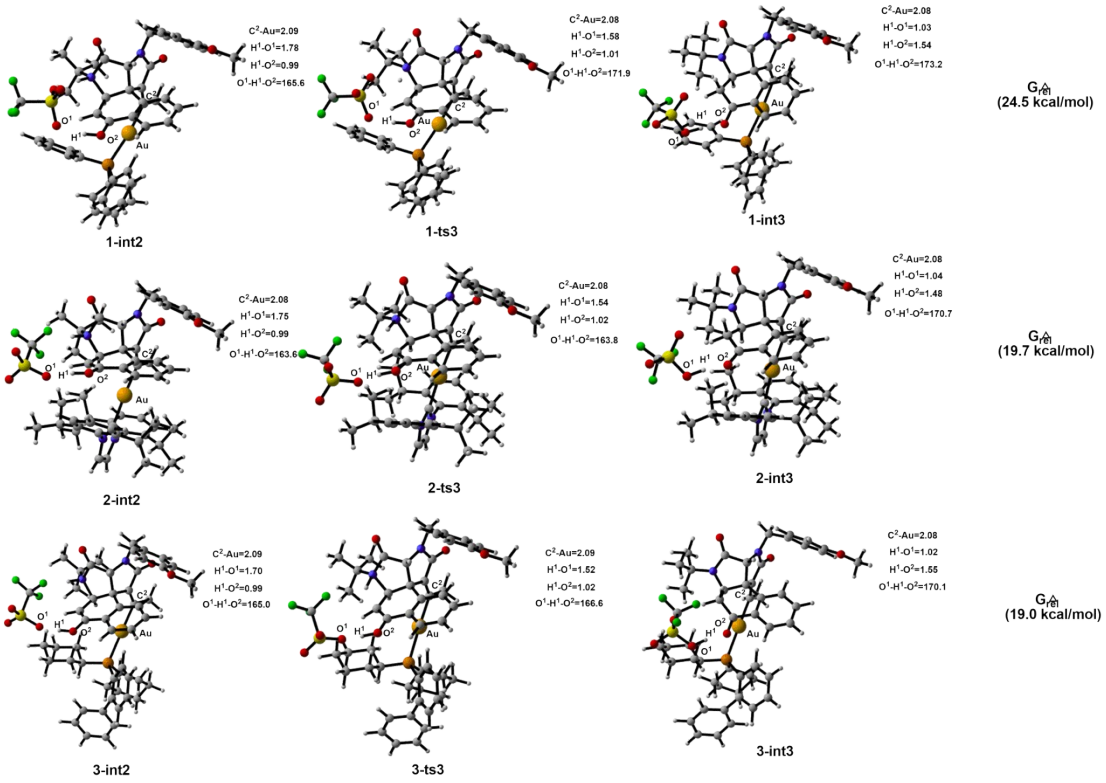

Fig. S11. Optimized transition states and intermediates for different ligands. Color scheme: C, gray; N, blue; O, red; Cl, green; P, orange; Au, yellow.

Table S1. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 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	19.4	19.0	19.4	19.0	27.4	18.8	27.4	18.8
A-int1	-5.5	-6.1			2.4	-5.1		
A-ts2	12.9	14.7	18.4	20.8	15.9	12.8	13.5	18.0
A-int2	7.6	10.0			1.4	4.8		
A-ts3	24.0	26.9	16.4	16.9	30.9	26.2	29.4	21.3
A-int3	-20.8	-17.7			-5.4	-14.9		
A-int4	-22.9	-20.2			-12.6	-16.0		
A-ts4	-14.4	-12.7	8.5	7.5	-5.3	-12.6	7.4	3.5
A-2	-41.2	-39.7			-40.0	-40.5		

A-int5	-5.9	-4.5			-6.2	-3.7		
A-ts5	47.3	49.3	53.3	53.9	54.9	49.4	61.1	53.1
A-int6	-9.9	-8.5			-8.8	-8.5		
A-int7	1.6	1.7			10.2	3.4		
A-ts6	7.4	7.6	5.8	5.9	14.9	6.5	4.7	3.1
A-int8	-9.0	-8.2			-12.8	-15.9		
A-ts7	3.5	6.8	12.6	15.0	8.3	2.7	21.1	18.6
A-int9	-13.0	-9.3			-14.7	-14.7		
A-ts8	17.7	19.9	30.7	29.2	19.4	12.1	34.2	26.8
A-int8	-9.0	-8.2			-12.8	-15.9		
A-ts9	3.0	4.3	12.1	12.5	8.8	4.2	21.5	20.1
A-int10	-9.6	-8.5			-8.0	-9.1		
A-ts10	18.6	20.0	28.2	28.5	23.9	18.3	31.9	27.4

Table S2. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 2

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	16.5	16.1	16.5	16.1	25.7	12.5	25.7	12.5
B-int1	-0.4	-1.5			5.6	-6.3		
B-ts2	5.0	5.4	5.4	6.9	10.0	0.5	4.4	6.9
B-int2	-3.0	-2.2			-3.8	-6.9		
B-ts3	20.8	21.5	23.9	23.7	30.5	17.0	34.4	23.9
B-int3	-8.4	-7.8			-5.3	-16.8		

B-ts4	21.7	24.0	30.1	31.7	32.9	21.1	38.2	37.8
B-2	-40.2	-40.9			-39.4	-47.5		
B-int1	-0.4	-1.5			5.6	-6.3		
B-ts5	41.9	42.9	42.3	44.4	53.5	38.9	47.9	45.3
B-int4	-15.0	-16.4			-17.7	-27.4		
B-ts6	-1.6	-1.9	13.4	14.5	4.5	-8.7	22.2	18.7
B-int5	-17.8	-16.4			-16.3	-22.6		
B-ts7	2.7	4.2	20.5	20.6	10.0	-1.8	26.2	20.8

Table S3. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 3a

System	ΔE^{rel}_{gas}	ΔG^{rel}_{gas}	$\Delta E^{\neq}_{gas}$	$\Delta G^{\neq}_{gas}$	ΔE^{rel}_{sol}	ΔG^{rel}_{sol}	$\Delta E^{\neq}_{sol}$	$\Delta G^{\neq}_{sol}$
C-1	0	0			0	0		
C-ts1	4.6	5.3	4.6	5.3	6.6	6.0	6.6	6.0
C-int1	5.2	4.4			13.0	5.0		
C-ts2	25.5	26.8	20.3	22.4	26.6	23.6	13.6	18.7
C-int2	22.2	23.3			16.3	18.2		
C-ts3	37.1	38.4	14.9	15.1	43.8	37.9	27.6	19.7
C-int3	-9.0	-7.2			1.8	-4.2		
C-int4	-8.0	-7.6			2.9	-3.7		
C-ts4	0.6	2.3	8.6	9.8	9.5	2.3	6.6	6.0
C-2	-26.5	-25.1			-24.4	-25.9		
C-int5	14.1	14.1			22.7	15.4		
C-ts5	16.7	16.9	2.6	2.8	25.1	16.2	2.4	0.8

C-int6	2.9	2.7			0.6	-4.7		
C-ts6	17.8	21.7	14.9	19.0	22.3	17.7	21.8	22.4
C-int7	1.2	5.3			-0.8	0.4		
C-ts7	31.1	32.9	30.0	27.6	32.8	25.6	33.6	25.2

Table S4. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 3b

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	22.2	22.3	22.2	22.3	25.4	22.9	25.4	22.9
D-int1	9.5	10.6			11.2	9.2		
D-ts2	20.5	22.0	11.0	11.4	20.4	21.7	9.2	12.6
D-int2	12.4	14.7			6.2	14.6		
D-ts3	36.6	37.0	24.2	22.4	40.0	36.3	33.8	21.7
D-int3	3.5	5.2			1.3	0.5		
D-ts4	39.3	41.8	35.8	36.5	44.9	42.1	43.6	41.6
D-2	-25.5	-27.7			-30.5	-30.2		
D-int1	9.5	10.6			11.2	9.2		
D-ts5	52.1	53.0	42.6	42.4	58.6	52.9	47.4	44.6
D-int4	-10.2	-10.1			-14.8	-13.3		
D-ts6	12.0	13.4	22.2	23.6	15.2	13.2	30.1	24.8
D-int5	1.1	2.2			-3.2	0.4		
D-ts7	18.4	20.9	17.3	18.6	19.4	19.2	22.6	18.4

Table S5. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Figure 4

System	ΔE^{rel}_{gas}	ΔG^{rel}_{gas}	$\Delta E^{\neq}_{gas}$	$\Delta G^{\neq}_{gas}$	ΔE^{rel}_{sol}	ΔG^{rel}_{sol}	$\Delta E^{\neq}_{sol}$	$\Delta G^{\neq}_{sol}$
E-1	0	0			0	0		
E-ts1	16.1	15.7	16.1	15.7	24.2	17.6	24.2	17.6
E-int1	-12.2	-9.6			-1.3	-4.7		
E-ts2	-2.2	0.2	10.1	9.8	11.7	9.4	13.0	14.1
E-int2	-9.7	-6.9			-5.7	0.6		
E-ts3	9.4	11.3	19.1	18.1	23.4	18.2	29.1	17.7
E-int3	-34.9	-33.4			-18.7	-23.9		
E-int4	-31.5	-29.3			-16.3	-21.2		
E-ts4	-17.6	-12.5	13.9	16.8	-2.2	-4.3	14.1	16.9
E-2	-45.9	-45.6			-40.1	-43.4		
E-int5	-7.1	-6.3			5.7	-0.9		
E-ts5	4.6	6.5			16.6	11.4	10.9	12.3
E-int6	-31.9	-31.9			-26.2	-28.2		
E-ts6	-12.1	-9.0	19.8	22.9	2.1	-2.8	28.3	25.4
E-int7	-26.4	-23.1			-20.6	-19.1		
E-ts7	0	3.9	26.4	27.0	12.0	6.9	32.5	25.9

The Cartesian coordinates of the stationary points discussed in the text

A-1

C	1.5961947	-2.2867893	2.0203450
C	0.5668267	-2.8928403	2.7675970
C	-0.6287073	-2.2361083	2.9316570

C	-0.8409333	-0.9604153	2.3566000
C	0.2048647	-0.3292583	1.6122920
C	1.4194867	-1.0413733	1.4684960
C	-2.1041773	-0.3124303	2.4965970
C	-2.2974753	0.9410237	1.9591410
C	-1.2630113	1.5481277	1.2340930
C	-0.0309083	0.9578827	1.0285000
C	-0.7187973	0.9817117	-1.9202840
C	0.7229437	0.6928867	-2.0501410
N	1.5248327	1.0432567	-1.0041100
C	0.9499967	1.7457827	0.1760880
C	-1.8423013	1.4385947	-2.1389100
N	2.3783487	3.6675117	0.8659090
C	2.0831657	2.3420067	1.0176540
O	2.7290877	1.6556927	1.7933150
O	1.1226327	0.1905017	-3.0900680
O	-3.0772853	-0.9777463	3.1420630
H	0.3640367	2.5819207	-0.2197870
Au	-1.9109673	-0.7942973	-1.1224300
C	-3.1404693	2.0365247	-2.3748440
C	1.8033677	4.7858117	0.0850250
C	0.4165397	5.1673127	0.5987150
C	1.7833997	4.4874217	-1.4134770
C	2.7508097	5.9600997	0.3227400
C	5.2048927	-1.5701413	0.4253820

C	4.9372687	-2.7249003	-0.3152750
C	4.0364577	-2.6704643	-1.3802120
C	3.4138737	-1.4653553	-1.6935940
C	3.6675867	-0.3088993	-0.9575470
C	4.5762547	-0.3789383	0.1033990
C	2.9796067	0.9873407	-1.2915540
O	5.5962177	-3.8435863	0.0774260
C	5.3599767	-5.0290643	-0.6389820
H	2.5521627	-2.7911343	1.8913700
H	0.7228827	-3.8686213	3.2227900
H	-1.4311633	-2.6716853	3.5220920
H	2.2421347	-0.5773873	0.9438280
H	-3.2630503	1.4319217	2.0448910
H	-1.4776453	2.5137717	0.7743710
H	3.1176367	3.9244277	1.5117300
H	-3.9407933	-0.6701463	2.7915000
H	-3.0052213	3.0165587	-2.8466860
H	-3.7416913	1.4064597	-3.0388700
H	-3.6986053	2.1528317	-1.4338880
H	0.4535337	5.3900927	1.6709720
H	0.0519937	6.0584087	0.0732580
H	-0.3205563	4.3712247	0.4478210
H	2.7846777	4.2093557	-1.7636630
H	1.4689547	5.3850877	-1.9590860
H	1.0907947	3.6841867	-1.6881720

H	2.4004517	6.8447237	-0.2194590
H	2.7980887	6.2172817	1.3885510
H	3.7630907	5.7235997	-0.0270090
H	5.9076237	-1.6380263	1.2518760
H	3.8184027	-3.5529893	-1.9747850
H	2.7160607	-1.4168053	-2.5274170
H	4.7595837	0.5073817	0.7090170
H	3.0758097	1.1923527	-2.3641700
H	3.4617157	1.8121047	-0.7581730
H	5.9743527	-5.8025153	-0.1733290
H	5.6485477	-4.9316533	-1.6956360
H	4.3039927	-5.3326783	-0.5880930
P	-2.5942453	-2.9648573	-0.5867520
C	-3.6142323	-3.2143313	0.8924170
H	-4.4955723	-2.5668363	0.8377860
H	-3.9137263	-4.2686703	0.9398110
H	-3.0559753	-2.9426653	1.7929350
C	-1.2071183	-4.1354603	-0.4174850
H	-1.5805103	-5.1530083	-0.2502850
H	-0.5932973	-4.1115163	-1.3232230
H	-0.5879803	-3.8268463	0.4337390
C	-3.6255543	-3.6070963	-1.9459240
H	-3.9598823	-4.6278113	-1.7248490
H	-4.4924713	-2.9452383	-2.0443940
H	-3.0607463	-3.5989023	-2.8830610

C	-7.0804483	0.2677477	-0.1403010
F	-7.5593273	-0.9705143	-0.1763750
F	-7.2958643	0.8430367	-1.3179190
F	-7.7241553	0.9503387	0.7947300
S	-5.2825893	0.2387837	0.2162740
O	-5.2193473	-0.4452583	1.5248340
O	-4.8919483	1.6537537	0.2285650
O	-4.7324083	-0.5515813	-0.9079770

Zero-point correction= 0.672491 (Hartree/Particle)

Thermal correction to Energy= 0.723396

Thermal correction to Enthalpy= 0.724340

Thermal correction to Gibbs Free Energy= 0.585155

Sum of electronic and zero-point Energies= -3051.436124

Sum of electronic and thermal Energies= -3051.385220

Sum of electronic and thermal Enthalpies= -3051.384276

Sum of electronic and thermal Free Energies= -3051.523460

A-ts1

C	0.6902811	-1.5513423	2.9223183
C	-0.5540559	-1.5992453	3.5774213
C	-1.5812429	-0.7994653	3.1412773
C	-1.3934839	0.0765017	2.0485803
C	-0.1183989	0.1800907	1.4244883
C	0.9068881	-0.6829933	1.8781823
C	-2.5075079	0.8098257	1.5224113
C	-2.3438429	1.6493347	0.4242383

C	-1.0856079	1.7981887	-0.1271857
C	0.0350781	1.0835237	0.3068993
C	-0.1094349	-0.4885743	-1.4381507
C	1.3031041	-0.3000333	-1.7526777
N	2.0698781	0.5083627	-0.9736197
C	1.3797011	1.5569947	-0.2263897
C	-1.1625109	-1.1481313	-1.6995257
N	2.2393721	3.4374607	1.1765853
C	2.2671681	2.0986687	0.9020203
O	2.9390131	1.3520877	1.5976183
O	1.7073361	-0.9091003	-2.7353097
O	-3.6816709	0.6527367	2.1177083
H	1.1609961	2.3890437	-0.9142587
Au	-2.7544369	-1.5755113	-0.3076107
C	-1.4643249	-1.9324703	-2.9530097
C	1.9898211	4.6571817	0.3691463
C	0.5086641	4.8654217	0.0722013
C	2.8113591	4.6422937	-0.9184007
C	2.4693211	5.8097337	1.2491943
C	5.5813961	-1.9181113	0.2843303
C	6.0230681	-2.6818023	-0.8011827
C	5.6206941	-2.3457293	-2.0928617
C	4.7796131	-1.2516943	-2.2832467
C	4.3385791	-0.4819983	-1.2133307
C	4.7509351	-0.8313393	0.0785833

C	3.4512381	0.7127787	-1.4379537
O	6.8356251	-3.7245523	-0.4962147
C	7.2980381	-4.5242653	-1.5547927
H	1.4963201	-2.2057273	3.2455033
H	-0.7029189	-2.2744363	4.4173833
H	-2.5587559	-0.8288873	3.6167873
H	1.8772811	-0.6523543	1.3949323
H	-3.2094339	2.1531697	0.0047353
H	-0.9783169	2.4599007	-0.9845687
H	2.8248281	3.5986827	1.9901033
H	-4.4088079	0.9488727	1.5054513
H	-0.6335959	-1.8559273	-3.6614847
H	-1.6388839	-2.9865903	-2.7127977
H	-2.3881539	-1.5473823	-3.3993207
H	-0.0934709	4.7285327	0.9774673
H	0.3482181	5.8830647	-0.3031507
H	0.1353411	4.1803867	-0.6940697
H	3.8788411	4.5262827	-0.6948547
H	2.6753741	5.5855177	-1.4613927
H	2.5135351	3.8317507	-1.5946297
H	2.3374351	6.7634247	0.7276213
H	1.8967821	5.8502077	2.1837833
H	3.5343181	5.7046967	1.4927333
H	5.9128621	-2.2012223	1.2803673
H	5.9437891	-2.9268623	-2.9514867

H	4.4443421	-1.0048113	-3.2888847
H	4.4075971	-0.2358203	0.9234173
H	3.4313531	0.9673667	-2.5074997
H	3.8449131	1.5801127	-0.8954927
H	7.9256371	-5.2992513	-1.1095477
H	7.8995891	-3.9453153	-2.2707417
H	6.4691511	-5.0028273	-2.0964127
P	-4.3236129	-2.7892723	0.9867283
C	-5.5041849	-1.9256093	2.0743833
H	-6.1254769	-1.2679673	1.4579023
H	-6.1325119	-2.6672263	2.5828253
H	-4.9622549	-1.3233803	2.8086303
C	-3.4786739	-3.9644523	2.1073253
H	-4.2080279	-4.5578863	2.6721273
H	-2.8427329	-4.6325263	1.5176063
H	-2.8374049	-3.4089423	2.8001183
C	-5.3753519	-3.8577243	-0.0510377
H	-6.0427259	-4.4603613	0.5769193
H	-5.9615549	-3.2097803	-0.7094077
H	-4.7455689	-4.5187953	-0.6547927
C	-6.6698999	1.3799867	-2.0603107
F	-7.8510719	1.5036507	-1.4711697
F	-6.8360749	0.7908187	-3.2369127
F	-6.1579429	2.5893577	-2.2541507
S	-5.5409449	0.3776287	-1.0211337

O	-5.4793319	1.1735777	0.2346633
O	-4.2833409	0.3533067	-1.7841557
O	-6.2271319	-0.9128243	-0.8775907

Zero-point correction= 0.671080 (Hartree/Particle)

Thermal correction to Energy= 0.722328

Thermal correction to Enthalpy= 0.723273

Thermal correction to Gibbs Free Energy= 0.581994

Sum of electronic and zero-point Energies= -2328.039615

Sum of electronic and thermal Energies= -2327.988366

Sum of electronic and thermal Enthalpies= -2327.987422

Sum of electronic and thermal Free Energies= -2328.128700

A-int1

C	-1.4200468	1.5176128	2.7401484
C	-0.3877228	1.2716958	3.6491104
C	0.7774872	0.6788028	3.2065724
C	0.9143762	0.3163658	1.8561434
C	-0.1296258	0.5511808	0.9404384
C	-1.2903898	1.1700458	1.4048664
C	2.1679382	-0.2643062	1.4058624
C	2.3749312	-0.4921312	-0.0005376
C	1.3799692	-0.2559942	-0.8740026
C	-0.0107578	0.1041768	-0.4987666
C	-0.6234578	1.1083528	-1.4777106
C	-1.9851578	0.6282398	-1.8215606
N	-2.1666158	-0.5810682	-1.1666826

C	-0.9062428	-1.1748472	-0.8004446
C	-0.0158078	2.2557998	-1.8471216
N	-0.2395568	-3.2799272	0.3447094
C	-0.9933008	-2.1365232	0.3771934
O	-1.6509518	-1.8609252	1.3687034
O	-2.8492268	1.1457948	-2.5091706
O	3.0707402	-0.5142602	2.2578204
H	-0.4489588	-1.6853592	-1.6641866
Au	1.7834412	2.8325878	-0.9691286
C	-0.6471838	3.2102808	-2.8117386
C	0.2043022	-4.1671622	-0.7626266
C	1.4467592	-3.6376662	-1.4722876
C	-0.9308018	-4.4192852	-1.7536926
C	0.5688532	-5.4865172	-0.0853436
C	-5.6228128	0.0895228	1.4397474
C	-6.6746398	0.6521548	0.7087844
C	-6.6660078	0.5804508	-0.6830156
C	-5.6049278	-0.0524812	-1.3276016
C	-4.5611388	-0.6252872	-0.6125876
C	-4.5804708	-0.5425262	0.7853664
C	-3.4196338	-1.3080792	-1.3203326
O	-7.6506458	1.2467528	1.4423234
C	-8.7229308	1.8311978	0.7485854
H	-2.3417858	1.9862278	3.0778764
H	-0.4996598	1.5485098	4.6940774

H	1.6060502	0.4829718	3.8821454
H	-2.1122148	1.3636168	0.7211004
H	3.3575232	-0.8024362	-0.3375966
H	1.5552332	-0.3973512	-1.9410696
H	-0.3686378	-3.7648152	1.2276414
H	4.0779422	-0.9896182	1.8736324
H	-1.6135888	2.8689768	-3.1934456
H	-0.7802808	4.1866758	-2.3261566
H	0.0363172	3.3922078	-3.6517286
H	2.2479612	-3.4248112	-0.7550776
H	1.8103352	-4.3908612	-2.1815186
H	1.2497002	-2.7248972	-2.0443296
H	-1.8113698	-4.8191942	-1.2362656
H	-0.6147218	-5.1519882	-2.5060236
H	-1.2320148	-3.5112202	-2.2895006
H	0.9176062	-6.2100402	-0.8296566
H	1.3719052	-5.3399202	0.6472104
H	-0.2997738	-5.9209952	0.4255594
H	-5.6557778	0.1596498	2.5245444
H	-7.4636398	1.0211378	-1.2737746
H	-5.5801628	-0.0789992	-2.4157646
H	-3.7569948	-0.9743712	1.3534024
H	-3.6534888	-1.4127792	-2.3906376
H	-3.2659908	-2.3153162	-0.9112516
H	-9.3938308	2.2476618	1.5031774

H	-9.2741438	1.0907088	0.1504484
H	-8.3866498	2.6403668	0.0838434
P	3.7198102	3.6397538	0.2022834
C	4.0040822	2.8466348	1.8234124
H	4.3227802	1.8117858	1.6591064
H	4.7876142	3.3774348	2.3775154
H	3.0742712	2.8532308	2.4030244
C	3.5224012	5.4099028	0.6312404
H	4.3842272	5.7695698	1.2064084
H	3.4259152	6.0017238	-0.2845146
H	2.6103732	5.5418588	1.2221304
C	5.3493672	3.5797158	-0.6163246
H	6.1042032	4.0680538	0.0117604
H	5.6309662	2.5331598	-0.7666186
H	5.2951762	4.0881668	-1.5837176
C	6.2635862	-1.9230682	-0.7213326
F	6.8099122	-3.0483142	-0.2981836
F	7.0334192	-1.3793842	-1.6492806
F	5.0742852	-2.1970682	-1.2588596
S	6.0693862	-0.7431362	0.6708014
O	5.1171802	-1.5326032	1.5580844
O	5.3918702	0.4167828	0.0831684
O	7.3935432	-0.5799652	1.2311984

Zero-point correction= 0.670874 (Hartree/Particle)

Thermal correction to Energy= 0.720883

Thermal correction to Enthalpy= 0.721827

Thermal correction to Gibbs Free Energy= 0.582559

Sum of electronic and zero-point Energies= -3051.444926

Sum of electronic and thermal Energies= -3051.394917

Sum of electronic and thermal Enthalpies= -3051.393973

Sum of electronic and thermal Free Energies= -3051.533241

A-ts2

C	2.2515415	-2.0631820	2.3999172
C	1.2704865	-2.1354380	3.3884672
C	0.0490005	-1.5173860	3.1850222
C	-0.1990105	-0.8171350	1.9961742
C	0.7826125	-0.7471350	0.9989382
C	2.0079515	-1.3776390	1.2181012
C	-1.5066035	-0.2110880	1.7656912
C	-1.8054695	0.4212570	0.5692622
C	-0.8177415	0.6321300	-0.4017778
C	0.5842065	0.0664880	-0.2682648
C	0.9301105	-0.7162410	-1.5432618
C	2.1349955	-0.1072220	-2.1462098
N	2.4158165	1.0732460	-1.4528178
C	1.6481575	1.2040040	-0.2361588
C	0.2081765	-1.7567010	-2.0197348
N	-0.3752325	2.6235250	-0.3673028
C	1.0538425	2.5908650	-0.1254778
O	1.7068435	3.5628180	0.1552782

O	2.8276005	-0.4905710	-3.0741528
O	-2.3773295	-0.3761380	2.7231112
Au	-1.5829245	-2.4001550	-1.1599908
C	0.6011085	-2.4850090	-3.2687638
C	5.5142945	0.9721680	1.8033262
C	6.0362075	-0.3069630	1.5913952
C	5.8691935	-0.9278940	0.3509222
C	5.1740945	-0.2676240	-0.6591548
C	4.6431505	1.0062810	-0.4580878
C	4.8288545	1.6175120	0.7869032
C	3.7675235	1.6353770	-1.5066598
O	6.6839535	-0.8612010	2.6442922
C	7.2409865	-2.1410120	2.4738202
H	3.2177745	-2.5404820	2.5488832
H	1.4621435	-2.6724690	4.3136592
H	-0.7331125	-1.5598720	3.9374582
H	2.7889685	-1.3247740	0.4587112
H	-2.8309075	0.7231560	0.3723742
H	-3.3078515	-0.0937510	2.4378892
H	1.4948555	-2.0878580	-3.7562888
H	0.7681515	-3.5433470	-3.0260048
H	-0.2375155	-2.4816820	-3.9778358
H	5.6616065	1.4338790	2.7762282
H	6.2770265	-1.9163080	0.1599392
H	5.0251615	-0.7562110	-1.6215858

H	4.4120835	2.6106800	0.9588822
H	4.1306455	1.4258570	-2.5181308
H	3.7048455	2.7228350	-1.3750268
H	7.7161165	-2.4026100	3.4213202
H	7.9991045	-2.1524250	1.6777992
H	6.4724425	-2.8926720	2.2397792
P	-3.7308785	-3.1096670	-0.3626728
C	-3.9249175	-3.2836720	1.4432322
H	-3.8908845	-2.2929450	1.9047752
H	-4.8956045	-3.7390470	1.6732362
H	-3.1188145	-3.9059250	1.8448002
C	-4.2189265	-4.7548510	-1.0019058
H	-5.2278155	-5.0154800	-0.6600008
H	-4.1999855	-4.7438020	-2.0962838
H	-3.5107925	-5.5125460	-0.6519518
C	-5.0964225	-2.0214470	-0.8870208
H	-6.0440095	-2.3355570	-0.4337568
H	-4.8950915	-0.9978900	-0.5575208
H	-5.1768915	-2.0497190	-1.9786708
C	-5.3646835	2.1411330	0.6160352
F	-4.2805565	2.7563720	1.1129662
F	-6.3268315	3.0355240	0.4799462
F	-5.0350495	1.6826770	-0.5986598
S	-5.8739025	0.7582900	1.7129232
O	-4.6375995	-0.0950490	1.6391642

O	-7.0049445	0.1603080	1.0174042
O	-6.0819755	1.3903370	3.0064712
H	2.3131805	1.0989130	0.6376352
H	-1.1519285	0.7402280	-1.4304918
H	-0.8459715	2.9643920	0.4764332
C	-0.8421725	3.4672250	-1.5375548
C	-0.0593215	3.0571000	-2.7755228
C	-2.3308715	3.1954130	-1.7069848
C	-0.6268655	4.9450580	-1.2259778
H	1.0123315	3.2695590	-2.6725188
H	-0.1751045	1.9912850	-3.0070258
H	-0.4293035	3.6270280	-3.6347118
H	-2.8825665	3.3841320	-0.7784248
H	-2.7332805	3.8638930	-2.4763528
H	-2.5426125	2.1676820	-2.0209888
H	-0.9952095	5.5463430	-2.0656798
H	-1.1896865	5.2422920	-0.3319198
H	0.4280275	5.1805300	-1.0632808

Zero-point correction= 0.673217 (Hartree/Particle)

Thermal correction to Energy= 0.722141

Thermal correction to Enthalpy= 0.723085

Thermal correction to Gibbs Free Energy= 0.588734

Sum of electronic and zero-point Energies= -3051.415542

Sum of electronic and thermal Energies= -3051.366618

Sum of electronic and thermal Enthalpies= -3051.365674

Sum of electronic and thermal Free Energies= -3051.500025

A-int2

C	-2.4669229	-2.1103482	-2.2273314
C	-1.5285389	-2.2657352	-3.2432304
C	-0.2930109	-1.6446212	-3.1364754
C	0.0159921	-0.8657532	-2.0169974
C	-0.9160739	-0.7293952	-0.9811864
C	-2.1580339	-1.3517722	-1.1053494
C	1.3201291	-0.1981572	-1.9249124
C	1.6640341	0.5483378	-0.8505334
C	0.7743921	0.7347258	0.3123316
C	-0.6583159	0.1367058	0.2436056
C	-1.0285329	-0.5915302	1.5415126
C	-2.2347909	0.0507908	2.1033526
N	-2.4652549	1.2328688	1.3839466
C	-1.6353219	1.3336558	0.2079156
C	-0.3466309	-1.6423362	2.0514476
N	0.6145471	2.2711988	0.5424206
C	-0.8404929	2.6046128	0.2700076
O	-1.1981219	3.7303398	0.1131596
O	-2.9653909	-0.2922522	3.0168056
O	2.1195141	-0.4098732	-2.9648824
Au	1.4249951	-2.3455652	1.1910836
C	-0.7702969	-2.3293642	3.3129946
C	-5.4958119	1.2537228	-1.9488364

C	-6.0871599	0.0051008	-1.7368074
C	-5.9767529	-0.6121152	-0.4878444
C	-5.2675439	0.0193088	0.5296486
C	-4.6667479	1.2618618	0.3286146
C	-4.7975269	1.8707938	-0.9239704
C	-3.7896569	1.8575018	1.3930636
O	-6.7445969	-0.5215672	-2.7959654
C	-7.3591209	-1.7764882	-2.6334784
H	-3.4438639	-2.5834502	-2.3019384
H	-1.7616479	-2.8647592	-4.1199634
H	0.4523701	-1.7421232	-3.9203854
H	-2.9022449	-1.2427072	-0.3160614
H	2.6754571	0.9499648	-0.7864004
H	3.0400631	-0.0933402	-2.7609254
H	-1.6550799	-1.8941932	3.7849466
H	-0.9714929	-3.3867252	3.0927256
H	0.0631181	-2.3396562	4.0281946
H	-5.6019489	1.7144118	-2.9274204
H	-6.4383979	-1.5766792	-0.2976244
H	-5.1636269	-0.4674042	1.4990626
H	-4.3381689	2.8459418	-1.0943654
H	-4.1899449	1.6793138	2.3965806
H	-3.6712979	2.9399658	1.2544636
H	-7.8284229	-2.0185792	-3.5889274
H	-8.1310329	-1.7533792	-1.8511494

H	-6.6269379	-2.5590692	-2.3863024
P	3.5835451	-2.9259342	0.3229326
C	3.7281011	-3.1085962	-1.4855014
H	3.2767461	-2.2494762	-1.9887584
H	4.7864001	-3.1553802	-1.7696774
H	3.2132091	-4.0227362	-1.7987414
C	4.3409401	-4.4636522	0.9653816
H	5.3556291	-4.5800332	0.5663486
H	4.3859061	-4.4226942	2.0581806
H	3.7366371	-5.3285182	0.6747766
C	4.7742641	-1.6280572	0.7855726
H	5.7421751	-1.7616712	0.2867566
H	4.3765141	-0.6636442	0.4594406
H	4.8964591	-1.6286072	1.8742546
C	5.5858581	2.0299428	-0.7436474
F	4.5309281	2.7983148	-1.0665484
F	6.6570761	2.8016298	-0.6863344
F	5.3495001	1.5481178	0.4848426
S	5.7938491	0.6675458	-1.9621734
O	4.4427191	0.0341788	-1.8844364
O	6.8448761	-0.1584832	-1.3735434
O	6.0677861	1.3638518	-3.2107794
H	-2.2456299	1.3625568	-0.7103974
H	1.2454371	0.3729428	1.2309896
H	1.1459761	2.7294928	-0.2110644

C	1.2108231	2.8378058	1.8702236
C	0.4321541	2.2615818	3.0366056
C	2.6786391	2.4368138	1.8894126
C	1.1039231	4.3552558	1.8281476
H	-0.6279999	2.5422318	2.9980026
H	0.4973101	1.1684678	3.0897746
H	0.8518751	2.6682448	3.9629566
H	3.2185531	2.8230778	1.0167906
H	3.1393641	2.8742738	2.7818116
H	2.8401881	1.3543418	1.9397026
H	1.6345221	4.7522138	2.7003496
H	1.5835511	4.7711598	0.9335696
H	0.0723421	4.7112558	1.8661616

Zero-point correction= 0.675880 (Hartree/Particle)

Thermal correction to Energy= 0.724747

Thermal correction to Enthalpy= 0.725691

Thermal correction to Gibbs Free Energy= 0.592285

Sum of electronic and zero-point Energies= -3051.423936

Sum of electronic and thermal Energies= -3051.375069

Sum of electronic and thermal Enthalpies= -3051.374125

Sum of electronic and thermal Free Energies= -3051.507531

A-ts3

C	2.3974291	-1.9118245	2.3833147
C	1.4658771	-1.8718915	3.4204887
C	0.2612981	-1.2204095	3.2266607

C	-0.0182379	-0.5939445	2.0025017
C	0.9094171	-0.6470155	0.9513567
C	2.1167941	-1.3139335	1.1628397
C	-1.3076399	0.0568065	1.8066987
C	-1.6264889	0.7135475	0.6202657
C	-0.6889799	0.7053845	-0.5603983
C	0.7161521	0.0922925	-0.3593083
C	1.1295981	-0.7417625	-1.5715553
C	2.3507041	-0.1365895	-2.1494943
N	2.5634361	1.0852835	-1.5101313
C	1.6976521	1.2866765	-0.3729253
C	0.4640771	-1.8364855	-2.0007673
N	-0.5081159	2.2221045	-0.6899203
C	0.8971591	2.5512945	-0.5615273
O	1.3456001	3.6657635	-0.6004823
O	3.1008871	-0.5567885	-3.0151563
O	-2.1312479	-0.0088795	2.8133737
Au	-1.3276449	-2.4553835	-1.1188533
C	0.9194401	-2.6328645	-3.1843643
C	5.5356911	1.2925965	1.8702017
C	6.1139771	0.0264845	1.7443177
C	6.0109041	-0.6660775	0.5353607
C	5.3248511	-0.0892115	-0.5297503
C	4.7379691	1.1711265	-0.4156043
C	4.8584501	1.8536245	0.7992057

C	3.8858621	1.7098505	-1.5314733
O	6.7512621	-0.4419945	2.8445637
C	7.3702331	-1.7014815	2.7602307
H	3.3530031	-2.4126195	2.5235667
H	1.6831061	-2.3459145	4.3738477
H	-0.4842039	-1.1769945	4.0152297
H	2.8523211	-1.3598205	0.3608557
H	-2.6912099	0.8542615	0.4197847
H	-3.0809529	0.2052395	2.5267457
H	1.8174341	-2.2356975	-3.6652503
H	1.1133671	-3.6672895	-2.8690673
H	0.1079431	-2.7028745	-3.9210363
H	5.6356511	1.8125995	2.8194427
H	6.4634911	-1.6455535	0.4103797
H	5.2286991	-0.6326805	-1.4693423
H	4.4078251	2.8420685	0.9017877
H	4.3099931	1.4753315	-2.5132583
H	3.7607781	2.7967165	-1.4546963
H	7.8295931	-1.8884775	3.7328787
H	8.1505621	-1.7211055	1.9861067
H	6.6438441	-2.5004335	2.5491407
P	-3.5125349	-2.9855055	-0.2775583
C	-3.7327389	-3.0423535	1.5331047
H	-3.3361739	-2.1315505	1.9881787
H	-4.8007029	-3.1028345	1.7757107

H	-3.2042479	-3.9135515	1.9335517
C	-4.1995629	-4.5892125	-0.8315913
H	-5.2269899	-4.7070185	-0.4670153
H	-4.1977609	-4.6311885	-1.9252853
H	-3.5840499	-5.4106465	-0.4520413
C	-4.7240049	-1.7688885	-0.8898123
H	-5.7084849	-1.9199325	-0.4306903
H	-4.3913429	-0.7633225	-0.6160983
H	-4.7878509	-1.8526285	-1.9801053
C	-5.8140479	1.9000325	0.6421057
F	-4.8870039	2.8089665	0.9640437
F	-6.9940309	2.4929635	0.6076807
F	-5.5253439	1.4532735	-0.5860733
S	-5.7907689	0.5211355	1.8528237
O	-4.3699749	0.0609425	1.6754837
O	-6.7553049	-0.4395745	1.3279707
O	-6.0517939	1.1571165	3.1343957
H	2.2863341	1.3759825	0.5550037
H	-1.1331629	0.3042105	-1.4749963
H	-1.1333039	2.0946885	0.4351717
C	-1.3066559	2.9534105	-1.7723353
C	-0.6311679	2.6636625	-3.1061243
C	-2.7445469	2.4489315	-1.7689613
C	-1.3247719	4.4444075	-1.4577273
H	0.3943131	3.0495145	-3.1326163

H	-0.6040939	1.5879125	-3.3225363
H	-1.1934059	3.1516275	-3.9103493
H	-3.2587359	2.6840555	-0.8315233
H	-3.2820629	2.9667465	-2.5708743
H	-2.8395969	1.3744665	-1.9654523
H	-1.9908789	4.9381505	-2.1744413
H	-1.7244189	4.6225415	-0.4522373
H	-0.3367419	4.9004165	-1.5255663

Zero-point correction= 0.670715 (Hartree/Particle)

Thermal correction to Energy= 0.718973

Thermal correction to Enthalpy= 0.719918

Thermal correction to Gibbs Free Energy= 0.587889

Sum of electronic and zero-point Energies= -3051.397837

Sum of electronic and thermal Energies= -3051.349579

Sum of electronic and thermal Enthalpies= -3051.348635

Sum of electronic and thermal Free Energies= -3051.480663

A-int3

C	2.6296720	-1.9626541	2.1902791
C	1.6402980	-2.3168371	3.1111231
C	0.3819480	-1.7587571	2.9940811
C	0.1147040	-0.8399191	1.9682511
C	1.0876710	-0.5181841	1.0063891
C	2.3543330	-1.0929421	1.1453691
C	-1.1700180	-0.1520031	1.9408691
C	-1.1794920	1.1614209	1.2215811

C	-0.6073960	1.0167189	-0.1879549
C	0.7805660	0.3474399	-0.1997069
C	1.0411360	-0.4561051	-1.4854579
C	2.3692980	-0.0177951	-2.0094869
N	2.7325770	1.1062979	-1.3035679
C	1.7462980	1.5331629	-0.3456969
C	0.2511640	-1.4237741	-1.9891689
N	-0.4265840	2.3139919	-0.8314229
C	0.8980210	2.6526169	-0.9514179
O	1.3733290	3.6297629	-1.4995039
O	3.0795140	-0.5255861	-2.8661279
O	-2.1671950	-0.5937381	2.5292381
Au	-1.5748560	-2.0476201	-1.1856009
C	0.6052700	-2.1578501	-3.2510439
C	5.8663110	1.1901679	1.9036101
C	6.4105520	-0.0834851	1.7210451
C	6.2358550	-0.7440731	0.5026361
C	5.5125070	-0.1262811	-0.5143669
C	4.9554710	1.1406109	-0.3416359
C	5.1491020	1.7902889	0.8805181
C	4.0506690	1.7095999	-1.4013779
O	7.0905770	-0.5922361	2.7796381
C	7.6700550	-1.8638781	2.6360751
H	3.6322190	-2.3767121	2.2788951
H	1.8621090	-3.0116731	3.9167611

H	-0.4106590	-1.9846161	3.7034831
H	3.1400930	-0.8635581	0.4274721
H	-2.1865030	1.5881299	1.2090301
H	-3.4442330	-0.0875341	1.9667311
H	1.5549170	-1.8374601	-3.6875389
H	0.6550410	-3.2368571	-3.0503169
H	-0.1975380	-2.0324181	-3.9906579
H	6.0243360	1.6853769	2.8583661
H	6.6601310	-1.7297171	0.3333701
H	5.3512810	-0.6455631	-1.4588989
H	4.7299920	2.7859029	1.0292751
H	4.4222730	1.4811269	-2.4064529
H	3.9382960	2.7966729	-1.3121419
H	8.1725490	-2.0864111	3.5797141
H	8.4099490	-1.8863871	1.8229771
H	6.9131320	-2.6393131	2.4439031
P	-3.7539070	-2.8551131	-0.5649519
C	-4.1495470	-3.1836151	1.1905071
H	-3.8450570	-2.3457001	1.8208671
H	-5.2238030	-3.3643911	1.3141861
H	-3.5909200	-4.0699651	1.5091321
C	-4.1211750	-4.4702001	-1.3498549
H	-5.1427780	-4.7920481	-1.1140779
H	-4.0116470	-4.3812531	-2.4353919
H	-3.4127630	-5.2246431	-0.9936749

C	-5.0987460	-1.7994971	-1.2127959
H	-6.0793740	-2.1640141	-0.8859149
H	-4.9704280	-0.7710881	-0.8669709
H	-5.0430140	-1.8134331	-2.3067309
C	-5.8340890	2.0868519	1.2736561
F	-4.8424340	2.8801029	1.6519221
F	-6.9812990	2.5790319	1.6975261
F	-5.8463050	1.9959879	-0.0466769
S	-5.5930790	0.4172659	1.9998791
O	-4.2193860	0.0952619	1.3050541
O	-6.6267670	-0.4228791	1.4376481
O	-5.4191620	0.5783979	3.4260781
H	2.2173740	1.8465639	0.5998271
H	-1.2971060	0.4007059	-0.7792009
C	-1.4900320	2.9071139	-1.6974769
C	-1.2857380	2.3687289	-3.1119089
C	-2.8788590	2.5210539	-1.1915999
C	-1.4031310	4.4316079	-1.6706849
H	-0.2942610	2.6448429	-3.4878839
H	-1.3699510	1.2735409	-3.1288319
H	-2.0401190	2.7823209	-3.7925009
H	-3.0836610	2.9543749	-0.2052649
H	-3.6206210	2.9349259	-1.8844479
H	-3.0548530	1.4377889	-1.1468589
H	-2.2464760	4.8451329	-2.2372119

H	-1.4725540	4.7979359	-0.6391389
H	-0.4688310	4.7934729	-2.1007079
H	-0.5342410	1.8474759	1.7933401

Zero-point correction= 0.676072 (Hartree/Particle)

Thermal correction to Energy= 0.724402

Thermal correction to Enthalpy= 0.725346

Thermal correction to Gibbs Free Energy= 0.593635

Sum of electronic and zero-point Energies= -3051.469194

Sum of electronic and thermal Energies= -3051.420863

Sum of electronic and thermal Enthalpies= -3051.419919

Sum of electronic and thermal Free Energies= -3051.551631

A-int4

C	0.8638585	-2.5309990	1.7247855
C	-0.0820825	-2.4093160	2.7439225
C	-0.7505195	-1.2079380	2.9066625
C	-0.4923845	-0.1325000	2.0475625
C	0.4125955	-0.2707300	0.9817895
C	1.1024935	-1.4789830	0.8513855
C	-1.1126185	1.1771260	2.3275525
C	-0.3995245	2.3495940	1.7085395
C	-0.1601105	2.1224950	0.2162915
C	0.5888695	0.8031510	-0.0731155
C	0.2458895	0.2424070	-1.4631965
C	1.5322865	0.0626920	-2.2032045
N	2.5231325	0.6354990	-1.4423335

C	2.0531825	1.2526670	-0.2259945
C	-0.9866095	-0.0986250	-1.8909985
N	0.6881725	3.1499630	-0.3776855
C	1.9993895	2.7649920	-0.4246015
O	2.9748795	3.4601790	-0.6522305
O	1.7452275	-0.5214190	-3.2560435
O	-2.0913105	1.3181330	3.0475335
Au	-2.6712405	0.0764570	-0.6501825
C	-1.2452715	-0.6053830	-3.2810165
C	5.3814135	-1.6783240	1.1194365
C	5.0621495	-2.9694650	0.6917315
C	4.4367685	-3.1559900	-0.5435255
C	4.1273145	-2.0489910	-1.3291325
C	4.4300575	-0.7541490	-0.9083045
C	5.0673485	-0.5873150	0.3242645
C	3.9383695	0.4243140	-1.7044615
O	5.3997315	-3.9727020	1.5400795
C	5.0901155	-5.2883990	1.1553075
H	1.4059245	-3.4650380	1.5931915
H	-0.2806625	-3.2452020	3.4095275
H	-1.4624335	-1.0591850	3.7159705
H	1.8173595	-1.6137520	0.0393105
H	-0.9823025	3.2573540	1.8998815
H	-1.3865535	-2.0021790	-0.7774025
H	-0.3412685	-0.6699160	-3.8919615

H	-1.7163875	-1.5970210	-3.2431165
H	-1.9777275	0.0454180	-3.7771755
H	5.8748315	-1.5619680	2.0810625
H	4.1887805	-4.1509200	-0.9019415
H	3.6171805	-2.1863610	-2.2824975
H	5.3182415	0.4179600	0.6641985
H	4.0304345	0.2479790	-2.7817255
H	4.4752145	1.3468550	-1.4522875
H	5.4302985	-5.9381800	1.9642925
H	5.6050105	-5.5744770	0.2267705
H	4.0079095	-5.4291110	1.0154075
P	-4.5967135	0.2752920	0.7669725
C	-4.5664985	-0.6129930	2.3576445
H	-3.7551545	-0.1959470	2.9636655
H	-5.5237225	-0.4790270	2.8762375
H	-4.3813795	-1.6750630	2.1761035
C	-6.1320535	-0.3142050	-0.0317935
H	-6.9959725	-0.1814490	0.6303305
H	-6.3007165	0.2292430	-0.9666285
H	-6.0119695	-1.3777620	-0.2640015
C	-4.9483505	2.0028200	1.2523215
H	-5.8675445	2.0675470	1.8467795
H	-4.1039355	2.3602910	1.8538545
H	-5.0440065	2.6299630	0.3600565
C	-3.1129255	-4.4305620	-1.7264625

F	-3.4572355	-3.4000650	-2.4843825
F	-4.1835315	-5.1522870	-1.4499675
F	-2.2211675	-5.1678410	-2.3535065
S	-2.4146805	-3.8053070	-0.1445445
O	-1.1976815	-2.9752500	-0.7213125
O	-1.8884355	-4.9381510	0.5719105
O	-3.4297945	-2.9330150	0.4152155
H	2.6955735	0.9845460	0.6270605
H	-1.1315345	2.0994860	-0.2902905
C	0.2319395	4.5276740	-0.6983295
C	0.8017085	4.9320240	-2.0580615
C	-1.2906905	4.5525670	-0.8036455
C	0.7100725	5.4934840	0.3840645
H	1.8930125	4.9616730	-2.0393305
H	0.4829705	4.2208310	-2.8296735
H	0.4255595	5.9259640	-2.3285685
H	-1.7945385	4.3038570	0.1386785
H	-1.6024105	5.5658740	-1.0807755
H	-1.6478525	3.8671150	-1.5835475
H	0.4081145	6.5184170	0.1350015
H	0.2803925	5.2432420	1.3619045
H	1.8015115	5.4636830	0.4612945
H	0.5742155	2.4626300	2.2134025

Zero-point correction= 0.675252 (Hartree/Particle)

Thermal correction to Energy= 0.724107

Thermal correction to Enthalpy= 0.725052

Thermal correction to Gibbs Free Energy= 0.592291

Sum of electronic and zero-point Energies= -3051.472645

Sum of electronic and thermal Energies= -3051.423790

Sum of electronic and thermal Enthalpies= -3051.422846

Sum of electronic and thermal Free Energies= -3051.555606

A-ts4

C	0.5338455	-3.0134318	1.7549254
C	-0.4870645	-2.8961508	2.6979754
C	-1.1445915	-1.6870728	2.8406784
C	-0.7938425	-0.5966468	2.0373014
C	0.1882475	-0.7303968	1.0419504
C	0.8610945	-1.9464178	0.9290964
C	-1.3906745	0.7205582	2.3102534
C	-0.5804585	1.8800312	1.7907664
C	-0.2558915	1.7086412	0.3087034
C	0.4344885	0.3467262	0.0035554
C	0.0430305	-0.1738168	-1.3831596
C	1.2530605	-0.1179568	-2.2630806
N	2.2997385	0.2860052	-1.4762426
C	1.9212865	0.7307872	-0.1524086
C	-1.1345395	-0.7407468	-1.7436006
N	0.6831575	2.7151822	-0.1743656
C	1.9696345	2.2547412	-0.1578446
O	2.9981515	2.9062242	-0.2374846

O	1.3420435	-0.4360228	-3.4367026
O	-2.4145855	0.8859272	2.9589484
Au	-2.9305745	-0.0425698	-0.6485096
C	-1.4132285	-1.1961818	-3.1540456
C	6.1794505	-0.9458598	0.6081414
C	6.0838845	-2.3273268	0.4196334
C	5.2122155	-2.8387918	-0.5451126
C	4.4535725	-1.9602518	-1.3125646
C	4.5473875	-0.5813138	-1.1401616
C	5.4147775	-0.0857718	-0.1635156
C	3.6754395	0.3403442	-1.9444716
O	6.8712525	-3.0870698	1.2198684
C	6.8098905	-4.4832728	1.0676534
H	1.0535305	-3.9607228	1.6369234
H	-0.7716445	-3.7520718	3.3030074
H	-1.9328355	-1.5497148	3.5772494
H	1.6232495	-2.0725318	0.1591804
H	-1.1259875	2.8105552	1.9835604
H	-1.5304685	-1.7292868	-0.9548696
H	-0.5951515	-1.8045278	-3.5535456
H	-2.3398315	-1.7775978	-3.1887356
H	-1.5132375	-0.3381888	-3.8297926
H	6.8609765	-0.5768518	1.3703674
H	5.1228455	-3.9086858	-0.7090106
H	3.7706125	-2.3539248	-2.0672446

H	5.4757105	0.9914042	-0.0075296
H	3.6350005	0.0480902	-3.0004536
H	4.0373005	1.3744342	-1.8800736
H	7.5086095	-4.9063868	1.7922374
H	7.1096585	-4.7965618	0.0571694
H	5.8021645	-4.8719728	1.2744044
P	-4.8207695	0.8029392	0.4598234
C	-5.2953815	-0.2218498	1.8837824
H	-4.4494135	-0.2413338	2.5796764
H	-6.1821205	0.1979802	2.3736914
H	-5.4811025	-1.2449078	1.5462604
C	-6.3204885	0.9019762	-0.5773116
H	-7.1707845	1.2669442	0.0110864
H	-6.1460515	1.5755622	-1.4218906
H	-6.5521105	-0.0933808	-0.9692206
C	-4.6166785	2.4824402	1.1447984
H	-5.5501745	2.8208542	1.6104424
H	-3.8269975	2.4424242	1.9055954
H	-4.3320735	3.1796992	0.3497224
C	-3.9193825	-4.0593308	-1.2762946
F	-4.2160035	-2.9828198	-2.0124176
F	-5.0467735	-4.5599028	-0.7936276
F	-3.3390265	-4.9565048	-2.0533216
S	-2.8104585	-3.5693938	0.1004364
O	-1.6189245	-3.0324108	-0.6666336

O	-2.5114095	-4.7901038	0.8244504
O	-3.5650295	-2.5132798	0.7839234
H	2.5873945	0.3068862	0.6124424
H	-1.1918715	1.7704532	-0.2595926
C	0.3350915	4.1448352	-0.3950206
C	1.0175125	4.6198512	-1.6776836
C	-1.1731785	4.2821912	-0.5874536
C	0.8001665	4.9834862	0.7938484
H	2.1050195	4.5756992	-1.5897996
H	0.7071045	3.9992382	-2.5269426
H	0.7241225	5.6560902	-1.8832176
H	-1.7485285	4.0035802	0.3041134
H	-1.3996245	5.3321672	-0.8038996
H	-1.5268075	3.6822992	-1.4365036
H	0.5806165	6.0431232	0.6138214
H	0.2909155	4.6865142	1.7187114
H	1.8797395	4.8735102	0.9358054
H	0.3627785	1.9209142	2.3593774

Zero-point correction= 0.669047 (Hartree/Particle)

Thermal correction to Energy= 0.717845

Thermal correction to Enthalpy= 0.718789

Thermal correction to Gibbs Free Energy= 0.584466

Sum of electronic and zero-point Energies= -3051.459083

Sum of electronic and thermal Energies= -3051.410285

Sum of electronic and thermal Enthalpies= -3051.409341

Sum of electronic and thermal Free Energies= -3051.543664

A-2

C	1.5813637	-1.5174890	-1.9711039
C	1.9254737	-0.4909020	-2.8522429
C	1.2266767	0.7029420	-2.8051429
C	0.1721017	0.8706490	-1.8951029
C	-0.1580173	-0.1488080	-0.9865399
C	0.5694977	-1.3388500	-1.0384139
C	-0.6387263	2.0962790	-1.9547649
C	-2.0415043	1.9349730	-1.4321649
C	-2.0269043	1.3471690	-0.0190699
C	-1.2375723	0.0216550	0.0670421
C	-0.6805623	-0.2076020	1.4680661
C	-1.1628533	-1.5232080	1.9660121
N	-2.0702833	-1.9908960	1.0456761
C	-2.3261473	-1.0654150	-0.0365489
C	0.1846287	0.5965400	2.0938381
N	-3.3619823	0.9854790	0.4492721
C	-3.6412243	-0.3388060	0.2267631
O	-4.7263183	-0.8882320	0.2839311
O	-0.8214523	-2.1285260	2.9697181
O	-0.2312813	3.1551780	-2.4161069
Au	2.8450027	1.5350170	0.1112221
C	0.8508907	0.3644060	3.4024531
C	-0.4916373	-4.8120750	-1.9815169

C	0.7672127	-5.0099020	-1.4053529
C	0.9364047	-4.8217480	-0.0310709
C	-0.1398263	-4.3926060	0.7374771
C	-1.3866913	-4.1317020	0.1650451
C	-1.5508393	-4.3700720	-1.2023589
C	-2.4307323	-3.4059710	0.9717441
O	1.7604097	-5.3661930	-2.2539809
C	3.0585977	-5.5188530	-1.7152579
H	2.1200727	-2.4637380	-1.9865709
H	2.7331147	-0.6305680	-3.5657179
H	1.4443837	1.5146130	-3.4968469
H	0.3654237	-2.1406280	-0.3305259
H	-2.5513603	2.9032670	-1.4708619
H	0.4036007	-0.4749740	3.9374311
H	1.9088507	0.1242080	3.2188111
H	0.8257087	1.2667800	4.0252151
H	-0.6021133	-4.9854460	-3.0491339
H	1.9052867	-4.9591950	0.4389031
H	0.0042487	-4.1994830	1.7992881
H	-2.5212183	-4.1891940	-1.6664259
H	-2.4753963	-3.7706500	2.0035621
H	-3.4325553	-3.4797980	0.5329921
H	3.7100687	-5.7679700	-2.5554619
H	3.0941787	-6.3378730	-0.9828379
H	3.4138747	-4.5951000	-1.2360009

P	2.8403357	3.7530280	-0.4612369
C	2.9142027	4.0998570	-2.2444769
H	1.9672457	3.7755420	-2.6908039
H	3.0489077	5.1753550	-2.4103199
H	3.7450207	3.5492730	-2.6958219
C	4.2653147	4.6389490	0.2546701
H	4.2379847	5.6983750	-0.0267839
H	4.2444337	4.5490600	1.3450231
H	5.1936197	4.1884160	-0.1096949
C	1.3801577	4.6724280	0.1258651
H	1.4940447	5.7407260	-0.0937299
H	0.4941587	4.2944640	-0.3958849
H	1.2607787	4.5308490	1.2046261
C	5.0033837	-1.2565600	1.9876501
F	5.3163137	0.0113080	2.2472551
F	6.1179967	-1.9603480	1.8746151
F	4.2852027	-1.7307530	2.9939231
S	4.0454327	-1.3384460	0.4241501
O	2.8423947	-0.4914110	0.8122871
O	3.6933347	-2.7408600	0.2500951
O	4.8876447	-0.6895390	-0.5765089
H	-2.3447933	-1.5855860	-1.0055499
H	-1.5736493	2.0838800	0.6587801
C	-4.4060733	1.9632000	0.8592621
C	-5.1207713	1.4273730	2.1001181

C	-3.7515373	3.2885030	1.2345091
C	-5.4024943	2.1652080	-0.2808679
H	-5.6404603	0.4910230	1.8878861
H	-4.3999453	1.2533190	2.9079301
H	-5.8527973	2.1675180	2.4448581
H	-3.2334783	3.7684130	0.3958071
H	-4.5337913	3.9792150	1.5684081
H	-3.0441393	3.1627010	2.0636061
H	-6.1959023	2.8552730	0.0319411
H	-4.9163913	2.5908830	-1.1674229
H	-5.8629473	1.2110630	-0.5550839
H	-2.5799603	1.2403850	-2.0970369
H	0.4813537	1.5112350	1.5606201

Zero-point correction= 0.675231 (Hartree/Particle)

Thermal correction to Energy= 0.724246

Thermal correction to Enthalpy= 0.725190

Thermal correction to Gibbs Free Energy= 0.590201

Sum of electronic and zero-point Energies= -3051.501736

Sum of electronic and thermal Energies= -3051.452721

Sum of electronic and thermal Enthalpies= -3051.451777

Sum of electronic and thermal Free Energies= -3051.586766

A-int5

C	1.4418499	1.5902733	-3.0321335
C	0.2303059	1.6720943	-3.7139045
C	-0.9453941	1.3117263	-3.0728755

C	-0.9239091	0.8752373	-1.7440535
C	0.2969269	0.7619623	-1.0652865
C	1.4707079	1.1294763	-1.7222815
C	-2.1699091	0.5924143	-1.0310885
C	-2.1872711	0.1973563	0.2568325
C	-0.9651381	-0.2658727	0.9476655
C	0.3899669	0.2247463	0.3500525
C	1.0733009	1.1816803	1.3295645
C	2.1340559	0.4229323	2.0311005
N	2.0952589	-0.8964367	1.5622365
C	1.2968189	-1.0198637	0.3645385
C	0.7160079	2.4693813	1.5379275
N	-0.9427491	-1.8172567	0.9336865
C	0.4181149	-2.2327737	0.4821535
O	0.7064419	-3.3720617	0.2715525
O	2.9408319	0.7827483	2.8721175
O	-3.2973001	0.8169863	-1.7303605
Au	-0.8881231	3.3430103	0.5388765
C	1.4087439	3.3358703	2.5447375
C	5.1321259	-2.5670977	-1.4422715
C	5.9747619	-1.4571547	-1.5476725
C	5.9345949	-0.4595637	-0.5707335
C	5.0585929	-0.5865017	0.5036655
C	4.2214339	-1.6948437	0.6249705
C	4.2654769	-2.6786977	-0.3674885

C	3.2402579	-1.7810527	1.7610585
O	6.7898949	-1.4375427	-2.6299395
C	7.6655469	-0.3472097	-2.7743915
H	2.3686649	1.8746573	-3.5243435
H	0.2046199	2.0092483	-4.7472235
H	-1.8989541	1.3490893	-3.5926935
H	2.4225879	1.0581803	-1.1938815
H	-3.1455731	0.0500483	0.7464195
H	-3.9883911	0.1960013	-1.3936595
H	2.2089069	2.8310943	3.0920075
H	1.8203449	4.2191603	2.0379205
H	0.6719319	3.7304293	3.2573845
H	5.1778989	-3.3246987	-2.2202825
H	6.5817869	0.4105023	-0.6315225
H	5.0240509	0.1882923	1.2694145
H	3.5991299	-3.5386787	-0.2958395
H	3.6911369	-1.4612047	2.7069095
H	2.8811109	-2.8121657	1.8821565
H	8.2314689	-0.5220887	-3.6916215
H	8.3664209	-0.2732587	-1.9304215
H	7.1210439	0.6037963	-2.8665895
P	-2.8198751	4.3264473	-0.4804875
C	-2.9706341	4.2012353	-2.2974315
H	-3.0998551	3.1443293	-2.5558135
H	-3.8402561	4.7695493	-2.6490235

H	-2.0633791	4.5756963	-2.7811485
C	-3.0450521	6.1118803	-0.1446025
H	-3.9740911	6.4800613	-0.5962335
H	-3.0765341	6.2785913	0.9366865
H	-2.1975161	6.6712593	-0.5525485
C	-4.3838881	3.5772153	0.0985785
H	-5.2481541	4.0963753	-0.3328815
H	-4.3984191	2.5285113	-0.2179305
H	-4.4372531	3.6202123	1.1906185
C	-5.0206301	-3.8610147	-0.5781145
F	-4.5728821	-5.0300987	-1.0111605
F	-6.3045211	-3.7475877	-0.8742855
F	-4.8855721	-3.8278317	0.7512705
S	-4.0625781	-2.4962397	-1.3407645
O	-2.6803951	-2.7994897	-0.8765505
O	-4.6468971	-1.2979407	-0.6886775
O	-4.2748281	-2.6162117	-2.7723805
H	1.9262129	-1.1320007	-0.5323575
H	-0.9756691	0.0093563	2.0072815
H	-1.6252551	-2.1396427	0.1803725
C	-1.4402991	-2.5282807	2.2313165
C	-0.4216201	-2.3121097	3.3365645
C	-2.7909461	-1.9239887	2.5914295
C	-1.6202831	-4.0124527	1.9329445
H	0.5475799	-2.7650067	3.0976215

H	-0.2598761	-1.2538807	3.5714895
H	-0.7970191	-2.7970687	4.2445625
H	-3.5063991	-2.0074227	1.7659035
H	-3.1940961	-2.4885487	3.4394095
H	-2.7198081	-0.8769367	2.9044955
H	-2.0821241	-4.4733197	2.8136425
H	-2.2850801	-4.1687217	1.0774565
H	-0.6725181	-4.5172947	1.7383585

Zero-point correction= 0.675324 (Hartree/Particle)

Thermal correction to Energy= 0.724197

Thermal correction to Enthalpy= 0.725141

Thermal correction to Gibbs Free Energy= 0.590253

Sum of electronic and zero-point Energies= -3051.445582

Sum of electronic and thermal Energies= -3051.396709

Sum of electronic and thermal Enthalpies= -3051.395765

Sum of electronic and thermal Free Energies= -3051.530653

A-ts5

C	0.0188718	-1.0239109	3.3090560
C	-1.1189202	-0.3205259	3.7087430
C	-1.8932372	0.3138021	2.7539050
C	-1.5374252	0.2194991	1.4035740
C	-0.3523722	-0.4181649	0.9967730
C	0.4064468	-1.0598229	1.9747870
C	-2.3887182	0.7364561	0.3671730
C	-2.0784992	0.7502261	-1.0239440

C	-0.6465222	0.5551141	-1.4052540
C	0.1250838	-0.4199929	-0.4443200
C	0.2016328	-1.8147009	-1.0675750
C	1.4997348	-1.8931229	-1.7852620
N	2.1700498	-0.6810509	-1.5888330
C	1.5709078	0.0928661	-0.5236310
C	-0.7470402	-2.7763999	-0.9995240
N	0.1440748	1.8622531	-1.4117960
C	1.5189688	1.5349751	-0.9437470
O	2.4171168	2.3227241	-0.9364980
O	1.9831898	-2.7980399	-2.4446640
O	-3.5289082	1.3020651	0.5376010
Au	-2.5904542	-2.5074289	-0.0633860
C	-0.5801992	-4.1051589	-1.6746780
C	5.6892118	-0.2561829	1.3398510
C	5.7843028	-1.5882519	1.7511360
C	5.1828728	-2.5939019	0.9907520
C	4.4994398	-2.2568839	-0.1741510
C	4.4056398	-0.9321239	-0.5992050
C	5.0041818	0.0634971	0.1789890
C	3.6083428	-0.5886049	-1.8279330
O	6.4745258	-1.8029439	2.8977690
C	6.6068838	-3.1281439	3.3473020
H	0.6292458	-1.5304099	4.0532120
H	-1.3818072	-0.2578709	4.7612490

H	-2.7607772	0.9137851	3.0188290
H	1.3094638	-1.6000529	1.6900440
H	-3.1881062	1.6382521	-0.6651810
H	0.3723098	-4.2236129	-2.1965870
H	-0.6911002	-4.9070989	-0.9326110
H	-1.4020022	-4.2563759	-2.3880030
H	6.1595898	0.5076531	1.9536400
H	5.2463358	-3.6361139	1.2897820
H	4.0301388	-3.0380309	-0.7719950
H	4.9185248	1.1054231	-0.1289760
H	3.8114568	-1.2882079	-2.6459620
H	3.8474128	0.4254681	-2.1739340
H	7.1904128	-3.0872089	4.2693110
H	7.1370768	-3.7553929	2.6162100
H	5.6301558	-3.5853599	3.5629470
P	-4.8118632	-2.1789479	0.7798550
C	-5.0233822	-1.2636959	2.3465090
H	-4.6809102	-0.2344649	2.1877170
H	-6.0799672	-1.2518309	2.6399730
H	-4.4251142	-1.7210129	3.1403770
C	-5.7731372	-3.7160009	1.0299380
H	-6.7991692	-3.4876989	1.3423930
H	-5.7963852	-4.2869449	0.0964230
H	-5.2899522	-4.3308399	1.7954410
C	-5.8393192	-1.2075959	-0.3798800

H	-6.8704292	-1.1284379	-0.0150610
H	-5.4102832	-0.2023549	-0.4594990
H	-5.8351642	-1.6779479	-1.3680330
C	-0.7844492	5.5302531	1.4474450
F	-0.0498612	5.4016811	2.5431050
F	-1.6979982	6.4693521	1.6480850
F	0.0081008	5.9139661	0.4480710
S	-1.6023592	3.9399491	1.0398230
O	-0.4213152	3.0316491	0.8335750
O	-2.3066662	4.2027781	-0.2219660
O	-2.3908332	3.6203311	2.2210930
H	2.1474218	0.0186531	0.4115810
H	-0.5523002	0.1484861	-2.4182240
H	-0.2319692	2.4617281	-0.5880040
C	0.0816758	2.7302711	-2.7003270
C	1.0198808	2.1279601	-3.7355340
C	-1.3502572	2.7553861	-3.2154900
C	0.4777048	4.1523571	-2.3234550
H	2.0715978	2.2280491	-3.4490040
H	0.8050518	1.0693421	-3.9280100
H	0.8829778	2.6662261	-4.6796560
H	-2.0348652	3.1501061	-2.4577080
H	-1.3669792	3.4307681	-4.0791210
H	-1.7040332	1.7769441	-3.5573340
H	0.4933078	4.7520801	-3.2410970

H	-0.2656302	4.5897891	-1.6486060
H	1.4646448	4.2050801	-1.8601410
H	-2.7652812	0.1016231	-1.5802390

Zero-point correction= 0.668926 (Hartree/Particle)

Thermal correction to Energy= 0.717581

Thermal correction to Enthalpy= 0.718525

Thermal correction to Gibbs Free Energy= 0.584806

Sum of electronic and zero-point Energies= -3051.360716

Sum of electronic and thermal Energies= -3051.312061

Sum of electronic and thermal Enthalpies= -3051.311116

Sum of electronic and thermal Free Energies= -3051.444836

A-int6

C	-0.2048942	1.1041868	3.2859863
C	1.0595438	0.6749818	3.6952963
C	1.9506558	0.1974018	2.7528933
C	1.5807528	0.1267818	1.4044693
C	0.2871728	0.4726758	0.9998883
C	-0.5880182	0.9955398	1.9577383
C	2.6203428	-0.1884672	0.4111283
C	2.2173298	-0.4218982	-1.0249307
C	0.7345158	-0.5578802	-1.3291277
C	-0.1982482	0.3061618	-0.4241187
C	-0.5728812	1.6015378	-1.1464107
C	-1.8523092	1.3385478	-1.8546267
N	-2.2510562	0.0294918	-1.5506637

C	-1.5077662	-0.4953352	-0.4278747
C	0.1370238	2.7524938	-1.1531917
N	0.2455878	-1.9910012	-1.2371077
C	-1.1402122	-1.9295042	-0.6770037
O	-1.8035982	-2.9019612	-0.4799597
O	-2.5148942	2.0590878	-2.5814767
O	3.8091838	-0.1666022	0.6894213
Au	1.9718748	2.9917608	-0.1909407
C	-0.3133312	3.9572378	-1.9248397
C	-5.5492452	-0.7394042	1.5391703
C	-5.9389632	0.5795188	1.7878963
C	-5.5945562	1.5869368	0.8838193
C	-4.8710502	1.2640398	-0.2605007
C	-4.4849032	-0.0496182	-0.5241977
C	-4.8287492	-1.0449242	0.3962523
C	-3.6476582	-0.3645332	-1.7334237
O	-6.6422852	0.7807488	2.9284593
C	-7.0664832	2.0897058	3.2172483
H	-0.9049252	1.5080208	4.0137073
H	1.3394568	0.7184618	4.7447903
H	2.9441588	-0.1530362	3.0235673
H	-1.5806982	1.3298628	1.6543873
H	2.7970628	-1.2870632	-1.3625667
H	-1.2578952	3.8202938	-2.4566627
H	-0.4005452	4.8139798	-1.2432617

H	0.4669488	4.2402058	-2.6445927
H	-5.8240322	-1.5032772	2.2619443
H	-5.8885602	2.6182588	1.0555193
H	-4.6009192	2.0471318	-0.9682237
H	-4.5136312	-2.0727112	0.2141773
H	-3.9919842	0.1860068	-2.6154677
H	-3.6887022	-1.4379042	-1.9609507
H	-7.6118312	2.0387118	4.1618003
H	-7.7362642	2.4818408	2.4384173
H	-6.2164002	2.7777768	3.3322373
P	4.1910868	3.2606798	0.6800443
C	4.5615268	2.5655288	2.3262223
H	4.4695358	1.4761828	2.2496593
H	5.5822378	2.8285098	2.6286963
H	3.8476888	2.9359538	3.0682063
C	4.7597368	4.9974938	0.7886153
H	5.8043578	5.0436918	1.1190393
H	4.6690228	5.4739498	-0.1926167
H	4.1323678	5.5472988	1.4969523
C	5.4338168	2.4583418	-0.3924767
H	6.4461938	2.6252778	-0.0052507
H	5.2234578	1.3824028	-0.4092177
H	5.3603798	2.8589248	-1.4085107
C	2.3628438	-5.2476802	1.4379703
F	1.7980758	-5.2703612	2.6358263

F	3.4939408	-5.9362222	1.4787873
F	1.5396078	-5.8332352	0.5693043
S	2.7069218	-3.5179372	0.9328073
O	1.3268868	-2.9168352	0.9181423
O	3.2472998	-3.6316432	-0.4297997
O	3.5675658	-2.9949452	1.9804493
H	-2.0857182	-0.4435672	0.5069563
H	0.5453718	-0.2511902	-2.3641157
H	0.8006978	-2.4834192	-0.4351767
C	0.3523948	-2.8735342	-2.5258607
C	-0.7859462	-2.5012832	-3.4643807
C	1.6962968	-2.6393242	-3.2019537
C	0.2810338	-4.3317472	-2.0936127
H	-1.7626662	-2.7944772	-3.0665387
H	-0.8073672	-1.4298272	-3.6976407
H	-0.6430352	-3.0405702	-4.4068387
H	2.5271358	-2.9272412	-2.5489797
H	1.7273128	-3.2938952	-4.0804077
H	1.8302648	-1.6136542	-3.5632567
H	0.2958138	-4.9509812	-2.9981657
H	1.1546808	-4.5980942	-1.4905047
H	-0.6284952	-4.5595592	-1.5347577
H	2.6035528	0.4427178	-1.5857107

Zero-point correction= 0.674856 (Hartree/Particle)

Thermal correction to Energy= 0.723721

Thermal correction to Enthalpy= 0.724665

Thermal correction to Gibbs Free Energy= 0.589757

Sum of electronic and zero-point Energies= -3051.451901

Sum of electronic and thermal Energies= -3051.403036

Sum of electronic and thermal Enthalpies= -3051.402092

Sum of electronic and thermal Free Energies= -3051.537000

A-int7

C	1.2830962	-1.8442496	2.8902380
C	0.3740102	-1.6127096	3.9243800
C	-0.7001718	-0.7728796	3.7026590
C	-0.8702608	-0.1497046	2.4593030
C	0.0478092	-0.3700376	1.4197570
C	1.1200032	-1.2360106	1.6559090
C	-2.0823768	0.6711994	2.2602220
C	-2.2416448	1.3067474	0.9509590
C	-1.3896538	1.0688904	-0.0527720
C	-0.1369848	0.2647784	0.0519900
C	-0.0770378	-0.8131746	-1.0499670
C	1.2473932	-0.7009116	-1.7199900
N	1.9415392	0.3198254	-1.0962210
C	1.0650102	1.2063624	-0.3724880
C	-1.0224478	-1.7527396	-1.2605260
N	1.3386302	3.1567544	1.1517740
C	1.7448062	1.8896734	0.8062390
O	2.5676062	1.3026654	1.4896160

O	1.7102632	-1.3489046	-2.6435460
O	-2.9603198	0.7703444	3.1170400
H	0.6530802	1.9754374	-1.0487840
Au	-2.6895778	-1.8933976	0.0049170
C	-0.8730318	-2.8223046	-2.3026470
C	0.9896092	4.3407824	0.3223410
C	-0.4677808	4.3287184	-0.1241100
C	1.9272892	4.4739404	-0.8764220
C	1.1950322	5.5404094	1.2449470
C	5.7479622	-1.4948816	0.1673970
C	6.3432202	-2.1722056	-0.9017740
C	5.9193532	-1.9169646	-2.2047190
C	4.9059182	-0.9858216	-2.4223630
C	4.3161702	-0.2976686	-1.3700840
C	4.7470272	-0.5684516	-0.0657810
C	3.2390692	0.7241394	-1.6226730
O	7.3182182	-3.0576136	-0.5692010
C	7.9346512	-3.7699896	-1.6104360
H	2.1303342	-2.5075666	3.0478560
H	0.5089682	-2.0915156	4.8912160
H	-1.4371658	-0.5692006	4.4764020
H	1.8440662	-1.4253776	0.8677800
H	-3.1353758	1.9125364	0.8153430
H	-1.5940428	1.4793014	-1.0447190
H	1.8354292	3.4072184	2.0017320

H	0.0496722	-2.7376406	-2.8817530
H	-0.9023598	-3.8058086	-1.8138260
H	-1.7313228	-2.8135786	-2.9884760
H	-1.1323308	4.1888534	0.7356590
H	-0.7119748	5.2841004	-0.6044270
H	-0.6794058	3.5360434	-0.8490010
H	2.9740532	4.4860754	-0.5486380
H	1.7251272	5.4111014	-1.4092000
H	1.8026422	3.6567934	-1.5970780
H	0.9439842	6.4690734	0.7214480
H	0.5527182	5.4638594	2.1307160
H	2.2398132	5.6114064	1.5734660
H	6.0968192	-1.7158026	1.1733310
H	6.3550962	-2.4396246	-3.0511130
H	4.5516922	-0.8090096	-3.4366470
H	4.2764412	-0.0451276	0.7660680
H	3.1520532	0.9109144	-2.7042010
H	3.5031222	1.6737284	-1.1391050
H	8.6775342	-4.4224386	-1.1461890
H	8.4422982	-3.0996036	-2.3197010
H	7.2135522	-4.3879106	-2.1654040
P	-4.6131988	-2.0238016	1.4346000
C	-4.2577998	-2.3348836	3.2001660
H	-3.7242868	-1.4613446	3.5944830
H	-5.1887078	-2.4758576	3.7626120

H	-3.6246438	-3.2207906	3.3083800
C	-5.8009268	-3.3275666	0.9566850
H	-6.6706868	-3.3251376	1.6245810
H	-6.1253678	-3.1437476	-0.0724900
H	-5.3119138	-4.3056396	1.0001330
C	-5.6267348	-0.5047566	1.4924690
H	-6.5014458	-0.6646846	2.1347920
H	-5.0171158	0.3046134	1.9117390
H	-5.9592268	-0.2443086	0.4831870
C	-5.2183598	1.2311614	-2.2867170
F	-4.5279878	1.4207664	-1.1690630
F	-6.5041898	1.3982374	-2.0375610
F	-4.8181548	2.0870124	-3.2027340
S	-4.9622258	-0.4946486	-2.8692110
O	-3.3797878	-0.5037186	-2.9506810
O	-5.4869928	-0.5710026	-4.2061880
O	-5.4301508	-1.3453576	-1.7924490
H	-2.9670098	-0.8753886	-2.1234590

Zero-point correction= 0.672481 (Hartree/Particle)

Thermal correction to Energy= 0.722808

Thermal correction to Enthalpy= 0.723752

Thermal correction to Gibbs Free Energy= 0.585293

Sum of electronic and zero-point Energies= -3051.433581

Sum of electronic and thermal Energies= -3051.383254

Sum of electronic and thermal Enthalpies= -3051.382310

Sum of electronic and thermal Free Energies= -3051.520769

A-ts6

C	1.5539089	-2.3615416	2.0471716
C	0.7319389	-2.4952916	3.1659396
C	-0.3939071	-1.7009116	3.2688536
C	-0.6988771	-0.7613576	2.2761586
C	0.1388549	-0.6026226	1.1596956
C	1.2569529	-1.4376816	1.0575476
C	-1.9660191	-0.0133766	2.4106856
C	-2.2469521	1.0006704	1.3922846
C	-1.4721681	1.1470374	0.3125356
C	-0.1998201	0.4063644	0.0644936
C	-0.2077401	-0.3084626	-1.2921944
C	1.1632409	-0.1650536	-1.8705664
N	1.8378049	0.7450224	-1.0904524
C	0.9483979	1.4581044	-0.1974264
C	-1.2632471	-0.9071426	-1.8884454
N	1.2840209	3.1978754	1.5429416
C	1.6206939	1.9567924	1.0734966
O	2.3857399	1.2456464	1.7059816
O	1.6263409	-0.7180706	-2.8515114
O	-2.7861271	-0.2646956	3.2919046
H	0.4820189	2.3053924	-0.7243444
Au	-2.6557661	-1.8252886	-0.4390354
C	-1.1525331	-1.6132786	-3.2125794

C	0.8855349	4.4611254	0.8696886
C	-0.5881421	4.4717504	0.4747396
C	1.7792989	4.7474684	-0.3356524
C	1.1066879	5.5487324	1.9187506
C	5.4442899	-1.4827256	0.1598896
C	6.0308759	-2.0737316	-0.9642554
C	5.6946989	-1.6198766	-2.2387754
C	4.7741199	-0.5832246	-2.3737744
C	4.1919609	0.0189144	-1.2649744
C	4.5394549	-0.4465456	0.0100136
C	3.2003459	1.1421334	-1.4312174
O	6.9083339	-3.0774106	-0.7125184
C	7.5184699	-3.7030106	-1.8129534
H	2.4439209	-2.9780446	1.9392916
H	0.9718039	-3.2163826	3.9434296
H	-1.0701441	-1.7757766	4.1174486
H	1.9323439	-1.3581926	0.2115726
H	-3.1692541	1.5637764	1.5123776
H	-1.7804301	1.8328234	-0.4783774
H	1.7681319	3.3406704	2.4240316
H	-0.5047361	-1.0855966	-3.9196904
H	-0.7119321	-2.6094416	-3.0738164
H	-2.1456931	-1.7440026	-3.6571174
H	-1.2178141	4.1680614	1.3186596
H	-0.8789901	5.4839654	0.1694696

H	-0.8038511	3.8100284	-0.3701574
H	2.8347309	4.7658564	-0.0375484
H	1.5279699	5.7248614	-0.7649594
H	1.6603869	4.0027854	-1.1319144
H	0.8407819	6.5289194	1.5094226
H	0.4836699	5.3690024	2.8034446
H	2.1580989	5.5884824	2.2307566
H	5.7266949	-1.8535886	1.1424196
H	6.1274899	-2.0682866	-3.1280694
H	4.4880909	-0.2510156	-3.3702684
H	4.0790999	0.0083064	0.8862916
H	3.2181569	1.5016934	-2.4707274
H	3.4644419	1.9861094	-0.7817834
H	8.1815039	-4.4704266	-1.4078174
H	8.1136649	-2.9938046	-2.4065474
H	6.7790049	-4.1807756	-2.4719564
P	-4.2665621	-2.7168666	1.0087476
C	-3.7242611	-3.4284026	2.5971126
H	-3.2855441	-2.6179006	3.1920416
H	-4.5799401	-3.8533416	3.1354016
H	-2.9698641	-4.2031066	2.4313516
C	-5.2931141	-3.9939386	0.2073126
H	-6.1076861	-4.3081996	0.8707136
H	-5.7095701	-3.5703456	-0.7126404
H	-4.6786681	-4.8608196	-0.0531864

C	-5.4533711	-1.4199446	1.4898456
H	-6.2689171	-1.8536516	2.0812646
H	-4.9260601	-0.6689576	2.0905656
H	-5.8530931	-0.9527776	0.5839226
C	-5.4345501	1.5479984	-1.3587814
F	-4.8858931	1.3976634	-0.1512044
F	-6.7358201	1.3232434	-1.2559924
F	-5.2311831	2.7889674	-1.7650374
S	-4.6977431	0.3459704	-2.5340344
O	-3.2212061	0.7037664	-2.4008664
O	-5.2515341	0.6852524	-3.8279744
O	-5.0074821	-0.9606906	-1.9486254
H	-2.4077621	-0.1656576	-1.9198934

Zero-point correction= 0.667544 (Hartree/Particle)

Thermal correction to Energy= 0.717436

Thermal correction to Enthalpy= 0.718381

Thermal correction to Gibbs Free Energy= 0.580595

Sum of electronic and zero-point Energies= -3051.424369

Sum of electronic and thermal Energies= -3051.374477

Sum of electronic and thermal Enthalpies= -3051.373533

Sum of electronic and thermal Free Energies= -3051.511319

A-int8

C	-1.9852766	2.7540145	1.6822360
C	-1.5603936	2.8181385	3.0074510
C	-0.5410026	1.9838925	3.4316040

C	0.0404144	1.0726955	2.5472030
C	-0.4092376	0.9761015	1.2167760
C	-1.4126456	1.8505975	0.7959620
C	1.1563464	0.2462155	3.0559750
C	1.9039314	-0.5367375	2.0356450
C	1.4409634	-0.6653725	0.7541070
C	0.1412084	-0.0959625	0.2919540
C	0.1283834	0.3068635	-1.1762990
C	-1.2088106	-0.0486155	-1.7277080
N	-1.8075586	-0.8644465	-0.7953160
C	-0.8430996	-1.3437345	0.1696150
C	1.1690984	0.7560345	-1.8844930
N	-0.9768806	-2.9376045	2.0499170
C	-1.4441386	-1.7793005	1.4939710
O	-2.2563276	-1.0813945	2.0823040
O	-1.7208936	0.2911955	-2.7799570
O	1.4958764	0.2175655	4.2271770
H	-0.2413826	-2.1592205	-0.2597530
Au	3.2474184	1.0046045	0.9361780
C	1.2146304	1.0125315	-3.3470410
C	-0.4383856	-4.1930095	1.4551400
C	1.0327704	-4.0759675	1.0632770
C	-1.2909256	-4.6474035	0.2716040
C	-0.5538376	-5.2292935	2.5709960
C	-5.4850216	1.2976085	0.2060210

C	-6.1918776	1.6175145	-0.9581360
C	-5.9001686	0.9547085	-2.1490630
C	-4.9043046	-0.0199525	-2.1607360
C	-4.2057256	-0.3558525	-1.0082770
C	-4.5053156	0.3208845	0.1806390
C	-3.1358106	-1.4158245	-1.0361780
O	-7.1342796	2.5864845	-0.8281260
C	-7.8683346	2.9400405	-1.9722370
H	-2.7785956	3.4094885	1.3295490
H	-2.0184706	3.5220365	3.6977560
H	-0.1636926	2.0096255	4.4511150
H	-1.7784866	1.8234065	-0.2272560
H	2.7268264	-1.1601355	2.3939840
H	1.9625324	-1.3184155	0.0450270
H	-1.4223126	-3.0656455	2.9535010
H	0.2362364	0.8916105	-3.8148850
H	1.5897054	2.0242725	-3.5493860
H	1.9333804	0.3168475	-3.8009590
H	1.6257264	-3.6951755	1.9029670
H	1.4181554	-5.0680535	0.8003780
H	1.2115654	-3.4359755	0.1921430
H	-2.3408966	-4.7546795	0.5710190
H	-0.9365696	-5.6202495	-0.0893790
H	-1.2428486	-3.9527085	-0.5752600
H	-0.1789456	-6.1983425	2.2256960

H	0.0375034	-4.9289935	3.4447320
H	-1.5983436	-5.3624215	2.8807320
H	-5.7320416	1.8309835	1.1211930
H	-6.4250626	1.1932155	-3.0693520
H	-4.6534346	-0.5152505	-3.0974980
H	-3.9489216	0.0767395	1.0853230
H	-3.1424286	-1.9274765	-2.0098960
H	-3.3216176	-2.1712885	-0.2625460
H	-8.5673126	3.7215455	-1.6662520
H	-8.4378836	2.0877665	-2.3710440
H	-7.2192456	3.3328135	-2.7686230
P	4.7738084	2.6699945	0.3353670
C	5.0261434	3.9796645	1.5794490
H	5.3551894	3.5311365	2.5215800
H	5.7825534	4.6939105	1.2331060
H	4.0828014	4.5044985	1.7573180
C	4.3362654	3.5663995	-1.1912400
H	5.0843924	4.3401125	-1.4008610
H	4.3007404	2.8598395	-2.0256680
H	3.3516444	4.0303545	-1.0764070
C	6.4254854	1.9701765	0.0366590
H	7.1260844	2.7561725	-0.2688690
H	6.7828784	1.4892885	0.9523530
H	6.3583674	1.2010475	-0.7383550
H	2.1188234	0.8963555	-1.3592040

C	4.9236834	-0.5944805	-2.5595210
F	6.2332044	-0.3631785	-2.4807600
F	4.3051764	0.5960125	-2.3823250
F	4.6372364	-1.0159845	-3.7786740
S	4.3826594	-1.7951285	-1.2769560
O	5.2201434	-2.9598265	-1.5161440
O	2.9438184	-1.9331815	-1.5710020
O	4.6649764	-1.0467265	-0.0250580

Zero-point correction= 0.674286 (Hartree/Particle)

Thermal correction to Energy= 0.724174

Thermal correction to Enthalpy= 0.725118

Thermal correction to Gibbs Free Energy= 0.588331

Sum of electronic and zero-point Energies= -3051.450546

Sum of electronic and thermal Energies= -3051.400658

Sum of electronic and thermal Enthalpies= -3051.399714

Sum of electronic and thermal Free Energies= -3051.536501

A-ts7

C	-1.0147162	0.3327170	3.0890079
C	-1.4613772	1.0813820	1.9966009
C	0.4309808	0.2430560	3.4364749
C	1.3963218	0.8653830	2.4945779
C	0.9249998	1.8133630	1.5653679
C	-0.4804102	1.7182360	1.0092939
C	-1.0058092	3.0475270	0.4988069
C	-1.6310702	2.8333980	-0.8335591

N	-1.3719092	1.5251300	-1.1834371
C	-0.4773632	0.8353860	-0.2784301
C	-0.9454532	4.2038860	1.1689719
N	1.8992668	1.5382830	-0.3483241
C	0.8946178	0.7158120	-0.9415231
O	1.0485928	0.0136040	-1.9150831
O	-2.2822662	3.6088110	-1.5112701
O	0.7991818	-0.2751870	4.4802509
Au	1.6023388	-1.1789290	1.4636569
C	-1.4255312	5.5318570	0.7029439
C	-2.2727992	-2.8559990	-2.5128491
C	-3.2796392	-3.0573040	-1.5651561
C	-3.8639192	-1.9572570	-0.9327411
C	-3.4204122	-0.6755710	-1.2468461
C	-2.3965492	-0.4614660	-2.1667881
C	-1.8328232	-1.5731200	-2.7981461
C	-1.8647872	0.9235870	-2.4126441
O	-3.5983972	-4.3498640	-1.3088391
C	-4.5883522	-4.6012510	-0.3401731
H	-1.8816982	5.4722630	-0.2866751
H	-2.1566962	5.9420890	1.4107589
H	-0.5909232	6.2447770	0.6780799
H	-1.8365282	-3.7279710	-2.9950981
H	-4.6518642	-2.0837200	-0.1958741
H	-3.8705342	0.1798660	-0.7436081

H	-1.0241252	-1.4267770	-3.5133961
H	-2.6363112	1.6127090	-2.7797671
H	-1.0645982	0.8903670	-3.1667321
H	-4.6946512	-5.6859210	-0.2777701
H	-5.5555922	-4.1633520	-0.6239121
H	-4.2976592	-4.2109890	0.6468889
P	0.9648288	-3.2061500	0.5058179
C	1.8059178	-4.7036170	1.1170649
H	1.6701638	-4.7858380	2.1996059
H	1.3965408	-5.5952540	0.6274379
H	2.8762938	-4.6279270	0.9055929
C	1.1458408	-3.2615830	-1.3029071
H	0.7610538	-4.2116600	-1.6934121
H	0.5914268	-2.4249430	-1.7421651
H	2.2014858	-3.1452850	-1.5587801
C	-0.8108652	-3.5193110	0.8046779
H	-1.1470512	-4.4297270	0.2910159
H	-0.9825602	-3.6112150	1.8825059
H	-1.3983632	-2.6688370	0.4343499
H	-0.8494262	-0.1821620	-0.0822141
H	1.3942938	2.7933280	1.5300409
C	2.5344928	2.6062970	-1.2207241
C	1.4580258	3.4817500	-1.8422791
C	3.4245708	3.4158170	-0.2861991
C	3.3911998	1.9635280	-2.3085961

H	0.7976338	2.9111940	-2.5099711
H	0.8450418	3.9839160	-1.0835311
H	1.9376508	4.2563970	-2.4509151
H	4.1477288	2.7652150	0.2213949
H	3.9896918	4.1524040	-0.8689241
H	2.8371718	3.9640710	0.4618619
H	3.8429788	2.7597850	-2.9137241
H	4.2047038	1.3742690	-1.8704861
H	2.7968628	1.3220200	-2.9656631
H	-0.4827302	4.1774660	2.1611009
H	2.3742048	1.0532940	2.9399559
H	2.6806898	0.9448110	0.0005989
C	-1.9261612	-0.3156810	3.9247139
C	-2.8371882	1.1788940	1.7735519
H	-1.5238392	-0.8637580	4.7735669
H	-3.2168932	1.7940720	0.9603429
C	-3.7401922	0.5177680	2.5972649
C	-3.2868002	-0.2401440	3.6746349
H	-4.8068502	0.6111290	2.4034979
H	-3.9943882	-0.7498640	4.3239869
C	4.7306058	-1.6471820	-0.7871591
F	3.7953008	-1.1734540	-1.6157111
F	4.2184628	-2.7366460	-0.1895211
F	5.7765498	-2.0257730	-1.5000341
S	5.1998338	-0.3793920	0.4606069

O	5.8166478	0.6734570	-0.3453541
O	6.0223108	-1.1073150	1.4128099
O	3.8515658	0.0230210	0.9872319

Zero-point correction= 0.672483 (Hartree/Particle)

Thermal correction to Energy= 0.721108

Thermal correction to Enthalpy= 0.722052

Thermal correction to Gibbs Free Energy= 0.590449

Sum of electronic and zero-point Energies= -3051.430531

Sum of electronic and thermal Energies= -3051.381906

Sum of electronic and thermal Enthalpies= -3051.380961

Sum of electronic and thermal Free Energies= -3051.512565

A-int9

C	-0.7063043	1.3182932	3.1504839
C	-1.3128563	1.4137202	1.8959079
C	0.7814197	1.3589842	3.2997949
C	1.5438097	1.2107742	2.0484849
C	0.9872807	1.9945582	0.8769479
C	-0.5354343	1.7737042	0.6369429
C	-1.2223773	2.9593072	-0.0296101
C	-1.7935813	2.5273632	-1.3299081
N	-1.4529703	1.1968302	-1.4868451
C	-0.6045103	0.6739352	-0.4400371
C	-1.3334123	4.1753152	0.5170149
N	1.7054887	1.5242562	-0.3972341
C	0.7967137	0.4950872	-0.9879711

O	1.1541637	-0.2856948	-1.8202481
O	-2.4469823	3.1616272	-2.1389121
O	1.2922247	1.4013922	4.4096799
Au	1.4259627	-0.9205658	1.6675409
C	-1.9785223	5.3726892	-0.0827551
C	-2.0682163	-3.3638638	-2.1745551
C	-3.1493523	-3.4759358	-1.2964511
C	-3.8351723	-2.3266158	-0.8941621
C	-3.4207953	-1.0843238	-1.3655781
C	-2.3303143	-0.9563018	-2.2235581
C	-1.6617793	-2.1165248	-2.6217631
C	-1.8438813	0.4038952	-2.6412281
O	-3.4417433	-4.7303488	-0.8782011
C	-4.4926153	-4.8867478	0.0455619
H	-2.4091853	5.1539822	-1.0611981
H	-2.7639643	5.7542602	0.5815859
H	-1.2447333	6.1837702	-0.1827131
H	-1.5526483	-4.2726728	-2.4766681
H	-4.6846643	-2.3870348	-0.2204901
H	-3.9557343	-0.1884728	-1.0487481
H	-0.8019473	-2.0373018	-3.2863581
H	-2.6185953	0.9938732	-3.1477121
H	-0.9972773	0.3047042	-3.3380941
H	-4.5577203	-5.9540928	0.2648059
H	-5.4526513	-4.5484638	-0.3687991

H	-4.2946563	-4.3391008	0.9791569
P	1.0007597	-3.1722278	1.0646049
C	1.9125127	-4.4987868	1.9262059
H	1.7420397	-4.4275108	3.0045469
H	1.5877667	-5.4832268	1.5686499
H	2.9826917	-4.3756888	1.7344279
C	1.2630167	-3.5257688	-0.7051331
H	0.9214897	-4.5407968	-0.9431421
H	0.7015557	-2.7976178	-1.3019041
H	2.3225547	-3.4186108	-0.9472481
C	-0.7638503	-3.5891048	1.3170049
H	-0.9886743	-4.5999448	0.9527489
H	-1.0122993	-3.5132208	2.3804419
H	-1.3828333	-2.8697498	0.7642099
H	-0.9740853	-0.2959038	-0.0742051
H	1.1886457	3.0700512	0.9685429
C	2.3208297	2.5752972	-1.3996741
C	1.2472177	3.4554422	-2.0055801
C	3.3269517	3.3775132	-0.5870631
C	3.0413817	1.8077932	-2.5003981
H	0.5069467	2.8739312	-2.5713311
H	0.7278787	4.0752432	-1.2688741
H	1.7364177	4.1268292	-2.7202011
H	4.0839897	2.7229832	-0.1423521
H	3.8365047	4.0692662	-1.2666091

H	2.8570877	3.9791702	0.1986849
H	3.5983307	2.5437192	-3.0914821
H	3.7726047	1.0920202	-2.1111481
H	2.3464387	1.2951552	-3.1705961
H	-0.8903953	4.3082642	1.5101349
H	2.6041967	1.4296592	2.2109049
H	2.5836387	0.9975262	-0.0952321
C	-1.4783393	1.0787822	4.2890589
C	-2.6943153	1.2219962	1.8020779
H	-0.9553073	1.0257142	5.2412339
H	-3.1876083	1.3067782	0.8340669
C	-3.4537303	0.9532642	2.9326569
C	-2.8475123	0.8956092	4.1871639
H	-4.5272693	0.8062742	2.8365509
H	-3.4444753	0.7030492	5.0754119
C	4.7372757	-1.7957348	-0.5944051
F	3.7591857	-1.6519208	-1.4936861
F	4.2593067	-2.5613838	0.3984939
F	5.7432767	-2.4389558	-1.1622211
S	5.2617647	-0.1569548	0.0413819
O	5.7296487	0.5411422	-1.1562921
O	6.2222867	-0.4651218	1.0869619
O	3.9520377	0.3674942	0.5484969

Zero-point correction= 0.675444 (Hartree/Particle)

Thermal correction to Energy= 0.723810

Thermal correction to Enthalpy= 0.724754

Thermal correction to Gibbs Free Energy= 0.594017

Sum of electronic and zero-point Energies= -3051.456908

Sum of electronic and thermal Energies= -3051.408542

Sum of electronic and thermal Enthalpies= -3051.407598

Sum of electronic and thermal Free Energies= -3051.538334

A-ts8

C	0.8856568	-0.7369663	2.9460918
C	1.6504548	-1.1727943	1.8551748
C	-0.5940202	-0.8986283	3.0059488
C	-1.2658472	-1.4504733	1.7954448
C	-0.4290592	-2.2793283	0.8254278
C	1.0189818	-1.7985403	0.6228308
C	1.9169408	-2.8721533	0.0190178
C	2.6303858	-2.2899823	-1.1529502
N	2.0875648	-1.0394763	-1.3571812
C	0.9203488	-0.7993103	-0.5458522
C	2.0728628	-4.1110803	0.4985988
N	-1.1468912	-2.0157593	-0.4753092
C	-0.3391602	-1.1834583	-1.3040552
O	-0.6094222	-0.8052693	-2.4155972
O	3.5400688	-2.7630373	-1.8111972
O	-1.2233672	-0.5751283	4.0025328
Au	-1.8549802	0.7238617	1.1482488
C	2.9401688	-5.1850283	-0.0533612

C	1.6486058	3.5215147	-2.2743742
C	2.4995168	3.9480277	-1.2518812
C	3.3524198	3.0312447	-0.6323822
C	3.3388808	1.7009497	-1.0424182
C	2.4939428	1.2612317	-2.0596522
C	1.6427938	2.1904907	-2.6631062
C	2.4704908	-0.1843963	-2.4677772
O	2.3992978	5.2565257	-0.9085622
C	3.2358288	5.7314367	0.1196948
H	3.4994338	-4.8445473	-0.9259952
H	3.6446418	-5.5322453	0.7128778
H	2.3314778	-6.0571053	-0.3262452
H	0.9939428	4.2545677	-2.7405542
H	4.0212798	3.3377557	0.1663718
H	3.9974938	0.9839247	-0.5518072
H	0.9635438	1.8584837	-3.4481372
H	3.4592288	-0.5422933	-2.7824292
H	1.7821298	-0.3287263	-3.3118582
H	3.0162398	6.7947377	0.2332748
H	4.2984758	5.6107957	-0.1327042
H	3.0362628	5.2195897	1.0733788
P	-1.6168152	2.9878787	0.6264878
C	-2.7327142	4.1797567	1.4348528
H	-2.6096802	4.1174377	2.5202538
H	-2.5043852	5.1980667	1.0984468

H	-3.7683642	3.9328727	1.1879238
C	-1.8007392	3.2835807	-1.1614872
H	-1.5886692	4.3332447	-1.3987562
H	-1.0978342	2.6357497	-1.6985622
H	-2.8176792	3.0232077	-1.4664942
C	0.0607618	3.5870077	1.0263958
H	0.2215248	4.6026977	0.6407978
H	0.1993938	3.5723227	2.1126668
H	0.8005428	2.9152627	0.5737318
H	0.8542478	0.2544977	-0.2277662
H	-0.4552822	-3.3500813	1.0550338
C	-2.0729442	-3.0711653	-1.0740662
C	-1.1965582	-4.1753913	-1.6519262
C	-2.9810992	-3.6017733	0.0280108
C	-2.9421102	-2.4423733	-2.1559332
H	-0.5171762	-3.7845163	-2.4201392
H	-0.5975292	-4.6774013	-0.8809972
H	-1.8364552	-4.9305253	-2.1228712
H	-3.6304062	-2.8098923	0.4195278
H	-3.6297492	-4.3676383	-0.4105532
H	-2.4302962	-4.0787953	0.8480778
H	-3.7253192	-3.1626813	-2.4171552
H	-3.4515362	-1.5501503	-1.7827132
H	-2.3748362	-2.1921843	-3.0533352
H	1.4956768	-4.3729643	1.3920478

H	-2.1933252	-1.9517453	2.0915098
H	-1.7359402	-1.0975463	0.4129148
C	1.5037898	-0.1286303	4.0429608
C	3.0342428	-0.9739023	1.8932378
H	0.8656128	0.1728737	4.8701818
H	3.6565088	-1.3270003	1.0735568
C	3.6383088	-0.3524353	2.9783288
C	2.8730548	0.0727267	4.0623288
H	4.7171418	-0.2134923	2.9824458
H	3.3471148	0.5485707	4.9171918
C	-5.0087032	1.0645917	-0.8710042
F	-3.9102482	0.8344737	-1.6084512
F	-4.7670822	2.1850797	-0.1651222
F	-6.0135432	1.3106827	-1.6923892
S	-5.3787682	-0.3520923	0.2458608
O	-5.6566992	-1.4412313	-0.6903502
O	-6.4726352	0.1504387	1.0651978
O	-4.0794102	-0.5168193	0.9605728

Zero-point correction= 0.668033 (Hartree/Particle)

Thermal correction to Energy= 0.716955

Thermal correction to Enthalpy= 0.717899

Thermal correction to Gibbs Free Energy= 0.584216

Sum of electronic and zero-point Energies= -3051.407973

Sum of electronic and thermal Energies= -3051.359051

Sum of electronic and thermal Enthalpies= -3051.358107

Sum of electronic and thermal Free Energies= -3051.491790

A-ts9

C	-1.0475529	-2.0284647	-0.6144175
C	-1.2133539	-1.2546617	0.5426425
C	-0.0791139	-1.5946467	-1.6665405
C	0.9745191	-0.6637267	-1.1990175
C	0.7587211	0.1871083	-0.0842545
C	-0.6140559	0.1499883	0.5476355
C	-0.7250309	0.8376463	1.8836025
C	-1.9983099	1.6117613	1.8943225
N	-2.4312989	1.6733893	0.5884835
C	-1.5697359	1.0017973	-0.3555455
C	0.1633101	0.7515993	2.8793805
N	0.5481161	2.1592373	-0.8375505
C	-0.8261189	2.0136323	-1.2233515
O	-1.3685729	2.6197383	-2.1119405
O	-2.5914949	2.0956043	2.8434415
O	-0.0781869	-2.0906747	-2.7813315
Au	2.4826981	-2.0002207	-0.2468145
C	0.0994221	1.4557113	4.1883325
C	-5.4482439	0.0463773	-2.4498945
C	-5.7591089	-1.1026067	-1.7180775
C	-5.4692079	-1.1555087	-0.3524545
C	-4.8653489	-0.0626257	0.2586595
C	-4.5348449	1.0821333	-0.4630105

C	-4.8324589	1.1200343	-1.8273145
C	-3.7426339	2.1746953	0.1981295
O	-6.3307609	-2.1118817	-2.4178305
C	-6.5668859	-3.3235097	-1.7459815
H	-0.8137739	2.0462523	4.2838905
H	0.1450331	0.7357823	5.0149915
H	0.9733131	2.1108623	4.3034175
H	-5.6769369	0.0577473	-3.5122795
H	-5.6960829	-2.0393617	0.2369495
H	-4.6251259	-0.1080717	1.3220385
H	-4.5533559	1.9959263	-2.4119585
H	-4.2033429	2.5297183	1.1282045
H	-3.6269359	3.0350203	-0.4759345
H	-6.9769679	-4.0147047	-2.4851275
H	-7.2929829	-3.2039017	-0.9287255
H	-5.6369399	-3.7454847	-1.3360585
P	4.4409631	-3.0991367	0.4025315
C	5.4130521	-3.5920237	-1.0554825
H	5.5631211	-2.6947297	-1.6653805
H	6.3796041	-4.0092507	-0.7487185
H	4.8606291	-4.3328187	-1.6412155
C	4.3307011	-4.6043477	1.4315465
H	5.3328781	-4.9962567	1.6425765
H	3.8276861	-4.3710607	2.3747245
H	3.7470831	-5.3668047	0.9069725

C	5.5435371	-1.9796117	1.3232385
H	6.4989941	-2.4756187	1.5321555
H	5.7003211	-1.0786207	0.7210275
H	5.0672871	-1.6787537	2.2611875
H	-2.1768289	0.3768123	-1.0281915
H	1.6108191	0.5928593	0.4558785
C	0.9477421	3.5106003	-0.2390505
C	-0.2274769	4.1857413	0.4552715
C	2.0570191	3.2705383	0.7733805
C	1.4536051	4.3752703	-1.3891755
H	-1.0675689	4.3778553	-0.2215365
H	-0.5830439	3.6154543	1.3215975
H	0.1166341	5.1558083	0.8310725
H	2.9064621	2.7396263	0.3373645
H	2.4093151	4.2391093	1.1490575
H	1.6893841	2.6903903	1.6296305
H	1.7389151	5.3650993	-1.0123895
H	2.3383761	3.9171283	-1.8493515
H	0.6776901	4.5045653	-2.1524915
H	1.0444821	0.1235193	2.7054465
H	1.1863821	1.9942603	-1.6267275
C	-1.7278329	-3.2317607	-0.7632205
C	-2.0465439	-1.7166877	1.5553255
H	-1.5738409	-3.7930157	-1.6822615
H	-2.1831499	-1.1287387	2.4610845

C	-2.7090569	-2.9358797	1.4117105
C	-2.5631739	-3.6879977	0.2510295
H	-3.3498359	-3.2924217	2.2155515
H	-3.0890489	-4.6341087	0.1429345
C	5.6398261	1.9398423	-1.2897605
F	5.2571201	3.1162413	-0.7992155
F	6.0737461	2.1153143	-2.5281795
F	6.6390251	1.4736183	-0.5464325
S	4.2388501	0.7580253	-1.2556095
O	3.9337241	0.6469563	0.1882835
O	4.7908781	-0.4666607	-1.8516355
O	3.1925531	1.4403473	-2.0427365
H	1.6986301	-0.3503897	-1.9605255

Zero-point correction= 0.672500 (Hartree/Particle)

Thermal correction to Energy= 0.721711

Thermal correction to Enthalpy= 0.722655

Thermal correction to Gibbs Free Energy= 0.587173

Sum of electronic and zero-point Energies= -3051.431293

Sum of electronic and thermal Energies= -3051.382082

Sum of electronic and thermal Enthalpies= -3051.381138

Sum of electronic and thermal Free Energies= -3051.516620

A-int10

C	-0.4998859	-2.4584815	-1.8482939
C	-1.4092409	-1.8173475	-1.0051969
C	0.9628011	-2.1825575	-1.7701739

C	1.3895231	-1.0053905	-0.9460329
C	0.5793661	-0.8271815	0.3295201
C	-0.9720899	-1.0237065	0.2113131
C	-1.5720469	-1.6789815	1.4498421
C	-2.5639209	-0.7574055	2.0561711
N	-2.5126449	0.4125585	1.3260201
C	-1.5772019	0.3886275	0.2226501
C	-1.2718739	-2.9109075	1.8768101
N	0.7944161	0.5975475	0.8473141
C	-0.4594409	1.3540015	0.5321861
O	-0.5212989	2.5439285	0.5672481
O	-3.3068729	-0.9360875	3.0057761
O	1.7381661	-2.8177305	-2.4664449
Au	3.5199051	-1.0039605	-0.7664109
C	-1.8201099	-3.6035225	3.0730051
C	-5.0057719	2.8241615	-1.6601619
C	-6.0471249	1.9100285	-1.8436129
C	-6.2412559	0.8817795	-0.9172849
C	-5.3944829	0.7855025	0.1825261
C	-4.3578299	1.6953985	0.3788461
C	-4.1704209	2.7124145	-0.5608459
C	-3.4232409	1.5269595	1.5423741
O	-6.8097069	2.1010935	-2.9455539
C	-7.8675309	1.2045235	-3.1797339
H	-2.5434689	-2.9823675	3.6037711

H	-2.3023219	-4.5439015	2.7772871
H	-1.0065219	-3.8805665	3.7560951
H	-4.8744709	3.6098625	-2.3994829
H	-7.0468769	0.1636075	-1.0379899
H	-5.5419839	-0.0131415	0.9114451
H	-3.3517049	3.4194975	-0.4260449
H	-3.9602059	1.2829495	2.4667811
H	-2.8425639	2.4440215	1.7143031
H	-8.3481409	1.5260995	-4.1057069
H	-8.6072359	1.2264045	-2.3665879
H	-7.5064299	0.1732985	-3.3040289
P	5.8859451	-0.9602285	-0.7100499
C	6.6366411	-0.3043895	-2.2368039
H	6.2531551	0.7085995	-2.3933839
H	7.7304211	-0.2952225	-2.1560619
H	6.3358671	-0.9265775	-3.0856109
C	6.6897201	-2.5937375	-0.5058969
H	7.7820331	-2.4956355	-0.5230339
H	6.3814691	-3.0395825	0.4450261
H	6.3728821	-3.2589785	-1.3153039
C	6.6277621	0.0482935	0.6170711
H	7.7208631	0.0591825	0.5279081
H	6.2237991	1.0642715	0.5507151
H	6.3451431	-0.3691665	1.5895641
H	-2.0639109	0.6833945	-0.7200979

H	0.9410351	-1.5080085	1.1064061
C	1.3208051	0.8047815	2.3196661
C	0.2777611	0.3235445	3.3099581
C	2.6224371	0.0294795	2.4500171
C	1.6039081	2.2877135	2.5256981
H	-0.6640179	0.8806795	3.2203661
H	0.0664021	-0.7479275	3.2236441
H	0.6638101	0.5046955	4.3189501
H	3.3842431	0.4207295	1.7644211
H	2.9864511	0.1720245	3.4742961
H	2.5053251	-1.0481965	2.2916501
H	2.0833051	2.3872175	3.5063841
H	2.2998171	2.6788375	1.7778611
H	0.6962201	2.8945115	2.5305141
H	-0.5417459	-3.4719875	1.2827321
H	1.5220731	1.0851875	0.2345121
C	-0.9649039	-3.2786895	-2.8832929
C	-2.7791269	-1.9723005	-1.2426879
H	-0.2199829	-3.7586465	-3.5132149
H	-3.5031349	-1.4695285	-0.6001009
C	-3.2312369	-2.7640065	-2.2872369
C	-2.3213369	-3.4364755	-3.1040609
H	-4.3003759	-2.8629495	-2.4611609
H	-2.6760409	-4.0664625	-3.9160689
C	3.5857211	4.2929445	-0.9661189

F	2.8798911	4.8057315	0.0371061
F	3.0186721	4.6419435	-2.1114909
F	4.8133861	4.7947435	-0.9232089
S	3.6511521	2.4671245	-0.8138139
O	4.2505251	2.2478265	0.5140691
O	4.4414541	2.0278565	-1.9626599
O	2.2047711	2.1094475	-0.8652509
H	1.2126841	-0.1330895	-1.6036219

Zero-point correction= 0.674485 (Hartree/Particle)

Thermal correction to Energy= 0.723560

Thermal correction to Enthalpy= 0.724504

Thermal correction to Gibbs Free Energy= 0.588916

Sum of electronic and zero-point Energies= -3051.451442

Sum of electronic and thermal Energies= -3051.402367

Sum of electronic and thermal Enthalpies= -3051.401423

Sum of electronic and thermal Free Energies= -3051.537011

A-ts10

C	-0.6573379	-0.6773634	-2.6807986
C	-1.5223279	-0.7907184	-1.5734176
C	0.8298151	-0.7021744	-2.5345256
C	1.2127831	-0.5218514	-1.0933696
C	0.4600941	-1.5191654	-0.2166226
C	-1.0222159	-1.1796714	-0.1898696
C	-1.8996409	-2.2440744	0.4482134
C	-2.7669369	-1.5788614	1.4673394

N	-2.2634289	-0.3152354	1.6380124
C	-1.0765339	-0.0512084	0.8624194
C	-1.9207399	-3.5367234	0.1069774
N	1.0309041	-1.2172654	1.1179944
C	0.1542061	-0.2781874	1.7529394
O	0.2901721	0.1546136	2.8651234
O	-3.7620949	-2.0169634	2.0230714
O	1.5948811	-0.7744514	-3.4756886
Au	3.4257831	-0.2042124	-1.0197256
C	-2.7590489	-4.6036924	0.7174444
C	-3.9268359	3.3192686	-0.3204896
C	-5.1649229	2.8323806	-0.7484166
C	-5.7144349	1.7011396	-0.1412366
C	-5.0148169	1.0677606	0.8824834
C	-3.7779439	1.5417586	1.3159174
C	-3.2435959	2.6790016	0.7005914
C	-2.9872759	0.7498766	2.3205484
O	-5.7550279	3.5246136	-1.7549026
C	-7.0021809	3.0741946	-2.2171006
H	-3.4265179	-4.1984924	1.4801684
H	-3.3588399	-5.1050324	-0.0525206
H	-2.1218449	-5.3788944	1.1639044
H	-3.5224409	4.2017546	-0.8091826
H	-6.6804479	1.3118656	-0.4499676
H	-5.4312639	0.1744656	1.3479194

H	-2.2745029	3.0627926	1.0223824
H	-3.6391399	0.2625036	3.0535614
H	-2.2589089	1.3688476	2.8575164
H	-7.3039769	3.7552856	-3.0155536
H	-7.7638339	3.0936176	-1.4240626
H	-6.9432989	2.0528336	-2.6229256
P	5.6472331	0.5961576	-1.0282456
C	5.8351361	2.0426766	-2.1159406
H	5.0758161	2.7730406	-1.8184576
H	6.8399491	2.4691596	-2.0129716
H	5.6624251	1.7530456	-3.1567996
C	7.0077681	-0.5289824	-1.4986886
H	7.9714971	-0.0103394	-1.4312276
H	7.0173011	-1.3958304	-0.8310106
H	6.8588511	-0.8818604	-2.5236206
C	6.0918021	1.1961596	0.6324934
H	7.0649851	1.7008076	0.6076544
H	5.3065501	1.8761236	0.9809354
H	6.1320601	0.3497276	1.3259454
H	-1.0696809	0.9647486	0.4474554
H	0.6594781	-2.5515034	-0.5197126
C	1.7475331	-2.2360564	1.9839534
C	0.7526471	-2.9176074	2.9177864
C	2.4011991	-3.2857954	1.0920844
C	2.8283381	-1.4953344	2.7652044

H	0.2963481	-2.2052254	3.6115924
H	-0.0431349	-3.4149614	2.3473024
H	1.2741251	-3.6797464	3.5089934
H	3.0309601	-2.8371594	0.3115834
H	3.0483781	-3.9095914	1.7187174
H	1.6692731	-3.9538244	0.6215664
H	3.3629061	-2.2122594	3.4004174
H	3.5439491	-1.0174274	2.0841304
H	2.3998521	-0.7103064	3.3908834
H	-1.2481889	-3.8496384	-0.6997306
H	2.0307251	-0.6128494	0.1457704
C	-1.1725809	-0.3930064	-3.9492986
C	-2.8850549	-0.5591144	-1.7686626
H	-0.4692869	-0.3205454	-4.7756796
H	-3.5742809	-0.6246384	-0.9273336
C	-3.3801719	-0.2364604	-3.0253556
C	-2.5282949	-0.1731734	-4.1263996
H	-4.4434689	-0.0379964	-3.1427866
H	-2.9207629	0.0652666	-5.1116456
C	2.4772481	4.0938026	1.5194004
F	1.8493631	4.0084136	2.6832684
F	1.9619991	5.0997596	0.8253954
F	3.7649821	4.3483136	1.7460134
S	2.3225061	2.5241106	0.5873734
O	2.9756591	1.5367746	1.4684754

O	3.0622121	2.7930026	-0.6617846
O	0.8700571	2.3360886	0.4191614
H	0.8575141	0.4897176	-0.8223536

Zero-point correction= 0.667635 (Hartree/Particle)

Thermal correction to Energy= 0.716875

Thermal correction to Enthalpy= 0.717819

Thermal correction to Gibbs Free Energy= 0.582431

Sum of electronic and zero-point Energies= -3051.406462

Sum of electronic and thermal Energies= -3051.357222

Sum of electronic and thermal Enthalpies= -3051.356278

Sum of electronic and thermal Free Energies= -3051.491666

B-1

C	1.5647494	1.5569145	2.1586954
C	2.4000174	0.8126065	3.0149284
C	2.1885524	-0.5361695	3.1638594
C	1.1386984	-1.1849625	2.4692854
C	0.2638284	-0.4339055	1.6218454
C	0.5318784	0.9498615	1.4845844
C	0.9226504	-2.5810315	2.6454144
C	-0.1490596	-3.1967925	2.0434984
C	-1.0130086	-2.4436705	1.2299564
C	-0.8355786	-1.0980705	0.9789894
C	-0.4485836	-1.8434595	-1.8926556
C	-0.7663476	-0.4181565	-2.1452056
N	-1.3581426	0.2697465	-1.1346926

C	-1.8694386	-0.4532865	0.0633394
C	-0.2825756	-3.0586055	-1.9748966
N	-4.1590676	0.3482265	0.6358904
C	-2.8194266	0.4692575	0.8429844
O	-2.3787036	1.3125875	1.6072894
O	-0.4368476	0.0430765	-3.2262066
O	1.8179314	-3.2342875	3.4179934
H	-2.4659336	-1.2887225	-0.3187756
Au	1.7090304	-1.7793245	-1.1177006
C	-0.1685076	-4.5033025	-2.0183086
C	-5.0245806	-0.5730815	-0.1405346
C	-4.9901246	-1.9826285	0.4456524
C	-4.6727476	-0.5732955	-1.6268766
C	-6.4362056	-0.0118925	0.0159364
C	0.1417264	4.4949675	0.2731794
C	1.3939884	4.4411435	-0.3472816
C	1.6166364	3.5221905	-1.3758516
C	0.5979404	2.6518035	-1.7540686
C	-0.6440176	2.6760055	-1.1196036
C	-0.8613296	3.6218015	-0.1122196
C	-1.7115946	1.6765485	-1.4694646
O	2.3221974	5.3035265	0.1241074
C	3.6021404	5.2816195	-0.4597986
H	1.7142744	2.6291885	2.0400754
H	3.1937324	1.3066325	3.5702674

H	2.8006254	-1.1248375	3.8428104
H	-0.1245646	1.5550855	0.8773824
H	-0.3341486	-4.2588955	2.1998714
H	-1.8439046	-2.9670805	0.7563934
H	-4.6541136	1.0027525	1.2339334
H	1.5258914	-4.1410805	3.5657374
H	-1.0794806	-4.9238005	-2.4594046
H	0.6784484	-4.8202445	-2.6352106
H	-0.0517086	-4.9182415	-1.0105646
H	-5.2604296	-1.9640405	1.5072404
H	-5.7054176	-2.6261725	-0.0800886
H	-4.0017606	-2.4490875	0.3582874
H	-4.6770986	0.4480215	-2.0254226
H	-5.4223986	-1.1534825	-2.1771286
H	-3.6972626	-1.0229675	-1.8457766
H	-7.1538686	-0.6385965	-0.5231926
H	-6.7375716	0.0090555	1.0706384
H	-6.5016096	1.0050035	-0.3888126
H	-0.0121206	5.2259705	1.0626564
H	2.5672394	3.4947295	-1.9016626
H	0.7692954	1.9437905	-2.5637566
H	-1.8170446	3.6389845	0.4093014
H	-1.9108306	1.6824835	-2.5467656
H	-2.6480886	1.9247735	-0.9625796
H	4.1963724	6.0323415	0.0639134

H	3.5669084	5.5350975	-1.5284186
H	4.0820624	4.2974515	-0.3421306
P	3.8988624	-1.2021325	-0.5701576
C	4.5509734	-1.9865445	0.9328984
H	4.5120354	-3.0750875	0.8291634
H	5.5889074	-1.6721145	1.0936474
H	3.9394564	-1.6908095	1.7918834
C	4.0613574	0.5939265	-0.3455406
H	5.1010234	0.8501575	-0.1093116
H	3.7567914	1.0977805	-1.2690366
H	3.4001484	0.9271105	0.4628544
C	5.0730994	-1.6340105	-1.8929966
H	6.0815834	-1.3022435	-1.6191846
H	5.0805884	-2.7170295	-2.0480836
H	4.7735994	-1.1490765	-2.8270146

Zero-point correction= 0.641983 (Hartree/Particle)

Thermal correction to Energy= 0.684697

Thermal correction to Enthalpy= 0.685641

Thermal correction to Gibbs Free Energy= 0.566104

Sum of electronic and zero-point Energies= -2090.030548

Sum of electronic and thermal Energies= -2089.987834

Sum of electronic and thermal Enthalpies= -2089.986889

Sum of electronic and thermal Free Energies= -2090.106427

B-ts1

C	0.0325509	-1.9418597	2.4006126

C	-1.2080131	-1.9547787	3.0656806
C	-2.1250761	-0.9665977	2.8125786
C	-1.8322091	0.0573543	1.8807646
C	-0.5700831	0.0887943	1.2150486
C	0.3470699	-0.9462557	1.5075686
C	-2.7857721	1.0752793	1.6038636
C	-2.5415641	2.0547303	0.6560706
C	-1.3091681	2.0840923	0.0121736
C	-0.3167161	1.1361523	0.2501556
C	-0.6331341	-0.2900257	-1.6470164
C	0.8239879	-0.3809087	-1.8116544
N	1.6435989	0.3336723	-1.0208674
C	1.0539529	1.4704473	-0.3127104
C	-1.7583451	-0.7900317	-1.9782664
N	2.5281759	3.2110133	0.6974506
C	1.9895899	1.9673143	0.7996736
O	2.2284759	1.2575293	1.7640706
O	1.1578209	-1.1502267	-2.7032624
O	-3.9403091	1.0412033	2.3039036
H	0.9008249	2.2846613	-1.0336304
Au	-3.5779671	-0.6999717	-0.8803374
C	-1.9451391	-1.6930287	-3.1857284
C	2.5535289	4.2784803	-0.3352224
C	1.1785309	4.9160553	-0.5231604
C	3.1125809	3.7689113	-1.6612224

C	3.5048619	5.3348573	0.2228416
C	4.2885999	-2.5532097	1.2082366
C	4.4961689	-3.6368607	0.3456766
C	4.2545549	-3.4881327	-1.0206914
C	3.8018369	-2.2648697	-1.5074394
C	3.5895099	-1.1814097	-0.6595924
C	3.8493469	-1.3408677	0.7089316
C	3.0999159	0.1339223	-1.2018194
O	4.9303149	-4.7744237	0.9288476
C	5.1894609	-5.8861267	0.1026516
H	0.7637199	-2.7222207	2.5979556
H	-1.4336761	-2.7406187	3.7815746
H	-3.0798131	-0.9473857	3.3307206
H	1.3178879	-0.9552227	1.0272106
H	-3.2984681	2.8072003	0.4382836
H	-1.1228051	2.8726263	-0.7137854
H	3.0901009	3.3997943	1.5219216
H	-4.4103311	1.8768793	2.1934876
H	-0.9912591	-1.8496877	-3.6967334
H	-2.3520211	-2.6581357	-2.8665144
H	-2.6723581	-1.2475027	-3.8722814
H	0.7364769	5.1761933	0.4453586
H	1.2738249	5.8333033	-1.1158004
H	0.4817699	4.2635723	-1.0609134
H	4.1145139	3.3458063	-1.5228914

H	3.1929049	4.6019373	-2.3693234
H	2.4783429	3.0079103	-2.1312594
H	3.6049519	6.1641493	-0.4845344
H	3.1285639	5.7426403	1.1691556
H	4.5035049	4.9144933	0.3923776
H	4.5007849	-2.6899817	2.2656096
H	4.4141419	-4.3108847	-1.7109714
H	3.5994659	-2.1564587	-2.5712504
H	3.6964359	-0.5023537	1.3875846
H	3.3172669	0.2106893	-2.2751504
H	3.5998729	0.9707293	-0.7025834
H	5.5370969	-6.6854687	0.7593296
H	5.9704699	-5.6655187	-0.6380694
H	4.2834189	-6.2210867	-0.4216864
P	-5.7436011	-0.9956577	0.0338796
C	-6.7654591	0.5167293	0.0601536
H	-6.8743421	0.9035403	-0.9576334
H	-7.7576011	0.3036133	0.4748256
H	-6.2772861	1.2814703	0.6710256
C	-5.8235871	-1.6460917	1.7343316
H	-6.8657651	-1.8374147	2.0160406
H	-5.2527441	-2.5776627	1.7983296
H	-5.3823841	-0.9149177	2.4183306
C	-6.7304111	-2.1737147	-0.9493814
H	-7.7357701	-2.2780587	-0.5248074

H	-6.8088241	-1.8208257	-1.9822194
H	-6.2387701	-3.1512897	-0.9538734

Zero-point correction= 0.645393 (Hartree/Particle)

Thermal correction to Energy= 0.687642

Thermal correction to Enthalpy= 0.688587

Thermal correction to Gibbs Free Energy= 0.568113

Sum of electronic and zero-point Energies= -1754.897663

Sum of electronic and thermal Energies= -1754.855413

Sum of electronic and thermal Enthalpies= -1754.854469

Sum of electronic and thermal Free Energies= -1754.974942

B-int1

C	0.8992200	-2.5417790	1.5918406
C	0.4038190	-2.3561870	2.8889316
C	-0.4482200	-1.3069150	3.1406596
C	-0.7892880	-0.4148250	2.1004096
C	-0.2496130	-0.5734050	0.7968726
C	0.5649720	-1.6773320	0.5591146
C	-1.6683720	0.6671090	2.3481236
C	-2.1026500	1.5418680	1.3182426
C	-1.6222040	1.3774500	0.0603076
C	-0.5321000	0.4430790	-0.2805134
C	-0.6872580	-0.1862330	-1.6664384
C	0.6692740	-0.2270500	-2.2847404
N	1.4989750	0.5488200	-1.4954504
C	0.7306860	1.3675710	-0.5896114

C	-1.8416900	-0.6990130	-2.1410484
N	1.9604400	3.1294970	0.6347816
C	1.5006940	1.8501190	0.6345506
O	1.7254090	1.1013520	1.5760296
O	1.0547980	-0.8661150	-3.2471454
O	-2.1150670	0.8180910	3.5799236
H	0.3293800	2.2373960	-1.1310634
Au	-3.5700530	-0.7835020	-0.9939144
C	-1.9358710	-1.3015560	-3.5067704
C	1.7748560	4.3076610	-0.2519684
C	0.3187160	4.7706100	-0.2445284
C	2.2733550	4.0418920	-1.6700424
C	2.6377900	5.4045760	0.3669986
C	4.3611620	-2.0159080	0.9246546
C	4.4016460	-3.1937490	0.1694396
C	4.0075380	-3.1695450	-1.1698014
C	3.5737400	-1.9730130	-1.7360484
C	3.5126680	-0.7976250	-0.9885864
C	3.9213610	-0.8363900	0.3494756
C	2.9610730	0.4636780	-1.5987044
O	4.8243380	-4.2982340	0.8261606
C	4.9621170	-5.4929360	0.0912646
H	1.5663230	-3.3753220	1.3824256
H	0.6826660	-3.0410200	3.6841276
H	-0.8635040	-1.1507360	4.1319506

H	0.9773710	-1.8625710	-0.4282304
H	-2.8411290	2.3099550	1.5450526
H	-1.9639250	2.0313190	-0.7421604
H	2.4703540	3.3114790	1.4937516
H	-2.6970750	1.5870530	3.6580606
H	-1.0035630	-1.2456670	-4.0749904
H	-2.2290620	-2.3566880	-3.4230454
H	-2.7408930	-0.8153670	-4.0730694
H	-0.0282190	4.9279830	0.7837806
H	0.2249310	5.7189570	-0.7862484
H	-0.3554040	4.0554070	-0.7309194
H	3.3306280	3.7524490	-1.6578504
H	2.1832260	4.9584640	-2.2643034
H	1.7111320	3.2601870	-2.1926204
H	2.5705530	6.3191260	-0.2307324
H	2.3050660	5.6440980	1.3848496
H	3.6907880	5.1012180	0.4027306
H	4.6870050	-2.0572040	1.9610056
H	4.0435800	-4.0660430	-1.7815914
H	3.2548840	-1.9559260	-2.7762554
H	3.8765510	0.0671280	0.9552076
H	3.2070700	0.5187820	-2.6667074
H	3.3842360	1.3515570	-1.1141314
H	5.3458250	-6.2418050	0.7863396
H	5.6722010	-5.3768060	-0.7388954

H	3.9982380	-5.8375750	-0.3098464
P	-5.6068810	-1.0435870	0.2565556
C	-5.5729960	-0.3504380	1.9508816
H	-5.3977510	0.7296370	1.8976556
H	-6.5227670	-0.5315090	2.4676736
H	-4.7615340	-0.8171110	2.5197146
C	-6.0915970	-2.7849460	0.5180726
H	-7.0226230	-2.8476370	1.0934736
H	-6.2331900	-3.2739350	-0.4506214
H	-5.2963850	-3.3124890	1.0536776
C	-7.0900100	-0.2828430	-0.4905764
H	-7.9745150	-0.4637140	0.1313376
H	-6.9388950	0.7951850	-0.6020324
H	-7.2563490	-0.7085000	-1.4849024

Zero-point correction= 0.642903 (Hartree/Particle)

Thermal correction to Energy= 0.684929

Thermal correction to Enthalpy= 0.685874

Thermal correction to Gibbs Free Energy= 0.565238

Sum of electronic and zero-point Energies= -2090.031195

Sum of electronic and thermal Energies= -2089.989168

Sum of electronic and thermal Enthalpies= -2089.988224

Sum of electronic and thermal Free Energies= -2090.108860

B-ts2

C	-0.7772721	-1.5804638	2.8221871
C	-1.8626941	-0.8793938	3.3487441

C	-2.3628591	0.2173202	2.6693531
C	-1.7660701	0.6328992	1.4701671
C	-0.6320401	-0.0334278	0.9681571
C	-0.1690251	-1.1590998	1.6469671
C	-2.3516901	1.6996422	0.6789211
C	-1.7276391	2.2292302	-0.4242429
C	-0.4589781	1.7467752	-0.7971009
C	0.0297979	0.4160152	-0.3043549
C	-0.1644221	-0.5184898	-1.5266469
C	1.1265479	-0.4844818	-2.2663959
N	2.0431029	0.2668292	-1.5234639
C	1.5636309	0.4868352	-0.1740569
C	-1.2826371	-1.1998518	-1.8562399
N	0.9835959	2.8497952	0.2224521
C	2.0327769	1.8564292	0.2753601
O	3.1784079	2.1072962	0.5403621
O	1.4141879	-1.0024918	-3.3278889
O	-3.5486551	2.1137162	1.0894941
Au	-3.0998331	-1.2313998	-0.8277779
C	-1.3340481	-2.0703998	-3.0778139
C	5.2255259	-1.8919248	1.0056851
C	4.9413549	-3.2118968	0.6410011
C	4.1932059	-3.4652518	-0.5118369
C	3.7426079	-2.3999708	-1.2856479
C	4.0234359	-1.0792798	-0.9338949

C	4.7693899	-0.8422918	0.2261701
C	3.4803399	0.0555132	-1.7581429
O	5.4288739	-4.1665068	1.4633591
C	5.2213939	-5.5147988	1.1119441
H	-0.3970821	-2.4589868	3.3368331
H	-2.3187361	-1.1968868	4.2826651
H	-3.2184531	0.7650232	3.0551721
H	0.6645359	-1.7290818	1.2402141
H	-2.2051811	3.0219942	-0.9963619
H	-3.8696121	2.8348952	0.5306761
H	-0.4061931	-2.0925898	-3.6524279
H	-1.6063121	-3.0932358	-2.7855059
H	-2.1501881	-1.7297598	-3.7292679
H	5.8138529	-1.7221628	1.9037521
H	3.9706129	-4.4819718	-0.8218929
H	3.1708389	-2.5988918	-2.1915389
H	4.9906509	0.1835782	0.5180001
H	3.5628429	-0.1501148	-2.8303339
H	4.0141779	0.9889422	-1.5463509
H	5.7091599	-6.1141978	1.8825781
H	5.6685749	-5.7520378	0.1367671
H	4.1518219	-5.7678568	1.0854351
P	-5.3046121	-1.4306638	0.0909871
C	-5.5652951	-1.0105688	1.8510321
H	-5.3129651	0.0426422	2.0144131

H	-6.6115221	-1.1789888	2.1324001
H	-4.9167641	-1.6277948	2.4807971
C	-5.9867131	-3.1186878	-0.0564209
H	-7.0157451	-3.1563188	0.3197891
H	-5.9741411	-3.4275318	-1.1062659
H	-5.3670951	-3.8178678	0.5133211
C	-6.5355811	-0.3896848	-0.7714329
H	-7.5404771	-0.5562868	-0.3659789
H	-6.2691091	0.6654162	-0.6516349
H	-6.5329671	-0.6256018	-1.8400219
H	1.9770279	-0.2647628	0.5183831
H	-0.0595761	2.0505072	-1.7628829
H	0.4638429	2.8397522	1.1049561
C	1.3667329	4.2663662	-0.1316699
C	2.2182239	4.2414122	-1.3940099
C	0.0685679	5.0175852	-0.3970819
C	2.1057939	4.9154532	1.0343821
H	3.2117239	3.8211962	-1.2148549
H	1.7333199	3.6664502	-2.1936659
H	2.3494329	5.2667562	-1.7555869
H	-0.6181361	4.9566012	0.4578111
H	0.2936249	6.0764562	-0.5638379
H	-0.4430881	4.6432682	-1.2914859
H	2.3543369	5.9507542	0.7734801
H	1.4741319	4.9451782	1.9321441

H	3.0314009	4.3854292	1.2697061

Zero-point correction= 0.647503 (Hartree/Particle)

Thermal correction to Energy= 0.688211

Thermal correction to Enthalpy= 0.689155

Thermal correction to Gibbs Free Energy= 0.572381

Sum of electronic and zero-point Energies= -1754.916253

Sum of electronic and thermal Energies= -1754.875545

Sum of electronic and thermal Enthalpies= -1754.874601

Sum of electronic and thermal Free Energies= -1754.991375

B-int2

C	0.7190289	-3.0189087	1.1238696
C	-0.1990141	-3.1795147	2.1589596
C	-1.0330811	-2.1275687	2.5045456
C	-0.9626591	-0.9110147	1.8143966
C	-0.0428621	-0.7476497	0.7705836
C	0.7949789	-1.8128377	0.4403796
C	-1.8512381	0.1954963	2.1588156
C	-1.7825741	1.4062653	1.5703486
C	-0.8252631	1.7093643	0.4794116
C	0.1283909	0.5603943	0.0177786
C	0.0467739	0.3857493	-1.5007584
C	1.3394329	0.7982313	-2.0892924
N	2.1543079	1.2859463	-1.0533414
C	1.5712339	1.0674393	0.2468756
C	-1.0282161	-0.1092467	-2.1553284

N	0.0676509	2.9035063	0.9057656
C	1.5054299	2.3768503	0.9680296
O	2.3468749	2.9825983	1.5491876
O	1.7317899	0.7440333	-3.2387124
O	-2.7714691	-0.1129487	3.0950226
Au	-2.7135141	-0.8340027	-1.1664514
C	-1.0692141	-0.2293567	-3.6468374
C	4.9561959	-1.6059367	0.9588476
C	4.8126879	-2.6989457	0.0974056
C	4.3383749	-2.4988387	-1.2029034
C	4.0010779	-1.2149547	-1.6214444
C	4.1295419	-0.1185027	-0.7676924
C	4.6197029	-0.3341867	0.5255046
C	3.6181089	1.2291963	-1.1896474
O	5.1545379	-3.8993987	0.6111606
C	5.0803769	-5.0287297	-0.2289864
H	1.3889819	-3.8306887	0.8501666
H	-0.2541051	-4.1179497	2.7039826
H	-1.7376921	-2.2319787	3.3249936
H	1.5228909	-1.7005257	-0.3643404
H	-2.5332611	2.1649553	1.8005236
H	-3.2812591	0.6710293	3.3335696
H	-0.1932941	0.1836113	-4.1528654
H	-1.1630031	-1.2895027	-3.9196834
H	-1.9793601	0.2476653	-4.0328744

H	5.3405609	-1.7862937	1.9592466
H	4.2394539	-3.3289247	-1.8960904
H	3.6235739	-1.0605107	-2.6318124
H	4.7387609	0.5144763	1.2012516
H	3.8212389	1.4361913	-2.2452874
H	4.0595679	2.0349313	-0.5890134
H	5.4141409	-5.8798327	0.3667636
H	5.7351629	-4.9252557	-1.1048434
H	4.0516539	-5.2124077	-0.5718224
P	-4.6813731	-1.7137927	-0.1177974
C	-4.3998821	-2.7807667	1.3380066
H	-3.9364371	-2.1837477	2.1316296
H	-5.3480761	-3.1954587	1.7002486
H	-3.7194181	-3.5970627	1.0761546
C	-5.7390491	-2.7234427	-1.2126854
H	-6.6310981	-3.0709447	-0.6784874
H	-6.0442611	-2.1300487	-2.0800154
H	-5.1738211	-3.5889077	-1.5717374
C	-5.8173391	-0.4318287	0.5242066
H	-6.6999851	-0.8873567	0.9884086
H	-5.2886571	0.1712353	1.2700656
H	-6.1352101	0.2251483	-0.2910554
H	2.1834979	0.3773763	0.8499706
H	-1.3614551	2.0616723	-0.4071884
H	-0.1639591	3.1297733	1.8813836

C	-0.1274131	4.2479023	0.1195266
C	0.2786109	4.0407223	-1.3257014
C	-1.5966181	4.6188243	0.2574676
C	0.7303719	5.3111913	0.7885696
H	1.3342499	3.7610533	-1.4193934
H	-0.3259261	3.2819413	-1.8359914
H	0.1353669	4.9872843	-1.8575114
H	-1.8838511	4.7481563	1.3090826
H	-1.7530741	5.5812473	-0.2409144
H	-2.2737341	3.8996003	-0.2140914
H	0.4951309	6.2734333	0.3214746
H	0.5111259	5.4024813	1.8596426
H	1.8008819	5.1327963	0.6693776

Zero-point correction= 0.644565 (Hartree/Particle)

Thermal correction to Energy= 0.685422

Thermal correction to Enthalpy= 0.686366

Thermal correction to Gibbs Free Energy= 0.570104

Sum of electronic and zero-point Energies= -2090.035396

Sum of electronic and thermal Energies= -2089.994539

Sum of electronic and thermal Enthalpies= -2089.993595

Sum of electronic and thermal Free Energies= -2090.109857

B-ts3

C	-0.2942590	-2.7448581	1.7735220
C	-1.2523640	-2.4560461	2.7511310
C	-1.8131520	-1.1962541	2.7979090

C	-1.4267900	-0.2154001	1.8621260
C	-0.4709620	-0.5051911	0.8691100
C	0.0917110	-1.7825161	0.8530310
C	-2.0419170	1.0828209	1.8818160
C	-1.6643010	2.1228239	1.0318850
C	-0.6380990	1.9094479	-0.0633650
C	0.0109330	0.4979579	-0.1533690
C	-0.0704780	-0.0109101	-1.5914960
C	1.2569040	0.2183769	-2.2178810
N	2.0894010	0.7933359	-1.2556420
C	1.5162390	0.7635399	0.0686610
C	-1.1700690	-0.5450061	-2.1660000
N	0.4158970	2.8686759	0.4651090
C	1.6543750	2.1447119	0.6584720
O	2.6398600	2.6054949	1.1667430
O	1.6379190	-0.0351401	-3.3450360
O	-2.9744620	1.2619229	2.8029120
Au	-2.9307820	-0.9577471	-1.1329450
C	-1.1971710	-0.9522631	-3.6074610
C	5.1878450	-1.6674521	1.0354880
C	5.0576700	-2.8844711	0.3586210
C	4.4489750	-2.9164651	-0.8992710
C	3.9833650	-1.7339831	-1.4666760
C	4.1150810	-0.5136461	-0.8039300
C	4.7208050	-0.4989231	0.4570310

C	3.5462520	0.7390859	-1.4091830
O	5.5461390	-3.9682881	1.0007860
C	5.5073980	-5.2086111	0.3340940
H	0.1598460	-3.7317241	1.7361700
H	-1.5402120	-3.2114631	3.4769990
H	-2.5445770	-0.9443591	3.5612870
H	0.8360950	-2.0241131	0.0948380
H	-2.4024510	2.9109809	0.8660870
H	-3.3394700	2.1576769	2.7635050
H	-1.4205330	-2.0250821	-3.6827070
H	-2.0292960	-0.4472471	-4.1156150
H	-0.2670810	-0.7458541	-4.1420450
H	5.6696430	-1.6698061	2.0097630
H	4.3484820	-3.8482661	-1.4480780
H	3.5157520	-1.7552821	-2.4509340
H	4.8282050	0.4475499	0.9878300
H	3.7267090	0.7870139	-2.4882830
H	3.9826290	1.6333819	-0.9456990
H	5.9754770	-5.9339411	1.0018280
H	6.0672100	-5.1774501	-0.6107670
H	4.4755600	-5.5270021	0.1270210
P	-4.9568900	-1.6238101	-0.0329320
C	-4.7824430	-3.2100081	0.8574930
H	-3.9791250	-3.1210401	1.5969440
H	-5.7172030	-3.4835281	1.3608850

H	-4.5088880	-3.9981611	0.1491660
C	-6.3911100	-1.8911891	-1.1315150
H	-7.2596620	-2.2369201	-0.5588360
H	-6.6438850	-0.9583131	-1.6445800
H	-6.1371950	-2.6395651	-1.8884950
C	-5.6008950	-0.4889651	1.2499570
H	-6.5204980	-0.8882781	1.6938610
H	-4.8496790	-0.3588741	2.0370270
H	-5.8148960	0.4875349	0.8032410
H	2.0233310	0.0275199	0.7123360
H	-0.9890560	2.2099349	-1.0545170
H	-0.5363310	2.7840489	1.4718620
C	0.5213850	4.2761679	-0.1329560
C	1.2425120	4.1745489	-1.4700820
C	-0.8764960	4.8516809	-0.3270300
C	1.2761250	5.1672409	0.8459960
H	2.2646060	3.7990019	-1.3508680
H	0.7140890	3.5223689	-2.1763950
H	1.3058680	5.1711959	-1.9208450
H	-1.3999600	4.9820449	0.6277090
H	-0.7707200	5.8470939	-0.7705980
H	-1.5012390	4.2671699	-1.0116730
H	1.2630550	6.1929519	0.4607850
H	0.7876260	5.1690969	1.8280070
H	2.3136210	4.8590129	0.9786580

Zero-point correction= 0.639545 (Hartree/Particle)

Thermal correction to Energy= 0.680112

Thermal correction to Enthalpy= 0.681056

Thermal correction to Gibbs Free Energy= 0.564787

Sum of electronic and zero-point Energies= -2089.997329

Sum of electronic and thermal Energies= -2089.956762

Sum of electronic and thermal Enthalpies= -2089.955818

Sum of electronic and thermal Free Energies= -2090.072087

B-int3

C	2.0788242	-2.8818355	0.7613342
C	1.1575902	-3.5803975	1.5614232
C	-0.0099248	-2.9624935	1.9313152
C	-0.2718978	-1.6328295	1.5089902
C	0.6315382	-0.9474115	0.6592112
C	1.8196872	-1.5983745	0.3131512
C	-1.3736638	-0.9007565	1.9996332
C	-1.3672388	0.5734065	1.9944132
C	-0.9066938	1.1444075	0.6414712
C	0.2869472	0.3738895	0.0316202
C	0.0952012	0.1115935	-1.4721928
C	1.3401632	0.5901745	-2.1518648
N	2.0530022	1.3232065	-1.2301058
C	1.4598372	1.3600485	0.0807082
C	-0.9756718	-0.4750355	-2.0362548
N	-0.4936838	2.5349945	0.7240102

C	0.8221062	2.7178295	0.3487102
O	1.4052742	3.7691245	0.1928592
O	1.7132902	0.3878915	-3.2940558
O	-2.3900098	-1.4557545	2.6047912
Au	-2.7200228	-1.0647725	-1.0401478
C	-1.0803788	-0.6879985	-3.5174438
C	5.6642202	-0.2417045	0.8792992
C	5.9150982	-1.3872865	0.1168712
C	5.4053912	-1.4803225	-1.1818898
C	4.6447352	-0.4333115	-1.6976948
C	4.3808552	0.7103435	-0.9436178
C	4.9105362	0.7928955	0.3489302
C	3.4296422	1.7518215	-1.4647078
O	6.6531622	-2.3460575	0.7206422
C	7.0178552	-3.4768725	-0.0359358
H	3.0179362	-3.3550005	0.4824142
H	1.3823882	-4.5852065	1.9054762
H	-0.6829728	-3.4801145	2.6150992
H	2.5495542	-1.1057685	-0.3289768
H	-2.3533138	0.9451195	2.2864172
H	-0.1902408	-0.3540845	-4.0579438
H	-1.2477088	-1.7517775	-3.7316648
H	-1.9600798	-0.1623505	-3.9127898
H	6.0885892	-0.1861845	1.8784652
H	5.6073762	-2.3492675	-1.8017098

H	4.2328572	-0.5087465	-2.7038488
H	4.7351902	1.6905875	0.9429412
H	3.5287872	1.8854695	-2.5468808
H	3.5699242	2.7245145	-0.9794968
H	7.6402012	-4.0964435	0.6119702
H	7.5944042	-3.1983455	-0.9285128
H	6.1381892	-4.0589995	-0.3493038
P	-4.9254928	-1.5812285	-0.2020008
C	-5.1798928	-2.9986115	0.9287792
H	-4.7021238	-2.7936845	1.8925792
H	-6.2505678	-3.1557365	1.1047502
H	-4.7523628	-3.9093975	0.4990272
C	-6.0898358	-1.9114095	-1.5697228
H	-7.1063818	-2.0609285	-1.1875658
H	-6.0858078	-1.0650775	-2.2637838
H	-5.7743878	-2.8045505	-2.1177948
C	-5.6917518	-0.1862855	0.6978412
H	-6.7180398	-0.4303905	0.9963732
H	-5.1040468	0.0467855	1.5926892
H	-5.7072388	0.6982695	0.0527512
H	2.2065462	1.1261615	0.8573062
H	-1.7561608	1.0478615	-0.0467558
C	-1.4885478	3.6518595	0.5693532
C	-1.6014838	3.9712145	-0.9193688
C	-2.8550708	3.2339275	1.1056562

C	-1.0298828	4.8665715	1.3715132
H	-0.6412718	4.3112645	-1.3194308
H	-1.9230788	3.0858695	-1.4865118
H	-2.3386098	4.7656925	-1.0837328
H	-2.8270928	3.0415915	2.1855902
H	-3.5495018	4.0659955	0.9478332
H	-3.2794068	2.3643635	0.5851562
H	-1.7976528	5.6465075	1.3082902
H	-0.9011918	4.6008455	2.4277092
H	-0.0879678	5.2684645	0.9973552
H	-0.6517818	0.8879905	2.7719162
H	-2.3367698	-2.4257485	2.5690682

Zero-point correction= 0.644576 (Hartree/Particle)

Thermal correction to Energy= 0.685488

Thermal correction to Enthalpy= 0.686432

Thermal correction to Gibbs Free Energy= 0.569625

Sum of electronic and zero-point Energies= -2090.043892

Sum of electronic and thermal Energies= -2090.002980

Sum of electronic and thermal Enthalpies= -2090.002036

Sum of electronic and thermal Free Energies= -2090.118843

B-ts4

C	3.2164418	-2.3779508	1.6857284
C	2.5498388	-3.1386138	2.6443574
C	1.2186148	-2.8707628	2.9383894
C	0.6017458	-1.8050208	2.2871114

C	1.2466638	-1.0482598	1.2970694
C	2.5683278	-1.3575218	0.9933504
C	-0.7548392	-1.3395698	2.4516144
C	-0.9335812	0.1041552	2.6657734
C	-0.8111842	0.5672852	1.1539474
C	0.3628048	-0.1522478	0.4367434
C	-0.0739782	-1.0700698	-0.7119296
C	0.8715178	-0.7532538	-1.8396836
N	1.3848818	0.5020652	-1.5815936
C	1.1698288	0.9479792	-0.2276296
C	-1.0607412	-2.0031548	-0.7494086
N	-0.6427542	1.9837952	0.8872874
C	0.3300428	2.2002482	-0.0856246
O	0.5024618	3.2125982	-0.7285216
O	1.0949888	-1.4073668	-2.8396126
O	-1.7487642	-2.0183768	2.0208084
Au	-3.1170402	-1.3443408	-0.5197676
C	-1.0740382	-3.0324458	-1.8565986
C	5.6542788	1.1351262	-0.3550396
C	6.1778748	-0.1359658	-0.6174736
C	5.5138148	-0.9896518	-1.5041116
C	4.3333428	-0.5667668	-2.1099176
C	3.7983078	0.6947932	-1.8499656
C	4.4811838	1.5418012	-0.9692686
C	2.4536368	1.0748502	-2.4039126

O	7.3218618	-0.4441038	0.0303144
C	7.9232618	-1.6896678	-0.2377386
H	4.2557738	-2.5921748	1.4471184
H	3.0673528	-3.9411708	3.1618094
H	0.6813248	-3.4405048	3.6923424
H	3.1008038	-0.8351688	0.1992584
H	-1.9260172	0.3424862	3.0494784
H	-0.0769312	-3.4442168	-2.0412256
H	-1.7619472	-3.8524298	-1.6272826
H	-1.3948632	-2.5875998	-2.8094736
H	6.1981298	1.7842932	0.3261334
H	5.9122188	-1.9724978	-1.7385546
H	3.8057668	-1.2351388	-2.7897526
H	4.0816978	2.5370992	-0.7684766
H	2.3051478	0.6786942	-3.4136736
H	2.3121128	2.1611592	-2.4280946
H	8.8354348	-1.7282848	0.3598674
H	8.1849358	-1.7931068	-1.2996056
H	7.2703448	-2.5264218	0.0516824
P	-5.3333812	-0.5888918	-0.8091566
C	-6.5930952	-1.9032188	-0.7207756
H	-6.5639762	-2.3795268	0.2637604
H	-7.5915372	-1.4843268	-0.8922756
H	-6.3857092	-2.6637868	-1.4795396
C	-5.5917982	0.2002932	-2.4318156

H	-6.6314522	0.5326472	-2.5341016
H	-4.9242332	1.0621052	-2.5325416
H	-5.3591052	-0.5107008	-3.2302656
C	-5.8876672	0.6649332	0.3948744
H	-6.9211662	0.9624032	0.1820124
H	-5.8310602	0.2596672	1.4100414
H	-5.2402542	1.5466192	0.3311024
H	2.1331248	1.1311262	0.2772484
H	-1.7559912	0.2308072	0.6997574
C	-1.8060512	2.9351692	0.9664494
C	-2.5398822	2.9201372	-0.3752556
C	-2.7737112	2.5183322	2.0684034
C	-1.2918892	4.3315112	1.3064734
H	-1.8997432	3.2868002	-1.1822016
H	-2.8696092	1.8989012	-0.6284446
H	-3.4268702	3.5641692	-0.3241486
H	-2.2954582	2.5194352	3.0550254
H	-3.5838772	3.2553112	2.1047094
H	-3.2393402	1.5401402	1.8849734
H	-2.1446882	5.0115932	1.4152804
H	-0.7479962	4.3143052	2.2579794
H	-0.6318762	4.7216962	0.5313174
H	-0.1445102	0.5448992	3.2803314
H	-1.5372792	-2.3971528	1.0345314

Zero-point correction= 0.639829 (Hartree/Particle)

Thermal correction to Energy= 0.679810

Thermal correction to Enthalpy= 0.680754

Thermal correction to Gibbs Free Energy= 0.567487

Sum of electronic and zero-point Energies= -2089.995906

Sum of electronic and thermal Energies= -2089.955925

Sum of electronic and thermal Enthalpies= -2089.954981

Sum of electronic and thermal Free Energies= -2090.068248

B-2

C	2.3000291	-3.1585919	-1.0204535
C	1.1822391	-3.9931189	-1.1086525
C	-0.0744759	-3.4560019	-0.9195995
C	-0.2196889	-2.0844449	-0.6404205
C	0.9010101	-1.2266569	-0.6127075
C	2.1623981	-1.7956229	-0.7944965
C	-1.5145629	-1.5738599	-0.2462305
C	-1.5072429	-0.2906619	0.5121925
C	-0.6634309	0.7752941	-0.1904685
C	0.7677601	0.2775961	-0.4789295
C	1.3848811	0.9555491	-1.7002525
C	2.7261581	1.4833211	-1.3111635
N	2.8082341	1.3687441	0.0533585
C	1.6016851	0.8733451	0.6675875
C	0.8451311	0.9829721	-2.9234335
N	-0.5035939	1.9509471	0.6524865
C	0.7674831	2.0518981	1.1723975

O	1.2156411	2.9442631	1.8614125
O	3.6155711	1.8998141	-2.0323105
O	-2.5632519	-2.2170359	-0.4713405
Au	-4.5626089	-1.5513639	-0.0115365
C	1.4252591	1.6059601	-4.1423705
C	4.9976161	-1.8030279	2.2946925
C	5.7351031	-2.3731899	1.2521205
C	5.9731841	-1.6361149	0.0885085
C	5.4631601	-0.3447879	-0.0218715
C	4.7177971	0.2304541	1.0069745
C	4.5003501	-0.5161299	2.1693005
C	4.0492281	1.5605291	0.7962175
O	6.1736161	-3.6348109	1.4632945
C	6.9817821	-4.2292389	0.4751535
H	3.2992581	-3.5724389	-1.1380215
H	1.3033401	-5.0547219	-1.3034735
H	-0.9642299	-4.0798769	-0.9397425
H	3.0563021	-1.1736409	-0.7583275
H	-2.5319469	0.0590311	0.6833925
H	2.4016591	2.0492731	-3.9413225
H	1.5304501	0.8548061	-4.9351955
H	0.7481681	2.3742371	-4.5366805
H	4.8429251	-2.3908909	3.1957715
H	6.5623501	-2.0495019	-0.7250675
H	5.6372141	0.2273671	-0.9331075

H	3.9407591	-0.0734989	2.9941295
H	4.6669961	2.2335381	0.1920255
H	3.8097201	2.0646371	1.7397575
H	7.2510181	-5.2188969	0.8481985
H	7.8989721	-3.6505559	0.2991655
H	6.4440801	-4.3410549	-0.4781915
P	-6.7235149	-0.8913289	0.4119935
C	-7.8091749	-1.0349349	-1.0389755
H	-7.8428089	-2.0750679	-1.3763845
H	-8.8221869	-0.7045679	-0.7814225
H	-7.4225839	-0.4159989	-1.8540675
C	-6.8277829	0.8459921	0.9393345
H	-7.8733179	1.1233491	1.1169085
H	-6.2552329	0.9866231	1.8612955
H	-6.4075359	1.4936271	0.1635505
C	-7.5206179	-1.8579519	1.7289775
H	-8.5428229	-1.4966719	1.8909605
H	-7.5509379	-2.9147549	1.4476755
H	-6.9503849	-1.7601609	2.6575235
H	1.8306771	0.1594561	1.4739135
H	-1.1509589	1.0455791	-1.1379775
C	-1.4458029	3.1131181	0.6234185
C	-0.8892359	4.1349811	-0.3645035
C	-2.8401789	2.6720421	0.1787365
C	-1.5814549	3.7119381	2.0217505

H	0.1048771	4.4692611	-0.0504515
H	-0.8090459	3.7030861	-1.3711465
H	-1.5429409	5.0133681	-0.4203485
H	-3.3050919	2.0005621	0.9135415
H	-3.4707339	3.5656571	0.1126175
H	-2.8590299	2.1948641	-0.8090145
H	-2.3337809	4.5092531	1.9973045
H	-1.9155069	2.9470241	2.7338805
H	-0.6383029	4.1257711	2.3794325
H	-1.0598919	-0.4917469	1.4987335
H	-0.1281929	0.4937951	-3.0500235

Zero-point correction= 0.645004 (Hartree/Particle)

Thermal correction to Energy= 0.685868

Thermal correction to Enthalpy= 0.686812

Thermal correction to Gibbs Free Energy= 0.567963

Sum of electronic and zero-point Energies= -2090.094543

Sum of electronic and thermal Energies= -2090.053679

Sum of electronic and thermal Enthalpies= -2090.052734

Sum of electronic and thermal Free Energies= -2090.171584

B-ts5

C	-2.8688051	-2.7813508	-1.3632559
C	-2.2642151	-3.9389538	-1.8514329
C	-0.8875651	-3.9773398	-1.9850099
C	-0.1509361	-2.8272178	-1.6934709
C	-0.7434861	-1.6487818	-1.1764679

C	-2.1227891	-1.6649838	-0.9918369
C	1.2860169	-2.7734908	-1.6456269
C	1.9298999	-1.5375448	-2.0748689
C	1.4028839	-0.4359268	-1.5255489
C	0.2425969	-0.6025578	-0.6003109
C	0.6283779	-1.2273338	0.7734061
C	-0.5054471	-0.7924438	1.6739851
N	-1.0409401	0.3383222	1.1034871
C	-0.3058591	0.7371462	-0.0889129
C	1.7225499	-1.9431858	1.1439831
N	-0.8494401	2.9271372	-1.1065509
C	-1.0738901	1.5802562	-1.1000899
O	-1.8630611	1.0748152	-1.8813119
O	-0.8806851	-1.2831518	2.7220331
O	1.9576989	-3.6146038	-0.9598159
H	0.5895139	1.3045242	0.2168291
Au	3.6495159	-1.2093168	0.4915911
C	1.8106209	-2.5950108	2.4991891
C	0.1473859	3.8306502	-0.4773819
C	1.5744309	3.4929112	-0.9181159
C	0.0339959	3.8462692	1.0444181
C	-0.2018951	5.2214882	-1.0032619
C	-5.4255181	0.5012012	-0.1410889
C	-5.8863581	-0.6828048	0.4457211
C	-5.1577111	-1.2714018	1.4830031

C	-3.9747191	-0.6781378	1.9134111
C	-3.4993631	0.4931462	1.3253831
C	-4.2477961	1.0793632	0.2993001
C	-2.1621351	1.0518532	1.7270841
O	-7.0359091	-1.1791098	-0.0608989
C	-7.5508201	-2.3646938	0.4993161
H	-3.9499151	-2.7395448	-1.2484349
H	-2.8649581	-4.8050558	-2.1130909
H	-0.3738061	-4.8669268	-2.3406619
H	-2.6385471	-0.8030278	-0.5858729
H	2.8599359	-1.5728988	-2.6360719
H	1.8692969	0.5436112	-1.6424629
H	-1.4098281	3.3556532	-1.8371889
H	2.2652829	-2.9526878	-0.0766499
H	0.8782319	-2.5253988	3.0647001
H	2.0732609	-3.6535918	2.3783581
H	2.6191979	-2.1534348	3.0973371
H	1.6281389	3.3981022	-2.0095969
H	2.2550899	4.2966182	-0.6124689
H	1.9510259	2.5665812	-0.4627429
H	-0.9737811	4.1484312	1.3524851
H	0.7415179	4.5762072	1.4551061
H	0.2607909	2.8783842	1.5059741
H	0.4678679	5.9707132	-0.5691459
H	-0.0986541	5.2697172	-2.0945449

H	-1.2300091	5.4921922	-0.7356489
H	-6.0148941	0.9433302	-0.9397619
H	-5.5030281	-2.1817628	1.9638301
H	-3.3945901	-1.1443208	2.7081931
H	-3.8925331	1.9940292	-0.1747719
H	-2.0131741	0.9719162	2.8106931
H	-2.0838961	2.1098922	1.4515661
H	-8.4719271	-2.5883778	-0.0413849
H	-7.7818511	-2.2423978	1.5664031
H	-6.8515951	-3.2054888	0.3800171
P	5.7370899	-0.1736238	0.1179301
C	5.8685309	0.5264522	-1.5632259
H	5.0586799	1.2466472	-1.7235629
H	6.8317619	1.0316492	-1.7001039
H	5.7759249	-0.2742328	-2.3040939
C	7.1931379	-1.2555218	0.2871631
H	8.1109349	-0.6931848	0.0794971
H	7.2381549	-1.6571608	1.3038941
H	7.1154229	-2.0936738	-0.4117409
C	6.0710949	1.2369532	1.2239151
H	7.0387979	1.6918312	0.9824001
H	5.2805669	1.9858462	1.1127851
H	6.0811089	0.8978162	2.2640971

Zero-point correction= 0.635948 (Hartree/Particle)

Thermal correction to Energy= 0.676637

Thermal correction to Enthalpy= 0.677581

Thermal correction to Gibbs Free Energy= 0.561580

Sum of electronic and zero-point Energies= -2089.963716

Sum of electronic and thermal Energies= -2089.923026

Sum of electronic and thermal Enthalpies= -2089.922082

Sum of electronic and thermal Free Energies= -2090.038084

B-int4

C	0.4570980	-1.8448237	2.4979803
C	-0.2307870	-1.3131727	3.5871183
C	-1.1202810	-0.2717617	3.3861933
C	-1.3096090	0.2532883	2.1049163
C	-0.5904770	-0.2584577	1.0045543
C	0.2766300	-1.3285777	1.2199043
C	-2.2983830	1.3347273	1.9446293
C	-2.6827530	1.6552873	0.5312993
C	-1.9301080	1.2108883	-0.5232097
C	-0.6760400	0.4186133	-0.3544167
C	-0.3931600	-0.5269127	-1.5103597
C	1.0759870	-0.4856387	-1.7785617
N	1.5796100	0.5571603	-1.0420997
C	0.5387140	1.4378133	-0.5676867
C	-1.2901100	-1.2518947	-2.1880247
N	0.5552310	3.5207823	0.7811933
C	0.9076840	2.2029353	0.6990423
O	1.4180780	1.6255703	1.6443983

O	1.7303420	-1.2217817	-2.4919547
O	-2.8492540	1.9135393	2.8620703
H	0.2301180	2.1398443	-1.3585137
Au	-3.8455190	-0.2924587	0.0477393
C	-1.0231170	-2.1767027	-3.3224807
C	0.4439110	4.5952673	-0.2453367
C	-0.9025450	4.5586903	-0.9627687
C	1.6040990	4.5352503	-1.2365637
C	0.5316800	5.9013033	0.5404763
C	4.4581120	-1.5717757	1.5117633
C	5.3165280	-2.3451757	0.7207463
C	5.4206250	-2.0827137	-0.6453407
C	4.6655520	-1.0539587	-1.2024297
C	3.8195270	-0.2724627	-0.4244537
C	3.7227280	-0.5462117	0.9459983
C	3.0187050	0.8416413	-1.0428587
O	5.9936180	-3.3189837	1.3699933
C	6.8956060	-4.1045667	0.6265643
H	1.1564790	-2.6649607	2.6420703
H	-0.0729940	-1.7152187	4.5841403
H	-1.6860930	0.1653103	4.2054753
H	0.8517460	-1.7518997	0.4001303
H	-3.4516080	2.4187003	0.3994163
H	-2.1532270	1.5603143	-1.5343297
H	0.8123020	3.8626513	1.7032693

H	0.0390150	-2.2126987	-3.5697207
H	-1.3569180	-3.1915087	-3.0689387
H	-1.5964800	-1.8736347	-4.2075307
H	-1.7248860	4.5726933	-0.2374447
H	-1.0007830	5.4397723	-1.6072737
H	-1.0172610	3.6792333	-1.6077517
H	2.5639500	4.5748493	-0.7080897
H	1.5570090	5.3936263	-1.9167127
H	1.5907620	3.6305773	-1.8565567
H	0.4456510	6.7565493	-0.1374367
H	-0.2765810	5.9710603	1.2785533
H	1.4929740	5.9831103	1.0622373
H	4.4037770	-1.7918987	2.5754443
H	6.0731170	-2.6716947	-1.2826367
H	4.7270210	-0.8687867	-2.2737287
H	3.0588960	0.0560643	1.5649893
H	3.3440660	1.0103533	-2.0791877
H	3.1620990	1.7788223	-0.4915837
H	7.3468960	-4.8076317	1.3290373
H	7.6878930	-3.4918977	0.1741823
H	6.3845610	-4.6687377	-0.1664757
P	-5.2359920	-2.1816297	-0.0133407
C	-5.4178380	-2.9606037	1.6198273
H	-5.8824180	-2.2579567	2.3179773
H	-6.0428340	-3.8574607	1.5381983

H	-4.4329860	-3.2376177	2.0078913
C	-4.5542850	-3.4705257	-1.1030957
H	-5.1991380	-4.3568707	-1.0872277
H	-4.4860380	-3.0931627	-2.1286167
H	-3.5507320	-3.7461307	-0.7627847
C	-6.9242730	-1.8643337	-0.6089147
H	-7.4991080	-2.7977117	-0.6108427
H	-7.4188230	-1.1379977	0.0427953
H	-6.8916390	-1.4581587	-1.6242137
H	-2.3433210	-1.1575267	-1.8907197

Zero-point correction= 0.642124 (Hartree/Particle)

Thermal correction to Energy= 0.684236

Thermal correction to Enthalpy= 0.685180

Thermal correction to Gibbs Free Energy= 0.563921

Sum of electronic and zero-point Energies= -2090.054412

Sum of electronic and thermal Energies= -2090.012300

Sum of electronic and thermal Enthalpies= -2090.011356

Sum of electronic and thermal Free Energies= -2090.132615

B-ts6

C	0.5846620	-0.6182094	3.0516145
C	-0.2781050	-0.0747294	2.0961405
C	2.0120310	-0.2282184	3.1122245
C	2.5366830	0.5947896	1.9604945
C	1.6005450	1.4397896	1.3093735
C	0.1437470	1.0418046	1.1415805

C	-0.7535290	2.2600916	1.3194185
C	-1.6043990	2.4218286	0.1172575
N	-1.1983990	1.4636096	-0.7986255
C	-0.1586170	0.5873196	-0.3271665
C	-0.7797960	3.0201166	2.4227905
N	2.0744100	1.5730336	-0.7739155
C	1.0725360	0.6439436	-1.2135765
O	1.2514010	-0.1171534	-2.1371685
O	-2.5049170	3.2126696	-0.0839165
O	2.7536610	-0.5598114	4.0153025
Au	2.9197090	-1.1845194	0.6954055
C	-1.6293010	4.2125426	2.6712055
C	-3.0129890	-2.5632514	-1.5947395
C	-4.1615020	-2.4688484	-0.8003335
C	-4.6410600	-1.2098554	-0.4240795
C	-3.9672550	-0.0658834	-0.8419935
C	-2.8191460	-0.1491864	-1.6284455
C	-2.3551050	-1.4148114	-2.0015795
C	-2.0334130	1.0908706	-1.9431385
O	-4.7315580	-3.6409174	-0.4552695
C	-5.9122910	-3.6077704	0.3161035
H	-2.2547990	4.4572926	1.8116475
H	-2.2736890	4.0340146	3.5410415
H	-1.0046340	5.0763986	2.9295535
H	-2.6720370	-3.5531844	-1.8876125

H	-5.5409090	-1.1105854	0.1756855
H	-4.3406410	0.9153236	-0.5472345
H	-1.4638500	-1.4940624	-2.6262245
H	-2.6829020	1.9546446	-2.1234085
H	-1.3963660	0.9509956	-2.8274065
H	-6.2020100	-4.6465694	0.4812155
H	-6.7238180	-3.0881684	-0.2109735
H	-5.7460080	-3.1232084	1.2885415
P	3.1163390	-2.9101924	-0.8884825
C	3.9957520	-4.4183124	-0.3749645
H	3.4828360	-4.8649844	0.4821145
H	4.0189110	-5.1411214	-1.1987365
H	5.0198080	-4.1740794	-0.0780085
C	3.9379670	-2.3277764	-2.4066765
H	3.9116160	-3.1070734	-3.1772025
H	3.4057140	-1.4413804	-2.7722195
H	4.9786180	-2.0640974	-2.1951175
C	1.4679300	-3.4607114	-1.4339255
H	1.5605260	-4.2342564	-2.2052045
H	0.9089340	-3.8595244	-0.5814725
H	0.9290470	-2.5978514	-1.8419175
H	-0.4973620	-0.4625194	-0.3575545
H	1.7794180	2.5137926	1.3239555
C	2.2338260	2.9239966	-1.4635095
C	0.9827420	3.7706256	-1.3198365

C	3.4207440	3.5890026	-0.7792875
C	2.5397760	2.6797546	-2.9371805
H	0.1216240	3.3271216	-1.8325265
H	0.7137200	3.9443986	-0.2711215
H	1.1701270	4.7471786	-1.7789115
H	4.3209870	2.9630516	-0.8345915
H	3.6481570	4.5366596	-1.2788875
H	3.2188160	3.8130226	0.2743235
H	2.7274420	3.6390586	-3.4327995
H	3.4324610	2.0544736	-3.0646445
H	1.7037360	2.1924596	-3.4506965
H	-0.1125470	2.7231626	3.2403375
H	3.4902450	1.0682336	2.2089035
H	2.9714400	1.0926166	-0.9036895
C	0.1290020	-1.5933524	3.9455875
C	-1.5909810	-0.5478974	2.0298465
H	0.8331540	-1.9764584	4.6803325
H	-2.2862800	-0.1436624	1.2936835
C	-2.0315390	-1.5324194	2.9033265
C	-1.1750690	-2.0522014	3.8742315
H	-3.0570510	-1.8877564	2.8272195
H	-1.5269260	-2.8131124	4.5655135

Zero-point correction= 0.694526 (Hartree/Particle)

Thermal correction to Energy= 0.733949

Thermal correction to Enthalpy= 0.734893

Thermal correction to Gibbs Free Energy= 0.614922

Sum of electronic and zero-point Energies= -1744.456958

Sum of electronic and thermal Energies= -1744.417535

Sum of electronic and thermal Enthalpies= -1744.416591

Sum of electronic and thermal Free Energies= -1744.536562

B-int5

C	0.7788133	-0.6278764	2.8503976
C	0.0769103	0.1064396	1.8878006
C	2.2429093	-0.8833904	2.7108876
C	2.7870653	-0.6225054	1.3496086
C	2.3180893	0.6896566	0.7621076
C	0.7813513	0.9265436	0.8164816
C	0.4204043	2.3980036	0.9872566
C	-0.3967137	2.8368476	-0.1694364
N	-0.4033497	1.7877036	-1.0842394
C	0.2513203	0.5987586	-0.5943304
C	0.7292503	3.1359446	2.0619856
N	2.7161163	0.6938166	-0.7220134
C	1.4367613	0.3150766	-1.4759924
O	1.4775663	-0.1129164	-2.5860464
O	-0.9840337	3.8848306	-0.3472634
O	2.8960973	-1.3932544	3.6035616
Au	1.9247433	-2.2977104	0.2856246
C	0.3923583	4.5623716	2.2998576
C	-3.6401167	-1.3046204	-1.4295074

C	-4.5943467	-0.7470054	-0.5699214
C	-4.5440647	0.6195006	-0.2759074
C	-3.5373407	1.4048536	-0.8292824
C	-2.5727847	0.8580186	-1.6755954
C	-2.6449597	-0.5075284	-1.9722934
C	-1.4164827	1.6953166	-2.1407594
O	-5.5169727	-1.6011674	-0.0865214
C	-6.5342307	-1.0848184	0.7449956
H	-0.1572597	5.0009046	1.4659826
H	-0.2105027	4.6542246	3.2120666
H	1.3060023	5.1412086	2.4850986
H	-3.7212237	-2.3628724	-1.6673144
H	-5.2868767	1.0789696	0.3693656
H	-3.4952627	2.4680856	-0.5929904
H	-1.9122587	-0.9465344	-2.6535744
H	-1.7139767	2.7276936	-2.3533794
H	-0.9515057	1.2788106	-3.0436234
H	-7.1765457	-1.9270914	1.0058376
H	-7.1319667	-0.3244484	0.2250196
H	-6.1208237	-0.6499774	1.6660566
P	0.6118073	-3.9439014	-0.8094964
C	1.0513153	-5.7025214	-0.6176784
H	1.0672163	-5.9652694	0.4442536
H	0.3207693	-6.3348404	-1.1354924
H	2.0462093	-5.8858244	-1.0340784

C	0.4702143	-3.6865044	-2.6102664
H	-0.2624337	-4.3767664	-3.0444494
H	0.1627563	-2.6535954	-2.8077364
H	1.4426483	-3.8472694	-3.0858654
C	-1.1024677	-3.8144584	-0.1940184
H	-1.7555577	-4.5410614	-0.6924564
H	-1.1189047	-3.9905524	0.8866376
H	-1.4837957	-2.8008994	-0.3754324
H	-0.4235027	-0.2729754	-0.6202754
H	2.8263763	1.5480066	1.2173696
C	3.5631163	1.8798546	-1.3053314
C	2.7447663	3.1532436	-1.3083714
C	4.8001923	1.9928676	-0.4269394
C	3.9730803	1.4865796	-2.7174114
H	1.8487633	3.0642086	-1.9344854
H	2.4445753	3.4630516	-0.3015214
H	3.3618533	3.9529506	-1.7316104
H	5.3523813	1.0459206	-0.3755624
H	5.4690663	2.7354156	-0.8746994
H	4.5818463	2.3303736	0.5905986
H	4.6596443	2.2524216	-3.0932244
H	4.5067663	0.5282046	-2.7382674
H	3.1267453	1.4274006	-3.4052424
H	1.2880203	2.6327646	2.8594926
H	3.8832993	-0.6699754	1.3829856

H	3.3176583	-0.1320534	-0.8493784
C	0.0900973	-1.2786474	3.8775566
C	-1.3186287	0.1326746	1.9421766
H	0.6781753	-1.8319574	4.6062696
H	-1.8895967	0.6948686	1.2014066
C	-1.9984967	-0.5466154	2.9448086
C	-1.2944067	-1.2393164	3.9295616
H	-3.0860617	-0.5218434	2.9615076
H	-1.8276677	-1.7538174	4.7246666

Zero-point correction= 0.644541 (Hartree/Particle)

Thermal correction to Energy= 0.685189

Thermal correction to Enthalpy= 0.686134

Thermal correction to Gibbs Free Energy= 0.570822

Sum of electronic and zero-point Energies= -2090.058888

Sum of electronic and thermal Energies= -2090.018239

Sum of electronic and thermal Enthalpies= -2090.017295

Sum of electronic and thermal Free Energies= -2090.132607

B-ts7

C	0.9235055	-0.1944323	3.0480058
C	1.4284045	0.7359007	2.1225618
C	0.8095065	-1.6353483	2.7460408
C	1.2797465	-2.0974953	1.3933078
C	2.1745475	-1.1629903	0.5699258
C	1.8685305	0.3355017	0.7245198
C	3.0031455	1.2148647	0.2094578

C	2.4272565	2.2322247	-0.7157602
N	1.0934805	1.9038667	-0.8793412
C	0.7866485	0.6058197	-0.3422622
C	4.2870525	1.1222907	0.5776088
N	1.7733645	-1.5216053	-0.8338142
C	0.9947605	-0.4703553	-1.3949762
O	0.5400615	-0.4515623	-2.5115642
O	2.9635905	3.1939267	-1.2292332
O	0.3294895	-2.4386103	3.5321838
Au	-0.9439865	-2.3082823	0.7230238
C	5.4169525	1.9687587	0.1157098
C	-3.4785195	1.8029747	-1.8855112
C	-3.9075555	2.3468447	-0.6710412
C	-2.9826825	2.9671077	0.1742708
C	-1.6472385	3.0455117	-0.2131972
C	-1.2087025	2.5150147	-1.4252422
C	-2.1429985	1.8817897	-2.2495882
C	0.2342785	2.5981047	-1.8292162
O	-5.2213265	2.1876917	-0.3874342
C	-5.7157305	2.7601847	0.8042978
H	5.0929595	2.7320497	-0.5928552
H	5.8933725	2.4562817	0.9754328
H	6.1928535	1.3441847	-0.3452422
H	-4.2186415	1.3312137	-2.5286612
H	-3.2911585	3.3991197	1.1216658

H	-0.9272995	3.5307047	0.4465368
H	-1.8123095	1.4517997	-3.1950022
H	0.5989385	3.6327697	-1.8539382
H	0.3677965	2.1848597	-2.8385752
H	-6.7886535	2.5624907	0.8215988
H	-5.5511295	3.8453467	0.8292118
H	-5.2509895	2.3060477	1.6924718
P	-3.1636185	-2.1105433	-0.0137672
C	-4.2789055	-3.5248673	0.2344688
H	-4.3730405	-3.7441603	1.3020228
H	-5.2682425	-3.2920723	-0.1761262
H	-3.8782195	-4.4088403	-0.2702712
C	-3.1358065	-1.7860823	-1.8037662
H	-4.1525945	-1.6173693	-2.1782692
H	-2.5255775	-0.8946613	-1.9940822
H	-2.6870035	-2.6366963	-2.3267742
C	-3.9747895	-0.6722973	0.7483078
H	-4.9189825	-0.4409153	0.2391848
H	-4.1620215	-0.8738813	1.8077468
H	-3.3108875	0.1972047	0.6626918
H	-0.2482735	0.5615347	0.0410598
H	3.2385725	-1.3623183	0.7327738
C	2.5941265	-2.4493983	-1.7103962
C	3.6805315	-1.6254843	-2.3875342
C	3.2095245	-3.5434463	-0.8460062

C	1.6679345	-3.1108353	-2.7283122
H	3.2510585	-0.8289053	-3.0049412
H	4.3555565	-1.1720743	-1.6506162
H	4.2794475	-2.2705683	-3.0402262
H	2.4434115	-4.1706323	-0.3737282
H	3.8037295	-4.1948973	-1.4951942
H	3.8888875	-3.1624403	-0.0758022
H	2.2266775	-3.8941313	-3.2523022
H	0.8160485	-3.5867643	-2.2228642
H	1.2839115	-2.4034683	-3.4636222
H	4.5421395	0.3396377	1.3010418
H	1.7113665	-3.0977413	1.5066658
H	0.8125915	-2.1931343	0.0017798
C	0.4988105	0.2232167	4.3155938
C	1.4734065	2.0804017	2.4985998
H	0.1322685	-0.5367923	5.0010878
H	1.8762085	2.8232557	1.8143788
C	1.0364565	2.4877357	3.7534048
C	0.5509195	1.5587507	4.6715368
H	1.0900195	3.5404217	4.0201508
H	0.2230385	1.8786957	5.6567278

Zero-point correction= 0.637688 (Hartree/Particle)

Thermal correction to Energy= 0.678185

Thermal correction to Enthalpy= 0.679130

Thermal correction to Gibbs Free Energy= 0.564166

Sum of electronic and zero-point Energies= -2090.026201

Sum of electronic and thermal Energies= -2089.985704

Sum of electronic and thermal Enthalpies= -2089.984759

Sum of electronic and thermal Free Energies= -2090.099723

C-1

C	-0.4151076	-1.0895392	2.3343378
C	0.5946514	-0.4657462	1.6136298
C	-1.6271106	-0.4310982	2.5732568
C	-1.7959816	0.8811818	2.1279648
C	-0.7844216	1.4879898	1.3993238
C	0.4127194	0.8282078	1.1122098
C	-0.3511486	1.2966158	-1.8660492
C	0.9883584	0.6992898	-2.0285492
N	1.8399574	0.8198648	-0.9716362
C	1.4292484	1.5426248	0.2555588
C	-1.4278796	1.8844878	-1.9577722
N	3.2768414	3.1224498	0.8119318
C	2.6834914	1.9169568	1.0524308
O	3.1737944	1.1347908	1.8510198
O	1.2521934	0.1213318	-3.0731942
O	-2.6080056	-1.0912942	3.2195488
H	0.9519384	2.4678848	-0.0840562
Au	-1.7435046	-0.3974312	-1.1032232
C	-2.6614646	2.6418098	-2.0476612
C	2.8706444	4.3414218	0.0780728

C	1.6462954	4.9891558	0.7229048
C	2.6402634	4.0662698	-1.4067322
C	4.0574524	5.2937258	0.2076368
C	3.8998454	-2.8858162	1.0550698
C	3.1417864	-3.8776682	0.4279508
C	2.4028564	-3.5635622	-0.7143792
C	2.4202494	-2.2621742	-1.2103912
C	3.1649654	-1.2627452	-0.5854922
C	3.9092874	-1.5961152	0.5501158
C	3.1454094	0.1474898	-1.1124212
O	3.1887484	-5.1080282	0.9962728
C	2.4309724	-6.1326072	0.4059288
H	-2.7311356	1.4041148	2.3079598
H	-0.9525996	2.4977298	1.0201158
H	4.0782444	3.2338458	1.4244598
H	-3.4620916	-0.6981362	2.9478498
H	-2.4384526	3.6777788	-2.3261672
H	-3.3246586	2.2086818	-2.8040342
H	-3.1978876	2.6262768	-1.0869312
H	1.8456344	5.2240738	1.7746898
H	1.3943614	5.9219528	0.2035908
H	0.7626634	4.3412378	0.6875368
H	3.4866614	3.5140498	-1.8321622
H	2.5452394	5.0180938	-1.9427022
H	1.7273884	3.4949318	-1.6028752

H	3.8383004	6.2418778	-0.2946062
H	4.2716544	5.5152628	1.2610578
H	4.9561044	4.8630678	-0.2503422
H	4.4664614	-3.1534722	1.9431398
H	1.8272924	-4.3252882	-1.2334172
H	1.8480494	-2.0178792	-2.1054342
H	4.4695274	-0.8193802	1.0662978
H	3.3656144	0.1577498	-2.1849042
H	3.9061454	0.7555328	-0.6128002
H	2.5882624	-7.0267782	1.0126008
H	2.7543574	-6.3387682	-0.6247722
H	1.3565364	-5.8925002	0.3969098
P	-2.5216946	-2.5713492	-0.7412672
C	-3.3808426	-2.9798222	0.8034908
H	-4.2391356	-2.3112232	0.9293198
H	-3.7133016	-4.0240592	0.7508768
H	-2.7232106	-2.8376852	1.6664108
C	-1.1847316	-3.8066942	-0.8734882
H	-1.5758326	-4.8222262	-0.7348382
H	-0.7127256	-3.7236242	-1.8585822
H	-0.4246846	-3.5927722	-0.1124552
C	-3.7164456	-3.0074802	-2.0457222
H	-4.0785556	-4.0332422	-1.9077042
H	-4.5507276	-2.3019522	-1.9755602
H	-3.2475206	-2.9102972	-3.0296772

C	-6.6949956	0.8876618	0.3293188
F	-7.1611636	1.5080918	1.4032508
F	-7.3164716	-0.2790422	0.2026188
F	-6.9541596	1.6283208	-0.7417812
S	-4.8867486	0.6274768	0.4837048
O	-4.3346186	1.9839078	0.5916458
O	-4.5407736	-0.0841772	-0.7677202
O	-4.7732206	-0.2013582	1.7016048
H	1.5284674	-0.9917742	1.4304188
H	-0.2859286	-2.1004582	2.7174648

Zero-point correction= 0.625393 (Hartree/Particle)

Thermal correction to Energy= 0.673634

Thermal correction to Enthalpy= 0.674579

Thermal correction to Gibbs Free Energy= 0.541211

Sum of electronic and zero-point Energies= -2897.962758

Sum of electronic and thermal Energies= -2897.914516

Sum of electronic and thermal Enthalpies= -2897.913572

Sum of electronic and thermal Free Energies= -2898.046939

C1INT1

C	-1.8213518	2.0497257	-1.8574129
C	-0.6627778	1.4621457	-1.3733939
C	-2.8695048	1.2526597	-2.3274559
C	-2.6860668	-0.1296393	-2.4047199
C	-1.5085648	-0.7057763	-1.9444559
C	-0.4949178	0.0712517	-1.3776649

C	-1.2252638	-2.4205253	0.7009751
C	0.1180192	-2.7800443	0.2076291
N	0.7979702	-1.9981143	-0.7032649
C	0.7837932	-0.5406043	-0.8240099
C	-2.2918068	-2.8398853	1.1696311
N	1.9276232	1.2085657	0.6115001
C	1.1538522	0.0902517	0.5291731
O	0.6783292	-0.3861083	1.5551371
O	0.5336172	-3.8778733	0.5440631
O	-4.0260448	1.8500937	-2.6626579
H	1.5833152	-0.3293003	-1.5392529
Au	-2.3085768	-0.4386643	1.0204281
C	-3.5403658	-3.3309043	1.7185811
C	2.8938232	1.9838657	-0.2076479
C	2.9393742	1.6044497	-1.6798699
C	4.2766662	1.7653607	0.4059981
C	2.5026112	3.4553027	-0.0702079
C	4.6992332	-2.0843983	1.2558481
C	5.7619562	-1.6481153	0.4549341
C	5.5873532	-1.5364223	-0.9236319
C	4.3470692	-1.8524773	-1.4794979
C	3.2817582	-2.2820203	-0.6955979
C	3.4791542	-2.4007233	0.6875171
C	1.9633802	-2.6400353	-1.3270609
O	6.9070312	-1.3421963	1.1118951

C	7.9702262	-0.8142343	0.3593591
H	-3.4939318	-0.7611493	-2.7639229
H	-1.4009798	-1.7870433	-1.9910749
H	1.9915902	1.4648587	1.5939031
H	-4.7619278	1.2363727	-2.4471359
H	-4.3572038	-3.1143803	1.0195301
H	-3.4653498	-4.4136283	1.8738661
H	-3.7606218	-2.8534923	2.6792861
H	1.9645382	1.6905937	-2.1737709
H	3.6202082	2.3003897	-2.1835029
H	3.3448562	0.5959877	-1.8248889
H	4.2951722	2.0812757	1.4570321
H	5.0309272	2.3524467	-0.1330239
H	4.5566922	0.7065377	0.3598971
H	3.2518752	4.0945217	-0.5521139
H	1.5308022	3.6601287	-0.5350879
H	2.4431212	3.7477787	0.9859951
H	4.8642782	-2.1661763	2.3271801
H	6.3942652	-1.2017813	-1.5688369
H	4.2135412	-1.7619113	-2.5585439
H	2.6607052	-2.7474523	1.3154901
H	1.7949952	-3.7194213	-1.2781699
H	1.9694632	-2.3498443	-2.3871919
H	8.7765482	-0.6016043	1.0640921
H	7.6804562	0.1188177	-0.1478739

H	8.3338622	-1.5284813	-0.3932829
P	-3.1835128	1.6365527	1.6589231
C	-4.3633768	2.5387187	0.6084111
H	-5.2561008	1.9163247	0.4923191
H	-4.6198098	3.4847557	1.1014431
H	-3.9558548	2.7346887	-0.3870699
C	-1.8386608	2.8262387	2.0118331
H	-2.2372878	3.7723227	2.3973151
H	-1.1601328	2.3825667	2.7485931
H	-1.2721848	3.0139147	1.0925021
C	-4.0756638	1.4727107	3.2408521
H	-4.4407248	2.4493347	3.5810461
H	-4.9211918	0.7987487	3.0689891
H	-3.4148118	1.0406687	3.9986351
C	-7.2106308	-1.7790993	-0.4691889
F	-8.2184938	-1.0005223	-0.0992569
F	-7.1456308	-2.8179733	0.3618521
F	-7.4424648	-2.2287083	-1.6947299
S	-5.6256358	-0.8617793	-0.4108009
O	-5.8206768	0.2335577	-1.3831429
O	-4.6356108	-1.8756993	-0.8063969
O	-5.5430798	-0.4251763	0.9951891
H	0.1098892	2.0992377	-0.9475289
H	-1.9571538	3.1296657	-1.8325039

Zero-point correction= 0.625480 (Hartree/Particle)

Thermal correction to Energy= 0.673367

Thermal correction to Enthalpy= 0.674312

Thermal correction to Gibbs Free Energy= 0.542313

Sum of electronic and zero-point Energies= -2897.955368

Sum of electronic and thermal Energies= -2897.907481

Sum of electronic and thermal Enthalpies= -2897.906537

Sum of electronic and thermal Free Energies= -2898.038536

C-int1

C	-0.8046086	-0.4536774	2.1281985
C	0.2146684	-0.5118534	1.2467655
C	-2.0799896	0.0743926	1.7291295
C	-2.3057806	0.4155366	0.3414865
C	-1.3208536	0.2320966	-0.5549665
C	0.0566804	-0.1721744	-0.1949555
C	0.5997674	-1.3562994	-1.0257485
C	2.0275524	-1.0472814	-1.3121505
N	2.2794884	0.2248856	-0.8195565
C	1.0546914	0.9601206	-0.6283635
C	-0.0969736	-2.4713164	-1.3286535
N	0.7373744	3.3130346	0.1413445
C	1.1730004	2.0552116	0.4245755
O	1.6200574	1.7899466	1.5330385
O	2.8786784	-1.7235724	-1.8616635
O	-2.9826996	0.2109026	2.6098955
H	0.6851504	1.3703116	-1.5826935

Au	-2.0239066	-2.8545314	-0.6316385
C	0.5182354	-3.5743714	-2.1369085
C	0.3490114	4.0334027	-1.0952485
C	-0.9791306	3.5326376	-1.6576015
C	1.4558284	3.9671626	-2.1455245
C	0.1706664	5.4866836	-0.6612695
C	5.5817664	-0.2244474	1.9961595
C	6.6767984	-0.8653824	1.4063455
C	6.7573034	-0.9620674	0.0184095
C	5.7423864	-0.4138364	-0.7636775
C	4.6586484	0.2367476	-0.1897835
C	4.5853454	0.3186176	1.2057775
C	3.5786004	0.8435656	-1.0447445
O	7.6016354	-1.3627054	2.2666665
C	8.7100144	-2.0292264	1.7189955
H	-3.2998476	0.7259176	0.0375865
H	-1.5103636	0.4042216	-1.6147625
H	0.8552004	3.8993157	0.9613695
H	-3.9577966	0.7383016	2.3010945
H	1.5400114	-3.3646934	-2.4639005
H	0.5176184	-4.4997104	-1.5447365
H	-0.1124126	-3.7868434	-3.0102095
H	-1.7531176	3.5144556	-0.8811445
H	-1.3129056	4.2000436	-2.4610055
H	-0.9013866	2.5283136	-2.0871975

H	2.3967594	4.3552156	-1.7374275
H	1.1813284	4.5784727	-3.0135645
H	1.6349994	2.9483087	-2.5080065
H	-0.1094176	6.1052066	-1.5201925
H	-0.6214666	5.5758586	0.0923345
H	1.1019324	5.8899817	-0.2442375
H	5.5428824	-0.1687734	3.0813185
H	7.5888144	-1.4686983	-0.4625715
H	5.7891424	-0.5150734	-1.8470425
H	3.7274294	0.8101527	1.6651115
H	3.8484624	0.7532047	-2.1079945
H	3.4716214	1.9141106	-0.8193905
H	9.3281514	-2.3510734	2.5599245
H	9.3045484	-1.3682954	1.0711595
H	8.4083444	-2.9131664	1.1382295
P	-4.1431896	-3.5258244	0.2688015
C	-4.5106156	-2.8438784	1.9215595
H	-4.6429206	-1.7618494	1.8314945
H	-5.4285036	-3.2860734	2.3268515
H	-3.6733316	-3.0473234	2.5976385
C	-4.1826866	-5.3365624	0.5435725
H	-5.1345586	-5.6389234	0.9968055
H	-4.0552856	-5.8564964	-0.4111875
H	-3.3586066	-5.6246203	1.2039765
C	-5.6547656	-3.2107454	-0.7019375

H	-6.5216756	-3.6599344	-0.2024505
H	-5.8055146	-2.1297933	-0.7798655
H	-5.5458896	-3.6416654	-1.7018425
C	-5.9778826	2.3862356	-0.0856545
F	-6.4012306	3.4613726	0.5540415
F	-6.7680796	2.1492236	-1.1200125
F	-4.7422306	2.6126136	-0.5357615
S	-5.9837906	0.9300936	1.0315955
O	-5.0001996	1.3888886	2.0900045
O	-5.4165896	-0.1530174	0.2192185
O	-7.3461836	0.8102547	1.5063035
H	1.2050024	-0.8363404	1.5589525
H	-0.6892076	-0.7329044	3.1715135

Zero-point correction= 0.623473 (Hartree/Particle)

Thermal correction to Energy= 0.670876

Thermal correction to Enthalpy= 0.671820

Thermal correction to Gibbs Free Energy= 0.537961

Sum of electronic and zero-point Energies= -2897.954444

Sum of electronic and thermal Energies= -2897.907040

Sum of electronic and thermal Enthalpies= -2897.906096

Sum of electronic and thermal Free Energies= -2898.039955

C-ts2

C	-0.8606655	-0.4921726	2.1831621
C	0.3220165	-0.6231596	1.5737191
C	-1.9948125	0.0653014	1.4557541

C	-1.8275225	0.6796184	0.2314551
C	-0.5222915	0.8104994	-0.3026489
C	0.5753935	-0.1074496	0.1971851
C	0.7888475	-1.2000826	-0.8716949
C	1.9509625	-0.7629886	-1.6828669
N	2.4111315	0.4590264	-1.1662129
C	1.9048735	0.6649174	0.1723621
C	-0.0224575	-2.2578796	-1.1078809
N	0.2403235	2.4683714	0.2829991
C	1.6601295	2.1407504	0.3902181
O	2.5225835	2.9599764	0.5600681
O	2.4679315	-1.2813066	-2.6564939
O	-3.1492465	-0.1150056	2.0424831
Au	-1.9042325	-2.6424206	-0.2624829
C	0.2991365	-3.2455146	-2.1923089
C	6.3708045	0.4920694	1.1929311
C	6.8160295	-0.8095606	0.9454051
C	6.2669355	-1.5409106	-0.1098079
C	5.2832025	-0.9631706	-0.9064459
C	4.8344575	0.3365454	-0.6735629
C	5.3910715	1.0538994	0.3910361
C	3.7491675	0.9287594	-1.5309909
O	7.7783755	-1.2714616	1.7798371
C	8.2683115	-2.5716216	1.5620651
H	-2.6956235	1.0351434	-0.3138039

H	-3.8932845	0.0683194	1.3850391
H	1.2518175	-3.0712636	-2.6971369
H	0.2844165	-4.2592566	-1.7712729
H	-0.5058345	-3.2336786	-2.9403599
H	6.8155515	1.0395684	2.0200951
H	6.6000715	-2.5524146	-0.3228769
H	4.8518455	-1.5303396	-1.7301949
H	5.0431005	2.0674374	0.5896461
H	3.8751355	0.6392654	-2.5795949
H	3.7654235	2.0241494	-1.4746129
H	9.0282765	-2.7495286	2.3255591
H	8.7289865	-2.6715966	0.5688351
H	7.4763375	-3.3277056	1.6630141
P	-4.1422475	-3.3027966	0.3181571
C	-5.0000715	-2.7147726	1.8215091
H	-5.3329025	-1.6834346	1.6690631
H	-5.8764815	-3.3476876	2.0058941
H	-4.3314245	-2.7500956	2.6861571
C	-4.1878115	-5.1265546	0.5067731
H	-5.2152945	-5.4753836	0.6666051
H	-3.7826905	-5.5954176	-0.3958439
H	-3.5676045	-5.4268296	1.3572741
C	-5.3492285	-2.9929486	-1.0152949
H	-6.3169765	-3.4410386	-0.7592959
H	-5.4692595	-1.9116276	-1.1397509

H	-4.9814845	-3.4268916	-1.9505209
C	-5.3334355	2.5288444	-0.0100789
F	-4.4837295	2.7397604	1.0059291
F	-6.2754595	3.4546094	0.0293871
F	-4.6413675	2.6702824	-1.1434109
S	-6.0379195	0.8365504	0.1162581
O	-4.7693345	0.0302774	0.0625891
O	-6.8682635	0.6806074	-1.0683099
O	-6.6647715	0.8073904	1.4338511
H	2.6248725	0.3132054	0.9337551
H	-0.4454435	1.0308354	-1.3684999
H	-0.1691705	2.4628974	1.2233451
C	-0.1304955	3.7724004	-0.4034189
C	0.6399205	3.8704644	-1.7126239
C	-1.6284675	3.7386554	-0.6767999
C	0.1944245	4.9371274	0.5258321
H	1.7118015	4.0228134	-1.5538569
H	0.4982355	2.9773204	-2.3338499
H	0.2606575	4.7279334	-2.2787189
H	-2.2183895	3.5423494	0.2264261
H	-1.9330275	4.7171054	-1.0652129
H	-1.9004355	2.9905894	-1.4284249
H	-0.0832035	5.8765724	0.0336901
H	-0.3886545	4.8696394	1.4537761
H	1.2576995	4.9744494	0.7746101

H	1.1488005	-1.1410996	2.0580071
H	-1.0580445	-0.8892296	3.1754031

Zero-point correction= 0.626281 (Hartree/Particle)

Thermal correction to Energy= 0.672437

Thermal correction to Enthalpy= 0.673381

Thermal correction to Gibbs Free Energy= 0.544054

Sum of electronic and zero-point Energies= -2897.922080

Sum of electronic and thermal Energies= -2897.875925

Sum of electronic and thermal Enthalpies= -2897.874981

Sum of electronic and thermal Free Energies= -2898.004308

C-int2

C	0.0214774	-0.4005731	2.4018504
C	0.9193004	-0.6985520	1.4626314
C	-1.2183366	0.3003809	2.0691824
C	-1.4897926	0.6824590	0.7981384
C	-0.5703036	0.3797349	-0.3199896
C	0.7781814	-0.3155871	0.0147454
C	1.0743514	-1.5127091	-0.8937656
C	2.3625104	-1.2603511	-1.5774616
N	2.7132994	0.0755249	-1.3378136
C	1.9011914	0.6892669	-0.3195396
C	0.2681094	-2.5894361	-1.0358676
N	-0.2187616	1.7234159	-1.0355396
C	1.2718194	1.9429250	-0.8555056
O	1.7791814	2.9908179	-1.1086946

O	3.0574654	-1.9929741	-2.2584446
O	-2.0197746	0.4906509	3.1100854
Au	-1.6229156	-2.7104411	-0.1479026
C	0.6347864	-3.7429361	-1.9190336
C	5.9575384	1.8455259	1.4390524
C	6.3410124	0.6478650	2.0489374
C	5.9928024	-0.5719021	1.4621774
C	5.2716494	-0.5788461	0.2726354
C	4.8917634	0.6096389	-0.3499566
C	5.2377154	1.8207189	0.2555434
C	4.0600624	0.5698729	-1.6011806
O	7.0403634	0.7713339	3.2007274
C	7.4540204	-0.4059271	3.8511614
H	-2.4557546	1.1280949	0.5635884
H	-2.8993766	0.8373259	2.8024634
H	1.5928694	-3.6272011	-2.4327426
H	0.6653224	-4.6594511	-1.3142676
H	-0.1610236	-3.9133201	-2.6564386
H	6.2360354	2.7799559	1.9192884
H	6.2830324	-1.5144031	1.9169954
H	5.0059934	-1.5293921	-0.1907096
H	4.9330654	2.7578420	-0.2111266
H	4.4745344	-0.1220041	-2.3437766
H	4.0008194	1.5667599	-2.0592146
H	7.9959234	-0.0922981	4.7454014

H	8.1239574	-1.0055371	3.2186174
H	6.5978174	-1.0267961	4.1513854
P	-3.8727446	-2.6777521	0.6819414
C	-4.0877696	-2.2818900	2.4484594
H	-3.5113326	-1.3888461	2.7038094
H	-5.1450496	-2.0803410	2.6586754
H	-3.7377186	-3.1250650	3.0528204
C	-4.8493116	-4.2106850	0.4654484
H	-5.8789566	-4.0535881	0.8082274
H	-4.8604676	-4.4932900	-0.5918676
H	-4.3980666	-5.0267351	1.0381914
C	-4.8273816	-1.4201901	-0.2255076
H	-5.8214196	-1.2648791	0.2121594
H	-4.2940066	-0.4692411	-0.1508116
H	-4.9086416	-1.7207351	-1.2758886
C	-5.1572006	2.5753599	0.1501564
F	-3.9866806	3.2293919	0.2486174
F	-6.0982916	3.4549129	-0.1450296
F	-5.0374176	1.7273249	-0.8810276
S	-5.5359006	1.6755779	1.7106144
O	-4.2850536	0.8732169	1.8671824
O	-6.6957926	0.8595859	1.3598894
O	-5.6999746	2.7411509	2.6884964
H	2.5098124	0.9765909	0.5562684
H	-1.0689436	-0.2136731	-1.0927376

H	-0.6794266	2.4648829	-0.4889676
C	-0.7526396	1.8807699	-2.4941076
C	-0.0411036	0.8705449	-3.3737386
C	-2.2563906	1.6522409	-2.4343376
C	-0.4803616	3.3066740	-2.9513076
H	1.0429624	1.0411950	-3.3970486
H	-0.2210426	-0.1644071	-3.0591816
H	-0.4170046	0.9796239	-4.3966686
H	-2.7476066	2.3484769	-1.7440926
H	-2.6676106	1.8340409	-3.4332286
H	-2.5362136	0.6315789	-2.1506636
H	-0.9608726	3.4432269	-3.9261356
H	-0.9169586	4.0417349	-2.2638736
H	0.5838144	3.5238619	-3.0621726
H	1.8522134	-1.2083441	1.7071754
H	0.1646194	-0.6717770	3.4446224

Zero-point correction= 0.627826 (Hartree/Particle)

Thermal correction to Energy= 0.674351

Thermal correction to Enthalpy= 0.675295

Thermal correction to Gibbs Free Energy= 0.545265

Sum of electronic and zero-point Energies= -2897.927325

Sum of electronic and thermal Energies= -2897.880800

Sum of electronic and thermal Enthalpies= -2897.879856

Sum of electronic and thermal Free Energies= -2898.009886

C-ts3

C	-0.2767177	-0.5041186	2.4344835
C	0.6812683	-0.8248246	1.5572135
C	-1.4659487	0.2080334	2.0084835
C	-1.6018257	0.6732484	0.7016525
C	-0.5441587	0.3753864	-0.3382855
C	0.7185973	-0.3968676	0.1237205
C	1.0679383	-1.5519546	-0.8084705
C	2.3188033	-1.1982746	-1.5207485
N	2.6268193	0.1247684	-1.1918975
C	1.8959093	0.5921044	-0.0387445
C	0.2852633	-2.6372176	-1.0003195
N	-0.1114867	1.8190864	-0.6095295
C	1.3089253	1.9496564	-0.3439415
O	1.9149223	2.9863234	-0.3929985
O	2.9975093	-1.8519576	-2.2933145
O	-2.3599697	0.3802504	2.9376355
Au	-1.6466997	-2.7857366	-0.2164535
C	0.6860663	-3.7479176	-1.9222905
C	6.0927033	1.5520584	1.4727415
C	6.7030203	0.3215544	1.7319395
C	6.4149893	-0.7801476	0.9229525
C	5.5242263	-0.6377896	-0.1368205
C	4.9160663	0.5861974	-0.4101545
C	5.2087433	1.6775384	0.4136205
C	3.9226373	0.7032934	-1.5325045

O	7.5530363	0.2970654	2.7864865
C	8.1984653	-0.9165026	3.0838755
H	-2.6149557	0.8849794	0.3572215
H	-3.2461007	0.6767584	2.5426035
H	1.6592503	-3.5990006	-2.3978325
H	0.6994443	-4.6927886	-1.3625365
H	-0.0805927	-3.8827186	-2.6972785
H	6.3326973	2.3920174	2.1196145
H	6.8799833	-1.7447796	1.1040215
H	5.2961593	-1.4939976	-0.7715525
H	4.7275323	2.6361474	0.2188605
H	4.2558113	0.1527904	-2.4193815
H	3.7788303	1.7552584	-1.8125095
H	8.8314123	-0.7271806	3.9531375
H	8.8286873	-1.2572736	2.2499315
H	7.4790333	-1.7103216	3.3317455
P	-3.9716727	-2.8417496	0.3790215
C	-4.4252357	-2.5257426	2.1172315
H	-3.9395877	-1.6136566	2.4700785
H	-5.5101207	-2.3897396	2.2012005
H	-4.1033127	-3.3730316	2.7313645
C	-4.8132757	-4.4257026	0.0123545
H	-5.8851977	-4.3432386	0.2283405
H	-4.6762567	-4.6784886	-1.0437125
H	-4.3824147	-5.2276266	0.6197295

C	-4.9005727	-1.6316936	-0.6191885
H	-5.9377867	-1.5399646	-0.2749995
H	-4.4370407	-0.6473706	-0.5132795
H	-4.8661157	-1.9439396	-1.6685815
C	-5.4853197	2.4182834	0.1038385
F	-4.4532497	3.2226374	0.3845065
F	-6.5394307	3.1644784	-0.1731155
F	-5.1591487	1.7185354	-0.9896385
S	-5.8093607	1.2933424	1.5171575
O	-4.4740737	0.6073554	1.5946755
O	-6.8631357	0.4048584	1.0384915
O	-6.0871627	2.1815344	2.6344695
H	2.5512253	0.6701104	0.8453685
H	-0.9353657	-0.0793766	-1.2529845
H	-0.8777307	1.9444854	0.4099965
C	-0.6549187	2.5196524	-1.8615135
C	0.1133043	1.9766204	-3.0583655
C	-2.1456397	2.2327624	-1.9941395
C	-0.4702887	4.0241804	-1.7074045
H	1.1825423	2.2103084	-2.9936545
H	0.0022493	0.8894004	-3.1572175
H	-0.2742527	2.4367384	-3.9742805
H	-2.7234447	2.6596614	-1.1676635
H	-2.4953657	2.7129394	-2.9146165
H	-2.3866527	1.1671354	-2.0812715

H	-0.9646397	4.5178294	-2.5517995
H	-0.9460757	4.3806074	-0.7861535
H	0.5788543	4.3212214	-1.6944975
H	1.5481573	-1.4011196	1.8811545
H	-0.2387817	-0.8153826	3.4747205

Zero-point correction= 0.622781 (Hartree/Particle)

Thermal correction to Energy= 0.668804

Thermal correction to Enthalpy= 0.669748

Thermal correction to Gibbs Free Energy= 0.540604

Sum of electronic and zero-point Energies= -2897.903598

Sum of electronic and thermal Energies= -2897.857575

Sum of electronic and thermal Enthalpies= -2897.856631

Sum of electronic and thermal Free Energies= -2897.985775

C-int3

C	0.2412650	-0.0739731	2.3439824
C	1.1281350	-0.4224011	1.3947514
C	-0.9393730	0.6778559	1.9673714
C	-0.8461920	1.4368059	0.6731694
C	-0.3465940	0.5366159	-0.4583486
C	0.9266660	-0.2260751	-0.0688326
C	1.0691700	-1.6111531	-0.7212636
C	2.4648320	-1.6863421	-1.2556316
N	2.9901090	-0.4140681	-1.1895256
C	2.0561880	0.5734119	-0.7261076
C	0.1367300	-2.5840091	-0.7252206

N	0.0078280	1.2861419	-1.6598296
C	1.3617610	1.2793379	-1.8942676
O	1.9507670	1.7022579	-2.8710386
O	3.0915500	-2.6529661	-1.6604336
O	-1.9396510	0.7283479	2.6989184
Au	-1.7805010	-2.4418281	0.1043254
C	0.3857240	-3.9076791	-1.3895696
C	6.3654730	1.9654729	0.9469404
C	6.5895670	1.0258249	1.9554114
C	6.0914150	-0.2721231	1.8164524
C	5.3799180	-0.6117621	0.6702814
C	5.1559070	0.3139049	-0.3475486
C	5.6537110	1.6084539	-0.1881696
C	4.3513220	-0.0812001	-1.5568676
O	7.2953400	1.4658099	3.0272854
C	7.5609320	0.5492189	4.0586944
H	-1.8043420	1.9045509	0.4289914
H	-3.1512040	1.0499779	1.9677934
H	1.3845510	-3.9935501	-1.8257386
H	0.2446890	-4.7193211	-0.6629276
H	-0.3695690	-4.0770571	-2.1692816
H	6.7601740	2.9693689	1.0817794
H	6.2573420	-1.0210911	2.5854324
H	4.9957570	-1.6262151	0.5547174
H	5.4799050	2.3466189	-0.9709656

H	4.7563220	-0.9829731	-2.0324326
H	4.3346480	0.7243139	-2.3025516
H	8.1398740	1.0869619	4.8124304
H	8.1492510	-0.3081881	3.7008064
H	6.6356110	0.1742979	4.5203064
P	-4.0554550	-2.4882771	0.8859784
C	-4.4221030	-1.9432811	2.5931694
H	-3.9408580	-0.9860601	2.8050024
H	-5.5044680	-1.8446161	2.7381064
H	-4.0255590	-2.6901091	3.2888234
C	-4.7315110	-4.1914431	0.8649554
H	-5.7810080	-4.1949361	1.1832154
H	-4.6598450	-4.5996391	-0.1482406
H	-4.1479090	-4.8304231	1.5350294
C	-5.2271590	-1.5968331	-0.1970926
H	-6.2463990	-1.6554201	0.2022744
H	-4.9424500	-0.5453441	-0.2775096
H	-5.1920590	-2.0537891	-1.1918866
C	-5.1854300	2.9432209	0.1812434
F	-4.0389980	3.6080729	0.1284404
F	-6.1875310	3.7958079	0.2586124
F	-5.3123840	2.2014039	-0.9083396
S	-5.1944550	1.8623739	1.6659434
O	-3.9426730	0.9946709	1.2861004
O	-6.3887240	1.0523009	1.5725274

O	-4.9138980	2.6973279	2.8123554
H	2.5475040	1.3017289	-0.0597656
H	-1.1334180	-0.1931021	-0.6935086
C	-0.9889880	1.5096419	-2.7502656
C	-0.9372660	0.3007649	-3.6819096
C	-2.3926680	1.6573939	-2.1673226
C	-0.6662810	2.7994499	-3.5010716
H	0.0630800	0.1925919	-4.1149756
H	-1.1817100	-0.6220291	-3.1379336
H	-1.6573500	0.4173559	-4.5011426
H	-2.4772840	2.5583229	-1.5482926
H	-3.0993680	1.7678329	-2.9978066
H	-2.7225840	0.7903999	-1.5791536
H	-1.4572220	2.9902549	-4.2366386
H	-0.6366240	3.6465509	-2.8049556
H	0.2941550	2.7412049	-4.0142346
H	-0.1144360	2.2449489	0.8291774
H	2.0379390	-0.9644291	1.6621774
H	0.3483870	-0.3654661	3.3856234

Zero-point correction= 0.627461 (Hartree/Particle)

Thermal correction to Energy= 0.673543

Thermal correction to Enthalpy= 0.674487

Thermal correction to Gibbs Free Energy= 0.546161

Sum of electronic and zero-point Energies= -2897.977040

Sum of electronic and thermal Energies= -2897.930958

Sum of electronic and thermal Enthalpies= -2897.930014

Sum of electronic and thermal Free Energies= -2898.058340

C-int4

C	0.6757400	0.4421622	2.1435752
C	-0.0021750	0.7849442	1.0369322
C	0.9730410	-0.9677128	2.4311702
C	0.1262730	-1.9587498	1.6705582
C	0.0594620	-1.6157778	0.1811292
C	-0.3639070	-0.1554338	-0.0678858
C	0.1769920	0.4044912	-1.3929888
C	-0.9967070	0.8643152	-2.1987698
N	-2.1301850	0.5611742	-1.4768968
C	-1.8806610	-0.2538628	-0.3132258
C	1.4816870	0.4914472	-1.7281798
N	-0.9419250	-2.3961048	-0.5365348
C	-2.1302220	-1.7278098	-0.6355548
O	-3.2116290	-2.1796948	-0.9768218
O	-1.0129460	1.4355762	-3.2767608
O	1.8064450	-1.3202298	3.2533872
Au	2.9933220	-0.0953218	-0.3850918
C	1.9329990	0.9983292	-3.0686098
C	-6.1089500	1.2744892	0.6993692
C	-5.9549020	2.6306962	0.9984242
C	-4.9934180	3.3855622	0.3232722
C	-4.2041450	2.7744612	-0.6466968

C	-4.3561220	1.4272252	-0.9634058
C	-5.3144060	0.6828962	-0.2693448
C	-3.4724180	0.7808352	-1.9917538
O	-6.7798770	3.1209642	1.9577142
C	-6.6670370	4.4824702	2.2860222
H	0.5234930	-2.9654078	1.8444312
H	2.0458330	2.2047052	-0.5216718
H	1.1044420	1.2384282	-3.7394098
H	2.5562190	1.8955352	-2.9502298
H	2.5858390	0.2520022	-3.5403638
H	-6.8605450	0.7094532	1.2450072
H	-4.8559880	4.4410272	0.5396132
H	-3.4520840	3.3610112	-1.1751968
H	-5.4210100	-0.3784558	-0.4923878
H	-3.3408710	1.4155242	-2.8762428
H	-3.9008390	-0.1774688	-2.3152958
H	-7.4095820	4.6786412	3.0623702
H	-6.8751110	5.1292612	1.4212592
H	-5.6686600	4.7269862	2.6774102
P	4.6789960	-0.7313228	1.1926492
C	4.6541210	0.1123682	2.8077552
H	3.7037890	-0.1133588	3.3044012
H	5.4863770	-0.2470438	3.4253272
H	4.7367670	1.1914282	2.6549882
C	6.3769450	-0.4455348	0.5772212

H	7.1236170	-0.7485058	1.3208702
H	6.5375730	-1.0022798	-0.3512078
H	6.4907480	0.6231102	0.3638962
C	4.6222410	-2.5040838	1.6353362
H	5.4470530	-2.7688888	2.3076252
H	3.6696630	-2.6914038	2.1456432
H	4.6733600	-3.1193538	0.7313992
C	4.5644240	3.6603702	-1.2230258
F	4.7268270	2.4035272	-1.6164008
F	5.7273210	4.1524802	-0.8387448
F	4.0752620	4.3730002	-2.2150488
S	3.4181100	3.7121642	0.2183812
O	2.0827410	3.1957652	-0.4608328
O	3.2277420	5.0976892	0.5541572
O	3.9266470	2.7383012	1.1639572
H	-2.5063580	0.0655042	0.5343142
H	1.0503350	-1.7768298	-0.2580428
C	-0.7738510	-3.8240378	-0.9149668
C	-1.3051240	-4.0257458	-2.3338658
C	0.7104790	-4.1801558	-0.9152818
C	-1.5360480	-4.7093638	0.0688382
H	-2.3751770	-3.8168028	-2.3927188
H	-0.7790660	-3.3653908	-3.0337978
H	-1.1309420	-5.0635038	-2.6423768
H	1.1773110	-4.0892648	0.0734472

H	0.8166920	-5.2243268	-1.2300138
H	1.2703550	-3.5574918	-1.6254788
H	-1.4466430	-5.7625548	-0.2250088
H	-1.1400700	-4.6082328	1.0868472
H	-2.5972830	-4.4414278	0.0757102
H	-0.8916010	-1.9257868	2.0923312
H	-0.2579010	1.8307452	0.8511232
H	1.0291040	1.1836512	2.8582672

Zero-point correction= 0.627575 (Hartree/Particle)

Thermal correction to Energy= 0.674124

Thermal correction to Enthalpy= 0.675068

Thermal correction to Gibbs Free Energy= 0.544111

Sum of electronic and zero-point Energies= -2897.975523

Sum of electronic and thermal Energies= -2897.928973

Sum of electronic and thermal Enthalpies= -2897.928029

Sum of electronic and thermal Free Energies= -2898.058986

C-ts4

C	-0.7938769	-0.8481811	2.0899480
C	0.0736771	-0.9957421	1.0798620
C	-1.3830819	0.4666039	2.3732800
C	-0.5660169	1.6267939	1.8568030
C	-0.2242119	1.4538339	0.3758030
C	0.3983461	0.0632109	0.0686420
C	0.0021401	-0.4549041	-1.3146010
C	1.2232341	-0.4631061	-2.1799120

N	2.2812261	-0.1221931	-1.3775800
C	1.9073671	0.3568379	-0.0643230
C	-1.1969919	-0.9792971	-1.6654690
N	0.7746391	2.4102309	-0.0879140
C	2.0337711	1.8787189	-0.0668010
O	3.0955741	2.4751639	-0.1351570
O	1.3021541	-0.7749471	-3.3552430
O	-2.4177769	0.6254969	3.0030540
Au	-2.9564379	-0.1639041	-0.5906310
C	-1.4987849	-1.4571311	-3.0622800
C	6.1646491	-1.1324151	0.8189910
C	6.1164301	-2.5262811	0.7262620
C	5.2738331	-3.1316101	-0.2089140
C	4.4948371	-2.3342051	-1.0416840
C	4.5420251	-0.9448161	-0.9660280
C	5.3820631	-0.3538211	-0.0179670
C	3.6601121	-0.1053571	-1.8453830
O	6.9180401	-3.2022131	1.5851660
C	6.8994891	-4.6072321	1.5334560
H	-1.1141539	2.5578539	2.0402710
H	-1.6341829	-1.9273321	-0.8448210
H	-0.6929829	-2.0790471	-3.4656970
H	-2.4331669	-2.0283091	-3.0706520
H	-1.6043109	-0.6085751	-3.7494340
H	6.8248401	-0.6889231	1.5600380

H	5.2190841	-4.2125701	-0.2976270
H	3.8336361	-2.8037041	-1.7709440
H	5.4042521	0.7328079	0.0643290
H	3.6200191	-0.4873341	-2.8723220
H	4.0215751	0.9306759	-1.8745590
H	7.6009761	-4.9559411	2.2940900
H	7.2213731	-4.9829491	0.5514690
H	5.9010051	-5.0100971	1.7567710
P	-4.8543689	0.6629979	0.5129420
C	-5.3472189	-0.4069841	1.8972030
H	-4.5218529	-0.4348581	2.6176540
H	-6.2577439	-0.0160611	2.3673270
H	-5.5047509	-1.4267811	1.5325580
C	-6.3344449	0.7754389	-0.5496570
H	-7.2019409	1.1128199	0.0298530
H	-6.1525659	1.4718699	-1.3738080
H	-6.5420569	-0.2140391	-0.9703780
C	-4.6621849	2.3194999	1.2515820
H	-5.5952339	2.6355259	1.7333160
H	-3.8677569	2.2573169	2.0056480
H	-4.3851049	3.0454519	0.4802990
C	-4.3138189	-3.8498651	-0.6302570
F	-4.5475309	-2.7327931	-1.3337200
F	-5.3886909	-4.1007061	0.1052650
F	-4.1166149	-4.8428661	-1.4763090

S	-2.8604719	-3.6188841	0.4712820
O	-1.7817119	-3.2140211	-0.5171790
O	-2.6203699	-4.9190041	1.0630760
O	-3.2672459	-2.5088951	1.3361430
H	2.5377691	-0.0937031	0.7155210
H	-1.1478639	1.5653179	-0.2062580
C	0.5119141	3.8627829	-0.2816180
C	1.2354561	4.3271839	-1.5454800
C	-0.9834579	4.0892879	-0.4875380
C	1.0087471	4.6463569	0.9318240
H	2.3178391	4.2229079	-1.4471950
H	0.9024391	3.7435719	-2.4121630
H	1.0002341	5.3819249	-1.7305840
H	-1.5837339	3.8229529	0.3908640
H	-1.1483759	5.1550229	-0.6810160
H	-1.3595569	3.5306179	-1.3545670
H	0.8591861	5.7210329	0.7705180
H	0.4659801	4.3643239	1.8422180
H	2.0770201	4.4662569	1.0880330
H	0.3701201	1.6684599	2.4358710
H	0.5072231	-1.9754671	0.8720500
H	-1.1216519	-1.6900841	2.6943870

Zero-point correction= 0.622034 (Hartree/Particle)

Thermal correction to Energy= 0.668081

Thermal correction to Enthalpy= 0.669025

Thermal correction to Gibbs Free Energy= 0.540498

Sum of electronic and zero-point Energies= -2897.961778

Sum of electronic and thermal Energies= -2897.915731

Sum of electronic and thermal Enthalpies= -2897.914787

Sum of electronic and thermal Free Energies= -2898.043315

C-2

C	-0.8463455	0.1549024	-1.5691296
C	-0.1289445	0.6184424	-0.5312736
C	-0.5911085	-1.1813566	-2.1103376
C	0.7619095	-1.7585786	-1.7682576
C	1.0652075	-1.6251116	-0.2731286
C	0.8906445	-0.1807636	0.2190554
C	0.5967405	-0.0702826	1.7093234
C	1.5441875	0.9201734	2.2975744
N	2.4909186	1.1793804	1.3343214
C	2.3019215	0.4210764	0.1213274
C	-0.4170815	-0.6692076	2.3411744
N	2.4558905	-1.9266606	0.0531024
C	3.2296645	-0.7929976	0.0929604
O	4.4435445	-0.7261696	0.1438454
O	1.5044775	1.4479654	3.3960464
O	-1.3980905	-1.7918326	-2.8001636
Au	-3.3324565	-0.5641436	0.2969704
C	-0.8067565	-0.5136286	3.7672734
C	2.7323805	4.7704564	-1.5418866

C	1.4286325	5.1951474	-1.2739716
C	0.7792855	4.7544874	-0.1182936
C	1.4320825	3.8784714	0.7382964
C	2.7253795	3.4258984	0.4726864
C	3.3661125	3.8875084	-0.6783046
C	3.3311626	2.3681814	1.3579194
O	0.8648685	6.0176294	-2.1907546
C	-0.4769725	6.3963334	-1.9803306
H	0.8002405	-2.7997976	-2.1084016
H	-0.1169755	0.1432964	4.2998404
H	-1.8148135	-0.0803606	3.8205854
H	-0.8542085	-1.4887126	4.2684324
H	3.2165836	5.1281234	-2.4472036
H	-0.2390915	5.0502274	0.1103174
H	0.9091965	3.5296514	1.6298764
H	4.3734725	3.5390404	-0.9072416
H	3.3771036	2.6808804	2.4076954
H	4.3430015	2.0963404	1.0321664
H	-0.7749765	6.9793834	-2.8542746
H	-0.5844845	7.0191814	-1.0808406
H	-1.1364305	5.5223414	-1.8807786
P	-3.8972715	-2.6190176	-0.5468396
C	-4.4832615	-2.5149616	-2.2638926
H	-3.6700675	-2.1012186	-2.8700586
H	-4.7606765	-3.5097146	-2.6322626

H	-5.3480735	-1.8466366	-2.3137946
C	-5.2480994	-3.4231406	0.3783644
H	-5.5143474	-4.3788046	-0.0885846
H	-4.9373115	-3.5969326	1.4129904
H	-6.1233474	-2.7663256	0.3865924
C	-2.5614615	-3.8611316	-0.5775496
H	-2.9652115	-4.8291056	-0.8980656
H	-1.7984125	-3.5372266	-1.2948636
H	-2.1191015	-3.9652036	0.4186664
C	-4.6917275	3.2318764	0.9494114
F	-5.6451095	2.3052814	0.9417024
F	-5.0985654	4.2747024	0.2430774
F	-4.4653595	3.6078714	2.1965934
S	-3.1646215	2.5401074	0.2025314
O	-2.8907725	1.3742874	1.1409504
O	-2.1542345	3.5828034	0.3108504
O	-3.5681045	2.0932214	-1.1314436
H	2.4605125	1.0565534	-0.7638796
H	0.3889255	-2.2875256	0.2856854
C	3.0383045	-3.2949196	0.0813824
C	3.9473385	-3.4197586	1.3040954
C	1.9229755	-4.3263306	0.2203344
C	3.8316755	-3.5426926	-1.2001456
H	4.7857666	-2.7226946	1.2488664
H	3.3812355	-3.2150026	2.2207064

H	4.3403066	-4.4419086	1.3624624
H	1.2290495	-4.3289926	-0.6291786
H	2.3763545	-5.3225456	0.2705054
H	1.3519545	-4.1752296	1.1452934
H	4.2953686	-4.5364556	-1.1695756
H	3.1842615	-3.4993436	-2.0848216
H	4.6240675	-2.7953146	-1.3061896
H	1.5231835	-1.1975966	-2.3337216
H	-1.0547175	-1.3312836	1.7390984
H	-0.3158165	1.6231054	-0.1405476
H	-1.6514835	0.7422904	-2.0109636

Zero-point correction= 0.627797 (Hartree/Particle)

Thermal correction to Energy= 0.673600

Thermal correction to Enthalpy= 0.674544

Thermal correction to Gibbs Free Energy= 0.545856

Sum of electronic and zero-point Energies= -2898.005066

Sum of electronic and thermal Energies= -2897.959264

Sum of electronic and thermal Enthalpies= -2897.958319

Sum of electronic and thermal Free Energies= -2898.087007

C-int5

C	-0.0055687	-1.6234559	2.5877163
C	0.6344393	-1.1633349	1.5034153
C	-1.3189297	-1.1117149	2.9882713
C	-1.8410677	0.0136201	2.1917373
C	-1.2325657	0.4238531	1.0724843

C	0.0377133	-0.1575839	0.5633773
C	-0.0654567	-0.8498409	-0.8185177
C	1.2595363	-0.6230649	-1.4815367
N	1.9406673	0.3008501	-0.7160467
C	1.0446033	0.9772421	0.1946123
C	-1.1181517	-1.5442859	-1.2996187
N	1.4443913	2.8548271	1.7642163
C	1.7325863	1.5683721	1.4112013
O	2.4805093	0.8866351	2.0976623
O	1.7096383	-1.1134329	-2.5023927
O	-1.9650277	-1.5900639	3.9159943
H	0.4671023	1.7517011	-0.3356637
Au	-2.8650887	-1.8754119	-0.1906937
C	-1.0908837	-2.1778499	-2.6630827
C	0.8844893	4.0227251	1.0402723
C	-0.6176367	3.8938691	0.7873543
C	1.6377053	4.2780061	-0.2636297
C	1.1098303	5.2052021	1.9805523
C	5.7058533	-1.6419409	0.3913343
C	6.3619283	-2.1378689	-0.7403337
C	5.9938543	-1.6881319	-2.0069997
C	4.9747443	-0.7449629	-2.1264247
C	4.3266344	-0.2350889	-1.0095257
C	4.7000854	-0.7020779	0.2564993
C	3.2390234	0.7966661	-1.1505277

O	7.3362703	-3.0535049	-0.5022827
C	8.0108793	-3.5910119	-1.6101707
H	-2.7807767	0.4549751	2.5228493
H	-1.6889747	1.2117911	0.4750523
H	1.9374813	3.0820011	2.6215693
H	-0.1699117	-1.9873149	-3.2199277
H	-1.2183497	-3.2634929	-2.5563667
H	-1.9571157	-1.8393689	-3.2499917
H	-1.1380427	3.5690591	1.6958173
H	-1.0233757	4.8662991	0.4842213
H	-0.8548637	3.1915431	-0.0199557
H	2.7100143	4.4046881	-0.0713787
H	1.2630653	5.1932591	-0.7377887
H	1.5115653	3.4629481	-0.9860087
H	0.7434463	6.1291131	1.5211903
H	0.5733123	5.0595581	2.9262963
H	2.1773223	5.3371511	2.1980643
H	6.0103393	-2.0147769	1.3662633
H	6.4773884	-2.0691329	-2.9016977
H	4.6648983	-0.4154189	-3.1170777
H	4.1824093	-0.3211269	1.1370323
H	3.1705773	1.1248511	-2.1986427
H	3.4707253	1.6797751	-0.5399127
H	8.7424633	-4.3003569	-1.2168967
H	8.5391743	-2.8145619	-2.1830877

H	7.3258863	-4.1226989	-2.2868437
P	-4.9009406	-2.2435219	0.9970133
C	-4.7322817	-2.8968449	2.6916893
H	-4.0785537	-2.2369209	3.2765023
H	-5.7140787	-2.9811429	3.1732883
H	-4.2589027	-3.8831389	2.6556733
C	-6.0714597	-3.3878719	0.1798043
H	-6.9954786	-3.4864079	0.7621723
H	-6.3098266	-3.0046199	-0.8180997
H	-5.6068477	-4.3722409	0.0674763
C	-5.8953606	-0.7253109	1.2142813
H	-6.8424436	-0.9548989	1.7172933
H	-5.3286986	-0.0034759	1.8102473
H	-6.0889996	-0.2657469	0.2399093
C	-4.9488797	0.6980891	-2.6884937
F	-4.7782017	0.9580281	-3.9657357
F	-6.1714446	1.0368321	-2.3129967
F	-4.7707197	-0.5970839	-2.4689877
S	-3.7595927	1.6789671	-1.6783787
O	-2.3867087	1.0585471	-2.1650457
O	-4.0271427	1.3295401	-0.2973157
O	-3.8183007	3.0352711	-2.1579397
H	1.6115453	-1.5554749	1.2257173
H	0.4189163	-2.4039999	3.2144903
H	-2.1263677	0.2357231	-1.6645947

Zero-point correction= 0.625459 (Hartree/Particle)

Thermal correction to Energy= 0.673098

Thermal correction to Enthalpy= 0.674042

Thermal correction to Gibbs Free Energy= 0.541388

Sum of electronic and zero-point Energies= -2897.940357

Sum of electronic and thermal Energies= -2897.892719

Sum of electronic and thermal Enthalpies= -2897.891775

Sum of electronic and thermal Free Energies= -2898.024429

C-ts5

C	-0.0458536	-1.3712207	2.6755321
C	0.5866794	-1.0316187	1.5436181
C	-1.3192506	-0.7597187	3.0705661
C	-1.8355816	0.2887863	2.1718731
C	-1.2386836	0.5740733	1.0093161
C	0.0192414	-0.0682767	0.5432351
C	-0.0932796	-0.8208437	-0.8021849
C	1.2345184	-0.6569867	-1.4726669
N	1.9383044	0.2847793	-0.7504979
C	1.0572284	1.0253893	0.1246931
C	-1.1626996	-1.4967197	-1.2718009
N	1.5065744	2.9602193	1.6156291
C	1.7608774	1.6541103	1.3139541
O	2.4909844	0.9825383	2.0291871
O	1.6694564	-1.2137377	-2.4655039
O	-1.9384826	-1.0995977	4.0734811

H	0.4970684	1.7858973	-0.4437809
Au	-2.8701906	-1.8385467	-0.1048469
C	-1.1329446	-2.1680817	-2.6183249
C	0.9951764	4.1157433	0.8394891
C	-0.5119416	4.0364463	0.6018841
C	1.7500804	4.2786843	-0.4781529
C	1.2758774	5.3311353	1.7211061
C	5.6061674	-1.7525947	0.4509351
C	6.2845484	-2.2823327	-0.6519649
C	5.9675034	-1.8434617	-1.9360569
C	4.9762774	-0.8776067	-2.1010629
C	4.3065954	-0.3347707	-1.0130349
C	4.6286274	-0.7908527	0.2709611
C	3.2503294	0.7210953	-1.2056729
O	7.2273944	-3.2182127	-0.3696409
C	7.9204534	-3.7915467	-1.4477499
H	-2.7620656	0.7803093	2.4686281
H	-1.6867696	1.3125123	0.3463811
H	2.0113494	3.2068023	2.4606951
H	-0.3538966	-1.7830507	-3.2826099
H	-0.9345076	-3.2399007	-2.4769069
H	-2.1119546	-2.1025887	-3.1092189
H	-1.0374846	3.7903503	1.5317081
H	-0.8793216	5.0046133	0.2413981
H	-0.7824336	3.2940863	-0.1574819

H	2.8269894	4.3790623	-0.2961449
H	1.4040404	5.1812033	-0.9964209
H	1.5934244	3.4336453	-1.1586919
H	0.9539504	6.2475283	1.2156021
H	0.7326294	5.2580833	2.6713811
H	2.3483494	5.4230813	1.9346481
H	5.8709954	-2.1174757	1.4403601
H	6.4680064	-2.2505857	-2.8096479
H	4.7045804	-0.5571477	-3.1059979
H	4.0952554	-0.3811207	1.1288681
H	3.1914154	0.9956093	-2.2697659
H	3.5079464	1.6280743	-0.6421019
H	8.6222034	-4.5116527	-1.0210819
H	8.4845794	-3.0385437	-2.0178229
H	7.2423694	-4.3180387	-2.1353869
P	-4.8692156	-2.2333407	1.1384661
C	-4.7107626	-2.2799147	2.9554481
H	-4.2821956	-1.3450397	3.3315761
H	-5.6869716	-2.4638967	3.4204311
H	-4.0132546	-3.0740377	3.2405541
C	-5.7337626	-3.7989407	0.7512771
H	-6.6879496	-3.8589277	1.2885401
H	-5.9180976	-3.8608817	-0.3258139
H	-5.1028596	-4.6447787	1.0417421
C	-6.1419616	-0.9566527	0.8365541

H	-7.0585176	-1.1836537	1.3944221
H	-5.7475246	0.0170863	1.1447041
H	-6.3642936	-0.8996087	-0.2349409
C	-5.0464206	0.4603543	-2.6791149
F	-5.0526486	0.8247143	-3.9417359
F	-6.2619396	0.5745153	-2.1648809
F	-4.6555816	-0.8019127	-2.5838459
S	-3.9170826	1.5555613	-1.7094459
O	-2.5066576	1.0146323	-2.1830539
O	-4.1528106	1.2342683	-0.3157619
O	-4.0698746	2.8899973	-2.2277939
H	1.5374354	-1.4914127	1.2782171
H	0.3608264	-2.1155917	3.3559791
H	-2.2285826	0.1804343	-1.6944309

Zero-point correction= 0.620556 (Hartree/Particle)

Thermal correction to Energy= 0.667735

Thermal correction to Enthalpy= 0.668679

Thermal correction to Gibbs Free Energy= 0.536728

Sum of electronic and zero-point Energies= -2897.936180

Sum of electronic and thermal Energies= -2897.889001

Sum of electronic and thermal Enthalpies= -2897.888057

Sum of electronic and thermal Free Energies= -2898.020008

C-int6

C	0.0213621	-1.2468881	-2.8442638
C	-0.5481379	-1.0442481	-1.6478848

C	1.2107421	-0.5089901	-3.2802768
C	1.8237641	0.3869909	-2.2550178
C	1.2968451	0.5112989	-0.9981838
C	0.0127311	-0.1286791	-0.5978188
C	-0.0119419	-0.8343391	0.7587522
C	-1.3789069	-0.6368301	1.3229412
N	-1.9777709	0.3371799	0.5557512
C	-0.9966239	1.0374099	-0.2471908
C	1.0131311	-1.4130931	1.3902122
N	-1.2260289	2.9792359	-1.7680238
C	-1.5835629	1.6965139	-1.4826368
O	-2.3094309	1.0604509	-2.2348848
O	-1.8997409	-1.1815961	2.2789322
O	1.6954341	-0.6063821	-4.3953048
H	-0.4327549	1.7602569	0.3622842
Au	3.3271081	-0.9707071	-1.1328618
C	1.0009871	-2.0009961	2.7556772
C	-0.6958969	4.1071459	-0.9536198
C	0.7832301	3.9405329	-0.6122878
C	-1.5315189	4.3125109	0.3079262
C	-0.8494429	5.3326449	-1.8518958
C	-5.7008659	-1.4699101	-0.8632498
C	-6.4571789	-1.9683391	0.2031892
C	-6.1751270	-1.5562211	1.5043082
C	-5.1403679	-0.6487831	1.7230462

C	-4.3921369	-0.1376491	0.6710842
C	-4.6808830	-0.5653181	-0.6304948
C	-3.2903529	0.8573219	0.9198882
O	-7.4364229	-2.8475201	-0.1297988
C	-8.2171889	-3.3792471	0.9096172
H	2.6147381	1.0609349	-2.5968818
H	1.7483711	1.1906599	-0.2699058
H	-1.6587229	3.2565829	-2.6434498
H	-0.0061949	-2.0399861	3.1733602
H	1.4288221	-3.0116691	2.7415582
H	1.6444331	-1.3971091	3.4094062
H	1.3602531	3.6836409	-1.5091528
H	1.1746701	4.8869459	-0.2209908
H	0.9798311	3.1898689	0.1612152
H	-2.5880579	4.4615339	0.0530252
H	-1.1787559	5.2013289	0.8443382
H	-1.4579289	3.4681949	1.0032882
H	-0.4965749	6.2278219	-1.3297488
H	-0.2578959	5.2209099	-2.7690448
H	-1.8998729	5.4938369	-2.1264618
H	-5.9419140	-1.8110861	-1.8670908
H	-6.7383510	-1.9383021	2.3505442
H	-4.9014969	-0.3474931	2.7419892
H	-4.0877099	-0.1797391	-1.4597888
H	-3.2817119	1.1491819	1.9806312

H	-3.4543769	1.7668269	0.3269572
H	-8.9384559	-4.0548801	0.4446712
H	-8.7627149	-2.5937921	1.4531142
H	-7.6079099	-3.9464531	1.6284902
P	5.0609931	-2.4380251	-0.5900978
C	5.5847141	-3.5442171	-1.9417878
H	5.8881631	-2.9462691	-2.8063208
H	6.4250271	-4.1701191	-1.6187648
H	4.7476551	-4.1821031	-2.2407538
C	4.6896161	-3.5541591	0.8026672
H	5.5429921	-4.2151111	0.9954402
H	4.4846021	-2.9558011	1.6950172
H	3.8063861	-4.1563531	0.5675082
C	6.5608711	-1.5327981	-0.1036488
H	7.3611501	-2.2322691	0.1651752
H	6.8842051	-0.8995001	-0.9353918
H	6.3302701	-0.8787751	0.7421712
H	1.9843901	-1.4194211	0.8849272
C	4.4811051	0.4921269	2.5870462
F	5.8124961	0.4377139	2.6006442
F	4.0415731	-0.7391691	2.2429312
F	4.0518761	0.7435149	3.8105052
S	3.8838491	1.7452719	1.3828802
O	4.5392491	2.9744479	1.8018072
O	2.4213541	1.6738249	1.5638012

O	4.3523121	1.1756139	0.0931312
H	-1.4692409	-1.5620601	-1.3839138
H	-0.4111309	-1.9278821	-3.5729588

Zero-point correction= 0.626347 (Hartree/Particle)

Thermal correction to Energy= 0.673959

Thermal correction to Enthalpy= 0.674903

Thermal correction to Gibbs Free Energy= 0.541801

Sum of electronic and zero-point Energies= -2897.958090

Sum of electronic and thermal Energies= -2897.910478

Sum of electronic and thermal Enthalpies= -2897.909534

Sum of electronic and thermal Free Energies= -2898.042637

C-ts6

C	-0.8086345	0.4671422	3.4623855
C	-1.2593795	1.1623982	2.4195005
C	0.6343685	0.2013142	3.6562095
C	1.5595505	0.6728652	2.5778695
C	1.0934155	1.6757592	1.7014325
C	-0.3718865	1.7330172	1.3375545
C	-0.8700595	3.1209422	0.9797005
C	-1.7279425	3.0134582	-0.2314455
N	-1.6263695	1.7085582	-0.6698875
C	-0.6543785	0.9126722	0.0460685
C	-0.6160695	4.2307862	1.6822275
N	1.7526015	1.3638432	-0.3484075
C	0.5878315	0.6893022	-0.8182755

O	0.5225765	0.0175092	-1.8225535
O	-2.4185515	3.8641362	-0.7624745
O	1.0478225	-0.3416788	4.6666945
Au	1.4264465	-1.3309028	1.5106555
C	-1.0761635	5.6090722	1.3667895
C	-3.1275335	-2.5254518	-1.9386465
C	-4.0013875	-2.6709328	-0.8577715
C	-4.3695935	-1.5493248	-0.1102785
C	-3.8511835	-0.3024198	-0.4500225
C	-2.9673105	-0.1457378	-1.5154655
C	-2.6130265	-1.2778008	-2.2537695
C	-2.3617635	1.1979232	-1.8150085
O	-4.4159444	-3.9350408	-0.6008255
C	-5.2569925	-4.1371848	0.5096945
H	-1.7051935	5.6302052	0.4752735
H	-1.6365355	6.0267132	2.2125265
H	-0.2109685	6.2683092	1.2179445
H	-2.8570865	-3.4132038	-2.5059595
H	-5.0541905	-1.6341998	0.7284225
H	-4.1374815	0.5722952	0.1349715
H	-1.9129665	-1.1765218	-3.0822385
H	-3.1197975	1.9609562	-2.0339995
H	-1.7014855	1.1253552	-2.6914345
H	-5.4646245	-5.2080038	0.5523055
H	-6.2064955	-3.5935728	0.4062325

H	-4.7699745	-3.8277948	1.4468265
P	0.5607285	-3.2791268	0.5540395
C	1.3664005	-4.8506868	1.0071485
H	1.3430105	-4.9742928	2.0940735
H	0.8481315	-5.6920578	0.5319075
H	2.4100935	-4.8319578	0.6816385
C	0.5083285	-3.2696998	-1.2652955
H	-0.0029755	-4.1691148	-1.6297485
H	-0.0275815	-2.3741288	-1.5997785
H	1.5257505	-3.2266618	-1.6610345
C	-1.1860415	-3.5056168	1.0436635
H	-1.6211495	-4.3860228	0.5530055
H	-1.2478785	-3.6176028	2.1310775
H	-1.7619845	-2.6182788	0.7501925
H	-1.0747625	-0.0802968	0.2751085
H	1.6583955	2.5993432	1.6029605
C	2.3536865	2.4171232	-1.2625615
C	1.2874465	3.4268632	-1.6582795
C	3.4625635	3.0793792	-0.4549685
C	2.9502625	1.7640422	-2.5066925
H	0.4740875	2.9628582	-2.2339465
H	0.8569255	3.9368092	-0.7874635
H	1.7408715	4.1890402	-2.3016865
H	4.1875355	2.3337292	-0.1059945
H	3.9976285	3.7927082	-1.0925165

H	3.0657005	3.6364322	0.4035505
H	3.3823815	2.5490882	-3.1401285
H	3.7547115	1.0716832	-2.2367285
H	2.1924645	1.2284792	-3.0860165
H	0.0088225	4.1195032	2.5746505
H	2.5953566	0.7552552	2.9104565
H	2.5093535	0.6811222	-0.1345005
C	4.2017725	-1.9710048	-1.1904215
F	3.1794405	-1.4089948	-1.8463225
F	3.7144575	-3.0400728	-0.5394755
F	5.0870025	-2.3974958	-2.0731855
S	4.9493475	-0.7757388	-0.0101965
O	5.4998406	0.2584122	-0.8867975
O	5.8644165	-1.5818308	0.7809905
O	3.7302815	-0.3089808	0.7298425
H	-2.3267305	1.3314282	2.2684945
H	-1.4717385	0.0716002	4.2281155

Zero-point correction= 0.626080 (Hartree/Particle)

Thermal correction to Energy= 0.671809

Thermal correction to Enthalpy= 0.672753

Thermal correction to Gibbs Free Energy= 0.548048

Sum of electronic and zero-point Energies= -2897.934342

Sum of electronic and thermal Energies= -2897.888613

Sum of electronic and thermal Enthalpies= -2897.887669

Sum of electronic and thermal Free Energies= -2898.012374

C-int7

C	-0.3380027	1.2045244	3.5825624
C	-0.9775837	1.5942394	2.4800364
C	1.1078943	0.8570524	3.5706324
C	1.7272503	0.7443674	2.2327654
C	1.2394613	1.7707064	1.2238664
C	-0.3064007	1.8878154	1.1648614
C	-0.8390527	3.2361024	0.6997314
C	-1.6745637	3.0355544	-0.5120776
N	-1.6213607	1.6866804	-0.8086106
C	-0.7327877	0.9285934	0.0403184
C	-0.6464427	4.3911584	1.3470294
N	1.6915583	1.3322464	-0.1772686
C	0.5259573	0.5695634	-0.7271356
O	0.6097933	-0.1503626	-1.6779866
O	-2.3085127	3.8500594	-1.1583066
O	1.6832763	0.5981714	4.6173774
Au	1.2123513	-1.2753806	1.6388544
C	-1.1426577	5.7340944	0.9465044
C	-3.1094767	-2.6212336	-1.8775326
C	-4.0122147	-2.6994936	-0.8139756
C	-4.3860177	-1.5350616	-0.1373876
C	-3.8457247	-0.3133996	-0.5294966
C	-2.9338467	-0.2236286	-1.5794306
C	-2.5726217	-1.3976046	-2.2448776

C	-2.3098697	1.0950424	-1.9435316
O	-4.4462557	-3.9429896	-0.4990966
C	-5.3114697	-4.0772496	0.6035514
H	-1.7585577	5.6864554	0.0469214
H	-1.7225857	6.1857084	1.7609244
H	-0.2941247	6.4083324	0.7679424
H	-2.8304077	-3.5411556	-2.3861676
H	-5.0894957	-1.5681696	0.6892394
H	-4.1312267	0.5924934	0.0062744
H	-1.8464837	-1.3499306	-3.0560186
H	-3.0520587	1.8420004	-2.2537666
H	-1.6115757	0.9603004	-2.7840446
H	-5.5303347	-5.1423656	0.6992804
H	-6.2532417	-3.5317516	0.4513564
H	-4.8387587	-3.7220266	1.5314574
P	0.3671063	-3.3506816	0.8674414
C	1.1711843	-4.8994016	1.4053154
H	1.1616693	-4.9617706	2.4975934
H	0.6481773	-5.7669516	0.9854504
H	2.2111933	-4.9016406	1.0664984
C	0.3174883	-3.4728656	-0.9513836
H	-0.2274247	-4.3741466	-1.2586086
H	-0.1808597	-2.5830596	-1.3538806
H	1.3371363	-3.4986196	-1.3418306
C	-1.3867887	-3.5674806	1.3444494

H	-1.8079357	-4.4767076	0.8960554
H	-1.4708537	-3.6181406	2.4347694
H	-1.9600997	-2.7009306	0.9899914
H	-1.2083097	0.0000414	0.3908564
H	1.6765423	2.7628014	1.4003444
C	2.3709383	2.3652984	-1.1569566
C	1.4237293	3.4912244	-1.5175346
C	3.6086683	2.8713984	-0.4306396
C	2.7833423	1.6160504	-2.4172866
H	0.5090753	3.1248634	-2.0032706
H	1.1487083	4.1155074	-0.6627906
H	1.9347933	4.1304394	-2.2462246
H	4.2789573	2.0451354	-0.1722506
H	4.1478193	3.5418284	-1.1087856
H	3.3683583	3.4448034	0.4712994
H	3.4048933	2.2995434	-3.0067606
H	3.3945413	0.7343554	-2.2044216
H	1.9243543	1.3291804	-3.0292216
H	-0.0407467	4.3465934	2.2586304
H	2.8196813	0.7497944	2.3100624
H	2.4800973	0.6238624	-0.0502336
C	4.0357913	-2.3392856	-1.1826816
F	3.0063903	-1.8888816	-1.9070136
F	3.5397743	-3.1823136	-0.2643476
F	4.8438163	-3.0216166	-1.9760446

S	4.9087683	-0.9414496	-0.3760936
O	5.3806373	-0.1365206	-1.5032826
O	5.8905283	-1.5773556	0.4856634
O	3.7707123	-0.3012126	0.3603794
H	-2.0521507	1.7877444	2.4891974
H	-0.8535317	1.0811054	4.5327724

Zero-point correction= 0.628608 (Hartree/Particle)

Thermal correction to Energy= 0.674234

Thermal correction to Enthalpy= 0.675179

Thermal correction to Gibbs Free Energy= 0.551067

Sum of electronic and zero-point Energies= -2897.960909

Sum of electronic and thermal Energies= -2897.915283

Sum of electronic and thermal Enthalpies= -2897.914339

Sum of electronic and thermal Free Energies= -2898.038450

C-ts7

C	-0.7506361	0.8045260	3.2972594
C	-1.5930001	1.1818710	2.3321014
C	0.7176809	0.9163150	3.1684944
C	1.2394799	1.4560000	1.8715934
C	0.2844479	2.3076660	1.0356184
C	-1.1726331	1.8219050	1.0415344
C	-2.1963901	2.8789410	0.6469314
C	-3.1163181	2.2791300	-0.3641156
N	-2.5812571	1.0517860	-0.6977166
C	-1.2640951	0.8569260	-0.1508256

C	-2.2868461	4.1064880	1.1707414
N	0.7918349	2.0665580	-0.3614166
C	-0.1795181	1.3339290	-1.1042966
O	-0.1504501	1.1034000	-2.2859696
O	-4.1502211	2.7296160	-0.8226056
O	1.4537959	0.5535720	4.0725934
Au	1.7687979	-0.6868610	1.1256364
C	-3.2878801	5.1525540	0.8331244
C	-2.0426961	-3.4322010	-1.8173966
C	-2.7324351	-3.9537210	-0.7200146
C	-3.5574151	-3.1204000	0.0395234
C	-3.6790851	-1.7780550	-0.3093536
C	-3.0009661	-1.2453550	-1.4039236
C	-2.1718811	-2.0910800	-2.1461446
C	-3.1277741	0.2112100	-1.7508116
O	-2.5121991	-5.2650450	-0.4533756
C	-3.2036951	-5.8398640	0.6305934
H	-4.0034531	4.8009420	0.0883144
H	-3.8302001	5.4597850	1.7361774
H	-2.7822351	6.0522610	0.4596004
H	-1.4081211	-4.1021650	-2.3934386
H	-4.1037381	-3.5027510	0.8967354
H	-4.3203271	-1.1269630	0.2852564
H	-1.6229291	-1.6875280	-2.9968686
H	-4.1749201	0.5207700	-1.8583316

H	-2.6195281	0.4205120	-2.7019976
H	-2.9107121	-6.8908970	0.6642504
H	-4.2924581	-5.7758330	0.4970264
H	-2.9336021	-5.3612460	1.5841394
P	1.5478239	-2.9744380	0.6865364
C	2.7790689	-4.1060130	1.4094384
H	2.7679039	-4.0077970	2.4991554
H	2.5475469	-5.1414920	1.1328804
H	3.7754689	-3.8407490	1.0476484
C	1.5411549	-3.3333950	-1.0987126
H	1.3481069	-4.3988630	-1.2740606
H	0.7546239	-2.7352370	-1.5731076
H	2.5056459	-3.0467380	-1.5248616
C	-0.0569701	-3.6069990	1.2849304
H	-0.2306471	-4.6338710	0.9368544
H	-0.0731761	-3.5743820	2.3793214
H	-0.8597291	-2.9635870	0.9046924
H	-1.0805921	-0.1976140	0.1163744
H	0.3415279	3.3750670	1.2785854
C	1.6793439	3.0982150	-1.0546976
C	0.7789899	4.2310300	-1.5308236
C	2.7180699	3.6033530	-0.0612836
C	2.4086499	2.4363550	-2.2175996
H	0.0189499	3.8721980	-2.2346966
H	0.2742299	4.7331250	-0.6947906

H	1.3896429	4.9792510	-2.0490956
H	3.3848459	2.7959820	0.2625664
H	3.3381349	4.3449950	-0.5760276
H	2.2756369	4.1033410	0.8091074
H	3.1817419	3.1267650	-2.5719096
H	2.9312749	1.5348780	-1.8850056
H	1.7403129	2.1926980	-3.0440336
H	-1.5414461	4.3797240	1.9255784
H	2.2057579	1.9415170	2.0416384
H	1.4700489	1.0985850	0.4072404
C	4.7419679	-1.0335720	-1.1919606
F	3.5808829	-0.8377200	-1.8375756
F	4.5822479	-2.1431120	-0.4463436
F	5.6777129	-1.2799840	-2.0914136
S	5.1801319	0.4114270	-0.1384626
O	5.3068679	1.4965820	-1.1112946
O	6.3790529	-0.0385340	0.5548344
O	3.9662599	0.5368870	0.7195384
H	-2.6679231	1.0305330	2.4452784
H	-1.1055671	0.3648880	4.2269174

Zero-point correction= 0.620415 (Hartree/Particle)

Thermal correction to Energy= 0.666912

Thermal correction to Enthalpy= 0.667857

Thermal correction to Gibbs Free Energy= 0.539130

Sum of electronic and zero-point Energies= -2897.913166

Sum of electronic and thermal Energies= -2897.866669

Sum of electronic and thermal Enthalpies= -2897.865725

Sum of electronic and thermal Free Energies= -2897.994451

D-1

C	0.9939333	-1.0635244	2.5297874
C	0.1725873	-0.3362314	1.6810724
C	0.7243533	-2.4095054	2.7852954
C	-0.3870167	-3.0170204	2.2023104
C	-1.2108777	-2.2712294	1.3649484
C	-0.9390747	-0.9338414	1.0768364
C	-0.6537377	-1.5419444	-1.8938806
C	-0.7306327	-0.0650944	-1.9969436
N	-1.2332277	0.5888526	-0.9175976
C	-1.8821757	-0.1641844	0.1807224
C	-0.6210017	-2.7610024	-2.0394466
N	-4.0305367	0.9863096	0.7190494
C	-2.7193037	0.8138286	1.0215504
O	-2.1821757	1.4549466	1.9122644
O	-0.2845077	0.4606116	-3.0026036
O	1.5973183	-3.0678154	3.5839354
H	-2.5533687	-0.8941794	-0.2866976
Au	1.4508603	-1.8073654	-0.9622496
C	-0.6703137	-4.2030644	-2.1898776
C	-4.9835117	0.3023676	-0.1897326
C	-5.2356207	-1.1328074	0.2671944

C	-4.5241167	0.3556036	-1.6450766
C	-6.2825457	1.0951826	-0.0671696
C	1.6989983	3.4793336	1.1227094
C	2.7318493	3.5773426	0.1832474
C	2.4984123	3.2041636	-1.1427356
C	1.2452213	2.7141736	-1.5090776
C	0.2132883	2.5990036	-0.5783036
C	0.4545393	3.0077406	0.7404234
C	-1.1373077	2.0694046	-0.9825226
O	3.9159203	4.0272786	0.6552894
C	4.9629443	4.2293626	-0.2649316
H	-0.6125927	-4.0624924	2.4095914
H	-2.0807437	-2.7519134	0.9150784
H	-4.4469487	1.6563316	1.3585554
H	1.2752433	-3.9565874	3.7738114
H	-1.6103977	-4.4853684	-2.6770726
H	0.1529703	-4.5665814	-2.8132026
H	-0.6247107	-4.7021194	-1.2151746
H	-5.5950137	-1.1500524	1.3020944
H	-5.9965207	-1.6014444	-0.3680656
H	-4.3336427	-1.7547214	0.2132174
H	-4.2779307	1.3833336	-1.9368276
H	-5.3342697	0.0036046	-2.2938646
H	-3.6538117	-0.2775724	-1.8499216
H	-7.0582067	0.6482986	-0.6972536

H	-6.6504607	1.0932986	0.9664564
H	-6.1401087	2.1338246	-0.3881396
H	1.8973863	3.8016496	2.1418064
H	3.2728183	3.3061596	-1.8982316
H	1.0628513	2.4242856	-2.5419566
H	-0.3499367	2.9398386	1.4731124
H	-1.3609507	2.3456276	-2.0182366
H	-1.9217217	2.4913966	-0.3507546
H	5.8039103	4.6295746	0.3037914
H	4.6828363	4.9487066	-1.0463036
H	5.2707313	3.2872526	-0.7440926
P	3.6068663	-1.4652934	-0.1451786
C	4.1298223	-2.5874734	1.1870774
H	4.1703483	-3.6104914	0.8000644
H	5.1280313	-2.2974644	1.5360704
H	3.4272683	-2.5598104	2.0266524
C	3.7929553	0.2336736	0.4719264
H	4.8172303	0.4013426	0.8259764
H	3.5579713	0.9364186	-0.3370316
H	3.0872273	0.4194936	1.2869434
C	4.8769763	-1.6392964	-1.4379706
H	5.8672783	-1.4203624	-1.0216356
H	4.8703833	-2.6586524	-1.8351626
H	4.6656293	-0.9442694	-2.2562206
H	0.3929163	0.7109276	1.4864554

H	1.8391403	-0.5997684	3.0358264

Zero-point correction= 0.594033 (Hartree/Particle)

Thermal correction to Energy= 0.634457

Thermal correction to Enthalpy= 0.635402

Thermal correction to Gibbs Free Energy= 0.519635

Sum of electronic and zero-point Energies= -1936.559135

Sum of electronic and thermal Energies= -1936.518711

Sum of electronic and thermal Enthalpies= -1936.517767

Sum of electronic and thermal Free Energies= -1936.633534

D-ts1

C	-1.8292047	-0.1510389	1.8169043
C	-0.7177267	-0.2610329	1.0032823
C	-2.6909527	0.9371771	1.6583733
C	-2.4786457	1.8804301	0.6398083
C	-1.3680977	1.7629281	-0.1674097
C	-0.4655257	0.6930551	-0.0109567
C	-1.1896537	-0.8516199	-1.5920757
C	0.1955803	-1.1042499	-1.9956537
N	1.1996813	-0.3783279	-1.4717827
C	0.8991263	0.7949871	-0.6593907
C	-2.4092817	-1.1915779	-1.7660527
N	2.8643903	1.9517871	0.3959613
C	1.9767323	0.9234441	0.4437623
O	2.0387573	0.0716621	1.3132143
O	0.3009903	-1.9979299	-2.8269297

O	-3.7227057	1.0499021	2.5209853
H	0.9045493	1.6817101	-1.3090887
Au	-4.1035087	-0.7505169	-0.5635647
C	-2.8323677	-2.1345689	-2.8826147
C	2.9227573	3.2548511	-0.3118807
C	1.6721353	4.0825321	-0.0280327
C	3.1524513	3.0972161	-1.8133567
C	4.1352033	3.9674471	0.2825813
C	5.5151663	-1.4133339	0.2481613
C	5.1336543	-2.6495159	0.7775463
C	3.9208403	-3.2245419	0.3882313
C	3.1052603	-2.5549349	-0.5155107
C	3.4676683	-1.3155379	-1.0352497
C	4.6868173	-0.7583479	-0.6464227
C	2.5591853	-0.6020629	-1.9953397
O	6.0014133	-3.2078519	1.6485203
C	5.6733203	-4.4611209	2.2012113
H	-3.1764057	2.7073911	0.5112843
H	-1.1889047	2.5033941	-0.9452247
H	3.5219843	1.8529541	1.1639643
H	-4.1028697	1.9354511	2.4676473
H	-1.9674717	-2.4479449	-3.4731267
H	-3.3209277	-3.0159369	-2.4538247
H	-3.5695407	-1.6391599	-3.5229647
H	1.5229523	4.1965231	1.0517113

H	1.7728453	5.0811601	-0.4690607
H	0.7682913	3.6281071	-0.4508417
H	4.0515553	2.5004221	-2.0084437
H	3.3024953	4.0850901	-2.2642177
H	2.3089343	2.6337521	-2.3377247
H	4.2649973	4.9489841	-0.1843907
H	4.0130503	4.1213101	1.3617703
H	5.0503893	3.3869941	0.1115773
H	6.4680893	-0.9934199	0.5591613
H	3.6102323	-4.1892389	0.7778383
H	2.1636783	-3.0102439	-0.8230927
H	4.9909583	0.2092721	-1.0473097
H	2.4236763	-1.1783719	-2.9179357
H	2.9789963	0.3724581	-2.2759667
H	6.4966603	-4.7320919	2.8643203
H	5.5710113	-5.2317219	1.4243193
H	4.7433013	-4.4149509	2.7852453
P	-6.1650157	-0.6612769	0.6002043
C	-6.9097457	0.9979551	0.7559693
H	-7.0924527	1.4137021	-0.2395437
H	-7.8574887	0.9418871	1.3039853
H	-6.2266757	1.6639231	1.2903243
C	-6.0878787	-1.3148529	2.2993973
H	-7.0766007	-1.2677809	2.7707803
H	-5.7526817	-2.3563189	2.2710213

H	-5.3695827	-0.7299709	2.8817563
C	-7.4661557	-1.6490879	-0.2108517
H	-8.3993357	-1.5954859	0.3620143
H	-7.6415417	-1.2739289	-1.2236617
H	-7.1458257	-2.6931649	-0.2790667
H	0.0022083	-1.0604529	1.1551303
H	-2.0272117	-0.8663449	2.6105963

Zero-point correction= 0.593319 (Hartree/Particle)

Thermal correction to Energy= 0.632826

Thermal correction to Enthalpy= 0.633770

Thermal correction to Gibbs Free Energy= 0.519166

Sum of electronic and zero-point Energies= -1936.523772

Sum of electronic and thermal Energies= -1936.484265

Sum of electronic and thermal Enthalpies= -1936.483321

Sum of electronic and thermal Free Energies= -1936.597925

D-int1

C	-1.0745047	-1.2994193	1.6349170
C	-0.3406287	-1.0068513	0.5101500
C	-1.8832467	-0.3026243	2.1772360
C	-2.0397167	0.9783537	1.5489810
C	-1.4425427	1.2079367	0.3621670
C	-0.5633267	0.2206357	-0.2845240
C	-1.0853397	-0.3079003	-1.6649130
C	0.1498263	-0.5533883	-2.4692120
N	1.2135863	0.0346807	-1.8085080

C	0.7828343	0.8673627	-0.7111330
C	-2.3610127	-0.5963613	-1.9857570
N	2.6145673	1.8739577	0.6582750
C	1.7310003	0.8669777	0.4894410
O	1.6770483	-0.0736123	1.2799950
O	0.2622653	-1.1946883	-3.4957940
O	-2.5257307	-0.5810343	3.2975660
H	0.5825543	1.8961037	-1.0535130
Au	-4.0245357	-0.4996713	-0.7337150
C	-2.7114257	-1.0965503	-3.3572850
C	2.6843263	3.2710377	0.1480310
C	1.4293163	4.0415617	0.5515480
C	2.9137613	3.3400057	-1.3580020
C	3.8952103	3.8809127	0.8487000
C	5.2569943	-1.2579813	0.1856410
C	4.8659533	-2.5776983	0.4309520
C	3.7559263	-3.1053723	-0.2352080
C	3.0482473	-2.3038413	-1.1236900
C	3.4148693	-0.9801713	-1.3595040
C	4.5376533	-0.4751393	-0.7010990
C	2.5869313	-0.1272353	-2.2802150
O	5.6237863	-3.2593943	1.3158840
C	5.2997153	-4.6067503	1.5696820
H	-2.6882617	1.7213557	2.0118300
H	-1.6146267	2.1429767	-0.1702780

H	3.1956383	1.6883867	1.4708690
H	-3.0184347	0.1838047	3.6271270
H	-1.8670317	-1.1328693	-4.0488130
H	-3.1335267	-2.1073573	-3.2731130
H	-3.5119757	-0.4786373	-3.7830270
H	1.2763083	3.9900797	1.6357780
H	1.5276263	5.0961167	0.2692520
H	0.5288913	3.6560787	0.0569430
H	3.8314653	2.8095357	-1.6379370
H	3.0323253	4.3885977	-1.6539190
H	2.0841333	2.9331937	-1.9464760
H	4.0327913	4.9186337	0.5289740
H	3.7663623	3.8806917	1.9383000
H	4.8087533	3.3259767	0.6022700
H	6.1350573	-0.8792283	0.7022720
H	3.4495563	-4.1355213	-0.0795170
H	2.1943963	-2.7223373	-1.6593630
H	4.8520253	0.5532187	-0.8834190
H	2.4787413	-0.5909593	-3.2688350
H	3.0520753	0.8550877	-2.4278100
H	6.0316453	-4.9700913	2.2929530
H	5.3639963	-5.2167483	0.6579890
H	4.2925033	-4.7071033	1.9983600
P	-6.0588707	-0.5443683	0.5299510
C	-5.8899887	-0.1323803	2.3061180

H	-5.5019577	0.8877177	2.4077950
H	-6.8578467	-0.1941793	2.8172120
H	-5.1936527	-0.8378093	2.7729500
C	-6.8725957	-2.1785263	0.5497730
H	-7.7999387	-2.1431153	1.1333350
H	-7.1030037	-2.4844593	-0.4752720
H	-6.1973387	-2.9216893	0.9847790
C	-7.3618997	0.5923057	-0.0566590
H	-8.2653037	0.4952997	0.5567180
H	-7.0026947	1.6249847	-0.0133990
H	-7.6068007	0.3594347	-1.0974720
H	0.3241473	-1.7526123	0.0813090
H	-0.9870527	-2.2473263	2.1553570

Zero-point correction= 0.595114 (Hartree/Particle)

Thermal correction to Energy= 0.633611

Thermal correction to Enthalpy= 0.634555

Thermal correction to Gibbs Free Energy= 0.522441

Sum of electronic and zero-point Energies= -1936.544046

Sum of electronic and thermal Energies= -1936.505548

Sum of electronic and thermal Enthalpies= -1936.504604

Sum of electronic and thermal Free Energies= -1936.616718

D-ts2

C	1.9231260	0.5389219	-1.6541154
C	0.7979750	-0.0517901	-1.2179974
C	2.5524830	1.5532359	-0.8382754

C	1.9398070	2.0817359	0.2739186
C	0.6558900	1.6166539	0.6249106
C	0.1455610	0.3260229	0.0577646
C	0.3131120	-0.7101271	1.2112976
C	-0.9848650	-0.6868721	1.9426646
N	-1.8752270	0.1325249	1.2437346
C	-1.3841070	0.4081039	-0.0894294
C	1.4161490	-1.4297161	1.5064306
N	-0.7607950	2.7801849	-0.3438434
C	-1.8244870	1.8063019	-0.4802044
O	-2.9557700	2.0886199	-0.7712384
O	-1.2864400	-1.2540601	2.9738186
O	3.7641360	1.9142269	-1.2513664
Au	3.2427530	-1.4306911	0.4908176
C	1.4365550	-2.3750621	2.6725756
C	-5.1512780	-1.8680071	-1.2894324
C	-5.0087450	-3.1991481	-0.8835554
C	-4.3216340	-3.4927581	0.2971956
C	-3.7881680	-2.4565631	1.0569606
C	-3.9269460	-1.1252181	0.6639786
C	-4.6164150	-0.8474361	-0.5222534
C	-3.3190530	-0.0232561	1.4856606
O	-5.5676000	-4.1226091	-1.6947914
C	-5.4938710	-5.4762381	-1.3104344
H	2.4348800	2.8465119	0.8682216

H	4.1372960	2.5961879	-0.6750464
H	0.5015220	-2.4167681	3.2340706
H	1.6959130	-3.3820161	2.3204266
H	2.2502720	-2.0888401	3.3524246
H	-5.6975310	-1.6665101	-2.2072604
H	-4.2079970	-4.5175491	0.6379196
H	-3.2601650	-2.6850571	1.9819946
H	-4.7361230	0.1876399	-0.8402214
H	-3.4015740	-0.2319221	2.5572736
H	-3.8113250	0.9354549	1.2858666
H	-6.0145950	-6.0457251	-2.0821324
H	-5.9862310	-5.6491271	-0.3435194
H	-4.4530270	-5.8243581	-1.2493334
P	5.3952730	-1.5893781	-0.5468644
C	5.4478740	-1.1166441	-2.3116664
H	5.1360160	-0.0716911	-2.4155114
H	6.4607260	-1.2331471	-2.7146174
H	4.7604740	-1.7486461	-2.8832324
C	6.1129070	-3.2679901	-0.5174804
H	7.0970520	-3.2772071	-1.0003494
H	6.2152380	-3.6052071	0.5185206
H	5.4474880	-3.9623281	-1.0395104
C	6.6901210	-0.5462611	0.2114496
H	7.6505980	-0.6884901	-0.2975534
H	6.3985640	0.5063959	0.1407606

H	6.7999700	-0.8034431	1.2692736
H	-1.7810650	-0.3167541	-0.8235934
H	0.2634220	1.8757129	1.6065786
H	-0.2337260	2.8242059	-1.2212304
C	-1.1310650	4.1785319	0.0940806
C	-2.0194580	4.0876679	1.3270676
C	0.1723980	4.8850249	0.4431866
C	-1.8244250	4.9152649	-1.0472674
H	-3.0184070	3.7115579	1.0901856
H	-1.5746700	3.4438359	2.0970186
H	-2.1338370	5.0880689	1.7575006
H	0.8813760	4.8667209	-0.3952694
H	-0.0383550	5.9349559	0.6730256
H	0.6521440	4.4438909	1.3248236
H	-2.0659130	5.9348039	-0.7251624
H	-1.1656120	4.9946749	-1.9221994
H	-2.7503550	4.4180989	-1.3446114
H	2.4282960	0.2384579	-2.5685004
H	0.3534880	-0.8755881	-1.7743284

Zero-point correction= 0.595198 (Hartree/Particle)

Thermal correction to Energy= 0.633321

Thermal correction to Enthalpy= 0.634265

Thermal correction to Gibbs Free Energy= 0.523204

Sum of electronic and zero-point Energies= -1936.526509

Sum of electronic and thermal Energies= -1936.488387

Sum of electronic and thermal Enthalpies= -1936.487443

Sum of electronic and thermal Free Energies= -1936.598503

D-int2

C	-1.8300818	0.3029730	1.8816629
C	-0.7539968	-0.2346110	1.2974579
C	-2.5053338	1.4378920	1.2662239
C	-1.9571808	2.1322260	0.2463349
C	-0.5945388	1.7875420	-0.2326821
C	-0.1308728	0.3301840	0.0612049
C	-0.2403708	-0.5249260	-1.2000481
C	1.0615512	-0.3897870	-1.9036701
N	1.9246692	0.3624260	-1.0791021
C	1.3902622	0.4440690	0.2563359
C	-1.3151028	-1.2418140	-1.6039881
N	0.4663432	2.7111910	0.4354859
C	1.6454072	1.8054870	0.8246139
O	2.5395202	2.2187440	1.4892249
O	1.4208582	-0.8089760	-2.9851151
O	-3.7192428	1.6817780	1.7929739
Au	-3.1120498	-1.4140370	-0.5608751
C	-1.3076818	-2.0043890	-2.8943921
C	5.0825482	-1.8380430	1.4066339
C	5.0110062	-3.1193070	0.8486349
C	4.4159162	-3.2973360	-0.4035271
C	3.9025202	-2.1976220	-1.0830271

C	3.9738162	-0.9152260	-0.5394891
C	4.5699802	-0.7531980	0.7166639
C	3.3784202	0.2541920	-1.2690051
O	5.5414622	-4.1118920	1.5923659
C	5.5320442	-5.4186950	1.0632389
H	-2.5115528	2.9261780	-0.2493391
H	-4.1240218	2.4447150	1.3604939
H	-0.3776248	-1.9256540	-3.4612851
H	-1.5196638	-3.0624310	-2.6915821
H	-2.1411518	-1.6608630	-3.5215571
H	5.5562002	-1.7262140	2.3783679
H	4.3566902	-4.2812810	-0.8588891
H	3.4414522	-2.3351780	-2.0604311
H	4.6383082	0.2432700	1.1553659
H	3.5190492	0.1695150	-2.3517601
H	3.8455352	1.1929310	-0.9397201
H	6.0164082	-6.0555480	1.8052059
H	6.0927542	-5.4763680	0.1202569
H	4.5078542	-5.7798680	0.8947459
P	-5.2395148	-1.7156500	0.4940689
C	-5.2213598	-1.7565220	2.3212659
H	-4.8748408	-0.7885970	2.6978299
H	-6.2256428	-1.9547830	2.7138629
H	-4.5376778	-2.5368120	2.6698709
C	-6.0922758	-3.2621490	0.0281239

H	-7.0653328	-3.3352570	0.5278109
H	-6.2390218	-3.2876760	-1.0559951
H	-5.4756818	-4.1210450	0.3101639
C	-6.4627888	-0.4100300	0.1200279
H	-7.4185158	-0.6168620	0.6156839
H	-6.0738388	0.5505800	0.4723679
H	-6.6206468	-0.3479490	-0.9608841
H	1.8231452	-0.3140580	0.9313509
H	-0.4838608	1.9694600	-1.3062161
H	0.0571482	3.0274360	1.3252719
C	0.8754892	4.0209070	-0.3248041
C	1.7842182	3.6561270	-1.4832921
C	-0.3970848	4.6956860	-0.8120671
C	1.5772852	4.9270850	0.6764109
H	2.7439402	3.2522230	-1.1438381
H	1.3284542	2.9415420	-2.1768051
H	1.9989642	4.5716450	-2.0446331
H	-1.0864148	4.9121560	0.0124649
H	-0.1148388	5.6534090	-1.2621211
H	-0.9213868	4.1215230	-1.5826011
H	1.8230952	5.8674500	0.1716179
H	0.9224572	5.1736760	1.5223409
H	2.5029342	4.4964740	1.0624959
H	-2.2798948	-0.1258680	2.7739529
H	-0.2966188	-1.1361710	1.7022679

Zero-point correction= 0.596877 (Hartree/Particle)

Thermal correction to Energy= 0.634479

Thermal correction to Enthalpy= 0.635423

Thermal correction to Gibbs Free Energy= 0.526122

Sum of electronic and zero-point Energies= -1936.539417

Sum of electronic and thermal Energies= -1936.501816

Sum of electronic and thermal Enthalpies= -1936.500872

Sum of electronic and thermal Free Energies= -1936.610173

D-ts3

C	-1.3987098	-0.3769082	2.1065010
C	-0.5065538	-0.7257932	1.1586410
C	-2.1282048	0.8442368	1.9700550
C	-1.8567188	1.7840298	0.9734120
C	-0.8209288	1.4839308	-0.1004540
C	-0.1040118	0.1079058	-0.0060350
C	-0.1721028	-0.6550902	-1.3211210
C	1.1307992	-0.4571902	-2.0114190
N	1.9309962	0.3373998	-1.1864460
C	1.3949512	0.4587558	0.1472370
C	-1.2563108	-1.3285982	-1.7658100
N	0.1890492	2.5467258	0.2914200
C	1.4653732	1.9124378	0.5551450
O	2.4295302	2.4846268	0.9829940
O	1.5031632	-0.8662122	-3.0930500
O	-3.0605618	1.0369568	2.8878700

Au	-3.0327748	-1.4743542	-0.6896630
C	-1.2689268	-2.0239252	-3.0915690
C	5.3857452	-1.2811842	1.3423570
C	5.4707052	-2.5917142	0.8597530
C	4.8794222	-2.9195172	-0.3635050
C	4.2154422	-1.9362702	-1.0900350
C	4.1318012	-0.6254562	-0.6228750
C	4.7245452	-0.3130922	0.6059950
C	3.3802042	0.4136448	-1.4045880
O	6.1405682	-3.4627862	1.6441220
C	6.3013852	-4.7847632	1.1830310
H	-2.6577288	2.4793258	0.7127980
H	-3.5124418	1.8847428	2.7633540
H	-0.3331488	-1.9290592	-3.6475880
H	-1.4926728	-3.0887842	-2.9439220
H	-2.0944048	-1.6362152	-3.7031080
H	5.8598442	-1.0518682	2.2931310
H	4.9405192	-3.9280722	-0.7613010
H	3.7602042	-2.1896052	-2.0471170
H	4.6675302	0.7085918	0.9829560
H	3.5121402	0.2805308	-2.4836920
H	3.7220102	1.4222168	-1.1386310
H	6.8844122	-5.3083372	1.9425360
H	6.8448862	-4.8163852	0.2287050
H	5.3340662	-5.2924002	1.0611980

P	-5.1218618	-1.7097982	0.4717280
C	-4.9695678	-2.0623532	2.2594470
H	-4.4603228	-1.2278632	2.7548840
H	-5.9577718	-2.1988822	2.7141840
H	-4.3771578	-2.9705962	2.4084110
C	-6.2031618	-3.0413542	-0.1528720
H	-7.1368208	-3.0834092	0.4200410
H	-6.4334868	-2.8638892	-1.2077750
H	-5.6865628	-4.0026132	-0.0723230
C	-6.1851838	-0.2223292	0.4280060
H	-7.1183278	-0.3904102	0.9782600
H	-5.6484328	0.6194498	0.8789340
H	-6.4185368	0.0360608	-0.6093370
H	1.9494272	-0.1659142	0.8677540
H	-1.1869628	1.6332268	-1.1203400
H	-0.7483968	2.5607478	1.2983710
C	0.2182662	3.8740888	-0.4789920
C	0.9303002	3.6415778	-1.8040590
C	-1.2095998	4.3497608	-0.7203080
C	0.9347172	4.9161598	0.3708440
H	1.9752772	3.3485978	-1.6563520
H	0.4359822	2.8724618	-2.4102850
H	0.9273752	4.5728368	-2.3811950
H	-1.7311548	4.5695508	0.2188200
H	-1.1589088	5.2874258	-1.2832770

H	-1.8092978	3.6554828	-1.3195320
H	0.8648722	5.8839348	-0.1381260
H	0.4555832	5.0161698	1.3523520
H	1.9881792	4.6805508	0.5242680
H	-1.6339678	-1.0199492	2.9501320
H	0.0124152	-1.6812002	1.2370580

Zero-point correction= 0.591554 (Hartree/Particle)

Thermal correction to Energy= 0.629778

Thermal correction to Enthalpy= 0.630722

Thermal correction to Gibbs Free Energy= 0.517809

Sum of electronic and zero-point Energies= -1936.500774

Sum of electronic and thermal Energies= -1936.462551

Sum of electronic and thermal Enthalpies= -1936.461607

Sum of electronic and thermal Free Energies= -1936.574520

D-int3

C	-0.3490607	-1.8935325	1.3879134
C	0.4949963	-1.3702485	0.4326084
C	-1.1587637	-1.0037745	2.0841294
C	-1.0256157	0.4685515	1.9484124
C	-0.6907737	0.8998865	0.5137634
C	0.3281623	-0.0410605	-0.1411146
C	-0.0037677	-0.4776175	-1.5851376
C	1.2685673	-0.2951605	-2.3676136
N	2.1252553	0.4426725	-1.5888846
C	1.6212493	0.7556935	-0.2818906

C	-1.1975977	-0.9406745	-2.0186256
N	-0.1022047	2.2278805	0.4097784
C	1.1607113	2.2047915	-0.1508046
O	1.8249883	3.1492295	-0.5182096
O	1.5227923	-0.7045685	-3.4844206
O	-2.0112827	-1.3911155	3.0045604
Au	-2.9381347	-1.1729065	-0.8692366
C	-1.4307967	-1.2351295	-3.4684936
C	5.9833723	-0.2315805	0.7785744
C	6.1113043	-1.6095425	0.5758304
C	5.3976423	-2.2282425	-0.4553896
C	4.5735273	-1.4607875	-1.2726526
C	4.4493203	-0.0845415	-1.0885616
C	5.1604963	0.5175245	-0.0463846
C	3.5130683	0.7100065	-1.9537346
O	6.9409293	-2.2532495	1.4254094
C	7.1685073	-3.6280185	1.2188554
H	-1.9369677	0.9445145	2.3243144
H	-0.5318957	-1.1340805	-4.0821816
H	-1.8383417	-2.2476555	-3.5841146
H	-2.2095587	-0.5622485	-3.8544246
H	6.5520153	0.2240265	1.5850034
H	5.4918283	-3.2947315	-0.6380596
H	4.0277593	-1.9381395	-2.0879296
H	5.0687763	1.5930705	0.1097824

H	3.5971913	0.4340975	-3.0108256
H	3.6958343	1.7871145	-1.8606966
H	7.8866733	-3.9405805	1.9787574
H	7.5916783	-3.8225545	0.2237304
H	6.2461663	-4.2149915	1.3361294
P	-5.0477147	-1.3867835	0.2572524
C	-5.4081747	-3.0296555	0.9714544
H	-4.6594277	-3.2796195	1.7298624
H	-6.4016427	-3.0386615	1.4348254
H	-5.3700877	-3.7912525	0.1867634
C	-6.4768537	-1.0555075	-0.8280966
H	-7.4152907	-1.1469375	-0.2688886
H	-6.3991677	-0.0452355	-1.2413556
H	-6.4813907	-1.7669975	-1.6595096
C	-5.2804227	-0.2392795	1.6608784
H	-6.2685227	-0.3782615	2.1150924
H	-4.5092207	-0.4177025	2.4182604
H	-5.1932627	0.7938775	1.3088094
H	2.3759553	0.5296855	0.4900374
H	-1.6213117	0.8559865	-0.0686166
C	-0.9704627	3.4476505	0.2840244
C	-1.2734577	3.6579735	-1.1973436
C	-2.2745857	3.2498275	1.0515664
C	-0.2559207	4.6538715	0.8866444
H	-0.3543147	3.8462165	-1.7605926

H	-1.7726297	2.7763485	-1.6254126
H	-1.9372187	4.5198525	-1.3315036
H	-2.0973847	3.1255585	2.1271964
H	-2.8827357	4.1522675	0.9286344
H	-2.8749197	2.4095835	0.6761014
H	-0.9269317	5.5199085	0.8514184
H	-0.0017147	4.4633135	1.9361574
H	0.6589643	4.8968235	0.3453284
H	-0.2107497	0.7765355	2.6243904
H	-2.0062087	-2.3557035	3.1144374
H	1.3037033	-1.9733285	0.0148104
H	-0.3449477	-2.9526815	1.6392084

Zero-point correction= 0.597809 (Hartree/Particle)

Thermal correction to Energy= 0.635854

Thermal correction to Enthalpy= 0.636798

Thermal correction to Gibbs Free Energy= 0.526165

Sum of electronic and zero-point Energies= -1936.553567

Sum of electronic and thermal Energies= -1936.515522

Sum of electronic and thermal Enthalpies= -1936.514578

Sum of electronic and thermal Free Energies= -1936.625211

D-ts4

C	0.5349400	-1.3433934	2.9164255
C	1.1688640	-1.1216024	1.7599995
C	-0.7709620	-0.7199654	2.8569735
C	-0.8110010	0.7239716	2.5923145

C	-0.5877090	0.6656096	1.0166635
C	0.4729420	-0.3955564	0.6346465
C	-0.0459880	-1.5442624	-0.2290465
C	0.9770370	-1.7091754	-1.3213325
N	1.7057820	-0.5377344	-1.3571395
C	1.4953640	0.3241196	-0.2242965
C	-1.1501470	-2.3130034	-0.0377335
N	-0.1855990	1.8876156	0.3531945
C	0.8712850	1.6708946	-0.5298055
O	1.2487150	2.4178236	-1.4049635
O	1.1070400	-2.6427934	-2.0876375
O	-1.8112980	-1.4144764	2.5928965
Au	-3.1276570	-1.4034704	-0.0345955
C	-1.2983790	-3.6138654	-0.7906045
C	6.0028980	0.6315886	-0.3442775
C	6.4723690	-0.6129734	0.0894635
C	5.7690130	-1.7743654	-0.2446675
C	4.6123660	-1.6770934	-1.0123985
C	4.1431720	-0.4433344	-1.4604605
C	4.8510500	0.7104726	-1.1087515
C	2.8605430	-0.3569454	-2.2371715
O	7.6044370	-0.5886454	0.8241705
C	8.1553850	-1.8172174	1.2398495
H	-1.7888360	1.1577716	2.8065865
H	-0.3529150	-4.1603334	-0.8583125

H	-2.0546290	-4.2552994	-0.3270215
H	-1.6146610	-3.4327034	-1.8280795
H	6.5699860	1.5177796	-0.0717095
H	6.1214470	-2.7514534	0.0724005
H	4.0708640	-2.5835884	-1.2858415
H	4.4880430	1.6819786	-1.4461865
H	2.7830730	-1.1490514	-2.9900945
H	2.7643790	0.6135736	-2.7377515
H	9.0676300	-1.5771234	1.7884105
H	8.4097550	-2.4564144	0.3832065
H	7.4719140	-2.3642444	1.9047815
P	-5.2853910	-0.5515264	-0.4656935
C	-6.2257700	-0.1357454	1.0401095
H	-5.6893970	0.6303346	1.6091615
H	-7.2210200	0.2406646	0.7763265
H	-6.3301830	-1.0248264	1.6690805
C	-6.3523820	-1.7109624	-1.3804995
H	-7.3406890	-1.2664714	-1.5460275
H	-5.8969600	-1.9492534	-2.3464315
H	-6.4642250	-2.6389374	-0.8117045
C	-5.3080300	0.9804416	-1.4545855
H	-6.3415000	1.3011426	-1.6305365
H	-4.7699680	1.7733346	-0.9235315
H	-4.8131190	0.8108336	-2.4160615
H	2.4499900	0.5019196	0.3024105

H	-1.5635100	0.3418586	0.6232755
C	-1.1848350	2.9687016	0.0377475
C	-1.8088640	2.6648396	-1.3238805
C	-2.2860950	3.0118516	1.0918425
C	-0.4793590	4.3217136	0.0427635
H	-1.0626410	2.7062516	-2.1214885
H	-2.2676290	1.6632526	-1.3268395
H	-2.5909560	3.3998826	-1.5506975
H	-1.8927450	3.2437896	2.0886385
H	-2.9766400	3.8196976	0.8255535
H	-2.8775200	2.0857396	1.1355915
H	-1.2148720	5.1118706	-0.1476365
H	-0.0236770	4.5105056	1.0216815
H	0.2958140	4.3765246	-0.7226115
H	-0.0047420	1.2733986	3.0839685
H	-1.6379550	-2.0763544	1.7507815
H	2.1235850	-1.5912414	1.5133555
H	0.8407760	-2.0363444	3.6938315

Zero-point correction= 0.592145 (Hartree/Particle)

Thermal correction to Energy= 0.629595

Thermal correction to Enthalpy= 0.630539

Thermal correction to Gibbs Free Energy= 0.521649

Sum of electronic and zero-point Energies= -1936.496502

Sum of electronic and thermal Energies= -1936.459051

Sum of electronic and thermal Enthalpies= -1936.458107

Sum of electronic and thermal Free Energies= -1936.566997

D-2

C	0.2149649	-1.5387442	1.9062547
C	-0.9047991	-0.8227412	1.6738747
C	1.4448919	-1.1873002	1.2464357
C	1.3812409	-0.1614522	0.1595057
C	0.3951009	0.9813448	0.4268847
C	-0.9602031	0.4657498	0.9332537
C	-1.7255641	1.4488828	1.8144167
C	-3.1338791	1.5087378	1.3139857
N	-3.1433831	0.8514248	0.1091837
C	-1.8442431	0.4135938	-0.3224223
C	-1.2335101	2.0588588	2.8987717
N	0.0803549	1.7106728	-0.7948163
C	-1.1932721	1.4465488	-1.2476463
O	-1.7665091	1.9598988	-2.1849763
O	-4.1049381	2.0027848	1.8554307
O	2.4970589	-1.8042762	1.5187517
Au	4.4215909	-1.5036912	0.5914747
C	-1.9575251	2.9965788	3.7959797
C	-4.7106611	-3.0177792	-1.8554673
C	-5.0827981	-3.6656542	-0.6739443
C	-5.2208371	-2.9290802	0.5067197
C	-4.9903051	-1.5576242	0.4870247
C	-4.6291171	-0.8990482	-0.6874783

C	-4.4864131	-1.6503692	-1.8564853
C	-4.3473141	0.5773848	-0.6616863
O	-5.2831241	-4.9986762	-0.7720483
C	-5.7261571	-5.6889052	0.3728077
H	2.3892689	0.2213798	-0.0436623
H	-2.9974221	3.1227058	3.4909507
H	-1.9286371	2.6265588	4.8283777
H	-1.4570731	3.9729758	3.8073157
H	-4.6139291	-3.6134272	-2.7594713
H	-5.5195991	-3.4102122	1.4334827
H	-5.1110771	-0.9775592	1.4034937
H	-4.2050151	-1.1496942	-2.7830313
H	-5.1473731	1.1398388	-0.1660683
H	-4.2197631	0.9813408	-1.6738173
H	-5.8571691	-6.7307282	0.0752437
H	-6.6862761	-5.2964752	0.7355777
H	-4.9895491	-5.6400932	1.1876677
P	6.4936429	-1.2141612	-0.3596723
C	7.8170159	-0.9752372	0.8631357
H	7.8814429	-1.8502282	1.5166617
H	8.7763159	-0.8335552	0.3519397
H	7.6004719	-0.0960942	1.4772167
C	6.5473629	0.2452098	-1.4437343
H	7.5469519	0.3554008	-1.8799083
H	5.8126619	0.1347648	-2.2472173

H	6.3037319	1.1424948	-0.8664933
C	7.0115009	-2.6191642	-1.3897293
H	7.9985349	-2.4203422	-1.8231993
H	7.0598479	-3.5275562	-0.7819883
H	6.2872319	-2.7757542	-2.1945943
H	-1.9027671	-0.5754002	-0.8050793
H	0.8272479	1.6568688	1.1786347
C	0.8571099	2.9009408	-1.2652623
C	0.1595379	4.1513178	-0.7364553
C	2.2895839	2.8497488	-0.7386753
C	0.9255289	2.9060708	-2.7906273
H	-0.8630841	4.2143788	-1.1216283
H	0.1185789	4.1403658	0.3612387
H	0.6986869	5.0533088	-1.0487403
H	2.8439499	1.9935728	-1.1469483
H	2.8057989	3.7563578	-1.0724373
H	2.3531749	2.8348128	0.3558917
H	1.5543959	3.7425548	-3.1173933
H	1.3776019	1.9751988	-3.1555143
H	-0.0621381	3.0102748	-3.2410683
H	1.0580819	-0.6960592	-0.7495803
H	-0.1869571	1.8563978	3.1547367
H	-1.8585591	-1.1590122	2.0862967
H	0.2204789	-2.4212072	2.5403527

Zero-point correction= 0.597055 (Hartree/Particle)

Thermal correction to Energy= 0.635655

Thermal correction to Enthalpy= 0.636599

Thermal correction to Gibbs Free Energy= 0.519145

Sum of electronic and zero-point Energies= -1936.599825

Sum of electronic and thermal Energies= -1936.561224

Sum of electronic and thermal Enthalpies= -1936.560280

Sum of electronic and thermal Free Energies= -1936.677734

D-ts5

C	0.2195453	-2.5486986	-2.0494115
C	-0.3959207	-1.7094086	-1.1844935
C	1.6129273	-2.2361616	-2.0879435
C	2.0081663	-0.8332606	-2.2471075
C	1.3674443	0.0205104	-1.4408145
C	0.3556493	-0.5623396	-0.5228435
C	0.9741743	-1.3114966	0.6864165
C	-0.1314517	-1.3094756	1.7052695
N	-1.0247327	-0.3272826	1.3337615
C	-0.5866547	0.4267504	0.1656295
C	2.1817103	-1.9278096	0.8135235
N	-2.2185277	2.1196854	-0.6771345
C	-1.7102557	0.8648654	-0.7789845
O	-2.1418197	0.0749384	-1.6095195
O	-0.2437857	-2.0246346	2.6820025
O	2.4722273	-3.0639546	-1.6284615
H	0.0073283	1.3007154	0.4806935

Au	3.9957253	-0.9007886	0.2055295
C	2.4675943	-2.7783316	2.0280865
C	-1.7085777	3.3953544	-0.1104135
C	-0.3773867	3.7765794	-0.7559555
C	-1.5907357	3.3583494	1.4097775
C	-2.7598277	4.4368474	-0.4850465
C	-5.5652017	-0.2319776	0.1923075
C	-5.6494317	-1.5894166	-0.1327185
C	-4.6497447	-2.4672806	0.2973665
C	-3.5779917	-1.9738816	1.0331035
C	-3.4720187	-0.6186766	1.3412225
C	-4.4880937	0.2416624	0.9208325
C	-2.2647717	-0.1127046	2.0800745
O	-6.7307257	-1.9535206	-0.8526235
C	-6.8811477	-3.3140176	-1.1871765
H	2.8714533	-0.5871006	-2.8603335
H	1.6530263	1.0683604	-1.3477635
H	-2.9672837	2.2296354	-1.3553195
H	2.6850893	-2.5714706	-0.5953955
H	1.6274163	-3.4328776	2.2783865
H	3.3668293	-3.3837756	1.8800545
H	2.6342843	-2.1499426	2.9135855
H	-0.4662717	3.7857434	-1.8483985
H	-0.0729727	4.7776944	-0.4287385
H	0.4297893	3.0864524	-0.4791215

H	-2.5583517	3.1220574	1.8682935
H	-1.2832247	4.3462444	1.7717765
H	-0.8489547	2.6376644	1.7716935
H	-2.4768007	5.4189254	-0.0929475
H	-2.8594117	4.5265834	-1.5739645
H	-3.7372087	4.1713894	-0.0637345
H	-6.3644857	0.4247904	-0.1408045
H	-4.7079197	-3.5294806	0.0793175
H	-2.8096377	-2.6618966	1.3901555
H	-4.4282447	1.3038114	1.1614105
H	-2.1168947	-0.6510996	3.0240285
H	-2.3701837	0.9519654	2.3183245
H	-7.8081497	-3.3912976	-1.7576775
H	-6.9589717	-3.9446096	-0.2906855
H	-6.0478757	-3.6723556	-1.8078835
P	6.0539313	0.2117864	-0.0806465
C	6.2773613	0.9071634	-1.7525745
H	5.4877643	1.6365764	-1.9592195
H	7.2530253	1.3999014	-1.8365615
H	6.2157013	0.1046884	-2.4945535
C	7.4991923	-0.8700636	0.1659915
H	8.4265763	-0.3074456	0.0073655
H	7.4901233	-1.2723216	1.1834925
H	7.4583353	-1.7074506	-0.5370855
C	6.3268793	1.6166624	1.0479335

H	7.3048203	2.0732314	0.8559425
H	5.5433343	2.3667104	0.9049635
H	6.2885173	1.2693084	2.0847755
H	-1.3437647	-1.9915536	-0.7309745
H	-0.1605307	-3.5337456	-2.2980575

Zero-point correction= 0.588597 (Hartree/Particle)

Thermal correction to Energy= 0.627307

Thermal correction to Enthalpy= 0.628251

Thermal correction to Gibbs Free Energy= 0.515550

Sum of electronic and zero-point Energies= -1936.476099

Sum of electronic and thermal Energies= -1936.437388

Sum of electronic and thermal Enthalpies= -1936.436444

Sum of electronic and thermal Free Energies= -1936.549146

D-int4

C	1.9556137	2.8660692	-1.3576939
C	1.0555477	1.8736582	-1.3147549
C	2.9266007	3.0997992	-0.2782889
C	2.7896337	2.2091302	0.9180551
C	1.8727707	1.1936952	0.9428411
C	0.9866267	0.8549092	-0.2247929
C	1.3550497	-0.5404508	-0.7391289
C	0.6358747	-1.5175098	0.1251501
N	-0.2979793	-0.7987858	0.8308401
C	-0.4368743	0.5684882	0.3781041
C	2.1452907	-0.8158418	-1.7846689

N	-2.4395033	1.6592292	-0.6600819
C	-1.4922963	0.6956692	-0.7314689
O	-1.4102723	-0.0685448	-1.6830419
O	0.8590827	-2.7092008	0.2468211
O	3.7847747	3.9587762	-0.3149149
H	-0.6428383	1.2230692	1.2341671
Au	4.1019887	0.2910122	0.5202871
C	2.4220277	-2.1713268	-2.3364529
C	-2.6785473	2.8106302	0.2472721
C	-1.4587003	3.7271122	0.3092791
C	-3.1068783	2.3576612	1.6387091
C	-3.8336023	3.5795602	-0.3891589
C	-4.9935383	-1.0270388	1.6439181
C	-5.2955113	-1.5843878	0.3970541
C	-4.2680433	-2.1081698	-0.3934879
C	-2.9578233	-2.0655958	0.0672141
C	-2.6413313	-1.4866638	1.2947001
C	-3.6798013	-0.9804368	2.0796141
C	-1.2168173	-1.4285478	1.7731511
O	-6.5987373	-1.5708748	0.0478991
C	-6.9662613	-2.1659768	-1.1762789
H	3.3099207	2.5330712	1.8217991
H	1.6866917	0.6383562	1.8660581
H	-3.0626463	1.5947272	-1.4590129
H	1.9747747	-2.9592628	-1.7268969

H	2.0196837	-2.2410768	-3.3547859
H	3.5022127	-2.3509488	-2.4306389
H	-1.1648833	4.0526432	-0.6955489
H	-1.6970243	4.6187122	0.9006711
H	-0.5899143	3.2515982	0.7829571
H	-3.9759453	1.6941382	1.5729221
H	-3.3764573	3.2318482	2.2429601
H	-2.3168703	1.8204832	2.1777671
H	-4.0824933	4.4564052	0.2170111
H	-3.5696713	3.9282512	-1.3951039
H	-4.7304043	2.9517502	-0.4559949
H	-5.8107353	-0.6420518	2.2486661
H	-4.4786343	-2.5557678	-1.3599059
H	-2.1628173	-2.4707838	-0.5567509
H	-3.4555583	-0.5415298	3.0524881
H	-0.8029293	-2.4317618	1.9373811
H	-1.1640723	-0.8863358	2.7295961
H	-8.0500013	-2.0659188	-1.2551809
H	-6.7014093	-3.2318228	-1.2023519
H	-6.4961673	-1.6589308	-2.0306009
P	5.6694687	-1.4271018	0.2275951
C	7.0839377	-1.3937238	1.3694921
H	6.7277057	-1.4297988	2.4031921
H	7.7334207	-2.2565298	1.1808931
H	7.6567097	-0.4724548	1.2281791

C	6.3911747	-1.4661298	-1.4419749
H	7.0453027	-2.3394958	-1.5466169
H	5.5969837	-1.5168558	-2.1932429
H	6.9735417	-0.5558668	-1.6138039
C	4.8522997	-3.0324298	0.4837891
H	5.5370467	-3.8521988	0.2374221
H	4.5473577	-3.1181018	1.5315451
H	3.9506457	-3.1017728	-0.1344529
H	0.3681137	1.7123372	-2.1455489
H	2.0075227	3.5551182	-2.1973009
H	2.5785947	0.0300952	-2.3275319

Zero-point correction= 0.594884 (Hartree/Particle)

Thermal correction to Energy= 0.634268

Thermal correction to Enthalpy= 0.635212

Thermal correction to Gibbs Free Energy= 0.520594

Sum of electronic and zero-point Energies= -1936.575403

Sum of electronic and thermal Energies= -1936.536019

Sum of electronic and thermal Enthalpies= -1936.535075

Sum of electronic and thermal Free Energies= -1936.649693

D-ts6

C	-0.2059108	-1.0141657	-3.3453932
C	-0.7290068	0.0075313	-2.6660232
C	-0.3754398	-2.4091987	-2.8987152
C	-1.1187018	-2.6182227	-1.5864402
C	-1.9537818	-1.5644747	-1.1684542

C	-1.5480978	-0.1350547	-1.4011942
C	-2.7053588	0.8466003	-1.4381552
C	-2.3010578	2.0689143	-0.6887752
N	-1.0800178	1.7854483	-0.1005662
C	-0.6731478	0.4100153	-0.2282412
C	-3.8610968	0.6539193	-2.0868672
N	-1.9447748	-1.3053617	1.0668728
C	-0.8725578	-0.3441087	1.0859668
O	-0.1708528	-0.1376837	2.0462858
O	-2.8772118	3.1324593	-0.5879002
O	0.0274032	-3.3600237	-3.5346902
Au	0.8010442	-2.5631037	-0.4400182
C	-5.0160438	1.5861443	-2.1447402
C	3.3918662	2.1496063	1.1742228
C	3.8848902	2.3487163	-0.1197512
C	3.0062722	2.7118183	-1.1450442
C	1.6508542	2.8637353	-0.8622892
C	1.1453732	2.6541853	0.4193058
C	2.0385562	2.2940523	1.4328928
C	-0.3298198	2.7537803	0.6908818
O	5.2088682	2.1357053	-0.2818082
C	5.7620362	2.3365613	-1.5649772
H	-4.8295228	2.5042163	-1.5855632
H	-5.2398748	1.8427203	-3.1875522
H	-5.9161118	1.0935243	-1.7551722

H	4.0969072	1.8794053	1.9576188
H	3.3658942	2.8890353	-2.1542312
H	0.9700352	3.1553263	-1.6627782
H	1.6618422	2.1233783	2.4409818
H	-0.7461178	3.7321413	0.4192188
H	-0.5262748	2.6046223	1.7631988
H	6.8304182	2.1339713	-1.4769102
H	5.6209082	3.3697303	-1.9085142
H	5.3240862	1.6488053	-2.3037812
P	2.8894632	-2.2057247	0.5778558
C	3.9267812	-3.6824337	0.8117408
H	4.0794852	-4.1856747	-0.1476102
H	4.8985292	-3.3926637	1.2280868
H	3.4351422	-4.3793437	1.4969058
C	2.7916422	-1.3943407	2.2009488
H	3.8029392	-1.2219987	2.5887228
H	2.2718642	-0.4359067	2.0895808
H	2.2284632	-2.0156887	2.9036198
C	3.8610532	-1.0698647	-0.4638452
H	4.7940182	-0.7825777	0.0373548
H	4.0877092	-1.5503387	-1.4209212
H	3.2718992	-0.1628267	-0.6514602
H	0.4052812	0.3565183	-0.4584452
H	-3.0064728	-1.7550187	-0.9742222
C	-3.1255398	-1.0304257	1.9893588

C	-3.5432788	0.4283513	1.9022198
C	-4.2548068	-1.9311017	1.5100618
C	-2.7278888	-1.3868977	3.4179758
H	-2.7443308	1.1130703	2.2139048
H	-3.8776538	0.7002803	0.8946858
H	-4.3863488	0.5920963	2.5817518
H	-3.9431018	-2.9827567	1.4713928
H	-5.1020958	-1.8621627	2.2013498
H	-4.6134358	-1.6312137	0.5172768
H	-3.5756558	-1.2141407	4.0909858
H	-2.4530098	-2.4469657	3.4983128
H	-1.8835728	-0.7818447	3.7621978
H	-3.9774578	-0.2910797	-2.6288042
H	-0.5683228	1.0372453	-2.9868932
H	0.3650402	-0.8724197	-4.2593782
H	-1.5420618	-3.6237087	-1.5301682
H	-1.5507498	-2.2031117	1.3625548

Zero-point correction= 0.593360 (Hartree/Particle)

Thermal correction to Energy= 0.631730

Thermal correction to Enthalpy= 0.632675

Thermal correction to Gibbs Free Energy= 0.521211

Sum of electronic and zero-point Energies= -1936.539997

Sum of electronic and thermal Energies= -1936.501626

Sum of electronic and thermal Enthalpies= -1936.500682

Sum of electronic and thermal Free Energies= -1936.612146

D-int5

C	1.0462239	0.4468157	3.0507563
C	-0.0697581	0.3338147	2.3284723
C	2.2325689	1.1709147	2.5469693
C	2.3201629	1.3793977	1.0752053
C	1.0166709	1.5013657	0.2993343
C	-0.2923001	1.0189877	1.0151903
C	-1.2538111	2.1889077	1.1873723
C	-2.2824671	2.1167177	0.1219173
N	-2.0258331	0.9610787	-0.6122047
C	-1.0328891	0.1152647	0.0091813
C	-1.1714571	3.1110227	2.1560573
N	1.1009739	0.7286587	-1.0242237
C	-0.0353121	-0.2757893	-1.0400807
O	-0.0245021	-1.2033553	-1.7863627
O	-3.1973421	2.8771027	-0.1197987
O	3.1382239	1.4934047	3.3013973
Au	3.6337779	-0.2958593	0.6357643
C	-2.0543931	4.2884727	2.3488703
C	-4.2911151	-2.9973963	-0.3336347
C	-5.3575611	-2.6273853	0.4940953
C	-5.6701971	-1.2746273	0.6591063
C	-4.9184321	-0.3112133	-0.0044377
C	-3.8593261	-0.6693893	-0.8370057
C	-3.5545241	-2.0266813	-0.9897937

C	-3.0358541	0.3893397	-1.5096767
O	-6.0185351	-3.6428033	1.0848083
C	-7.1259411	-3.3328893	1.9018473
H	-2.8274851	4.3570117	1.5827103
H	-2.5261001	4.2404917	3.3382653
H	-1.4558841	5.2079947	2.3469383
H	-4.0740551	-4.0560173	-0.4487827
H	-6.4981061	-0.9656383	1.2899323
H	-5.1648961	0.7431847	0.1195763
H	-2.7297581	-2.3220993	-1.6398687
H	-3.6481031	1.2404227	-1.8283727
H	-2.5308011	-0.0164413	-2.3979947
H	-7.5194181	-4.2847593	2.2617943
H	-7.9101311	-2.8110303	1.3367003
H	-6.8327941	-2.7173293	2.7635873
P	5.1590129	-2.0795803	0.2414813
C	6.8913739	-1.6586873	0.6232183
H	6.9779689	-1.3697353	1.6750733
H	7.5436299	-2.5181223	0.4291023
H	7.2130639	-0.8140853	0.0064543
C	5.1937219	-2.6600803	-1.4880237
H	5.9111309	-3.4809983	-1.6020997
H	4.1985539	-3.0093643	-1.7810907
H	5.4841019	-1.8366433	-2.1481307
C	4.8203339	-3.5790633	1.2219953

H	5.5614069	-4.3552573	0.9982713
H	4.8606049	-3.3394263	2.2888823
H	3.8201199	-3.9564783	0.9889413
H	-1.4795531	-0.7936193	0.4448543
H	0.8504879	2.5425167	0.0043093
C	1.3317069	1.5495037	-2.3384737
C	0.0778759	2.3281467	-2.6809967
C	2.5153619	2.4710347	-2.0833187
C	1.6888179	0.5549137	-3.4338867
H	-0.7763761	1.6719437	-2.8806207
H	-0.2061611	3.0437687	-1.9013397
H	0.2741289	2.9018367	-3.5932917
H	3.4130459	1.9112307	-1.7922957
H	2.7395509	2.9970837	-3.0174057
H	2.3148989	3.2335057	-1.3244287
H	1.9684299	1.1208077	-4.3288007
H	2.5517779	-0.0623653	-3.1483767
H	0.8609999	-0.1073633	-3.6956987
H	-0.3714131	2.9798807	2.8919263
H	-0.9413211	-0.1850913	2.7299233
H	1.1255959	0.0334207	4.0536433
H	2.9715299	2.2419027	0.8889883
H	1.9560719	0.1447997	-0.9323957

Zero-point correction= 0.596385 (Hartree/Particle)

Thermal correction to Energy= 0.634058

Thermal correction to Enthalpy= 0.635002

Thermal correction to Gibbs Free Energy= 0.523725

Sum of electronic and zero-point Energies= -1936.557334

Sum of electronic and thermal Energies= -1936.519661

Sum of electronic and thermal Enthalpies= -1936.518717

Sum of electronic and thermal Free Energies= -1936.629995

D-ts7

C	-0.9417292	-0.7347267	-3.3011256
C	-1.2927762	0.3531683	-2.6047276
C	-0.9579832	-2.0840037	-2.7198606
C	-1.4518202	-2.2033277	-1.2958546
C	-2.2845522	-1.0453827	-0.7297946
C	-1.8394462	0.3439543	-1.2078456
C	-2.9125782	1.4178873	-1.0750206
C	-2.3073962	2.5983493	-0.3923216
N	-1.0349382	2.2177843	-0.0013476
C	-0.8097762	0.8085623	-0.1614536
C	-4.1559282	1.3345983	-1.5652916
N	-1.9531312	-1.0988187	0.7321494
C	-1.1645122	0.0303763	1.0959854
O	-0.7997652	0.3028643	2.2115314
O	-2.7822332	3.6991553	-0.2023406
O	-0.5458482	-3.0600217	-3.3232486
Au	0.7354928	-2.3849687	-0.5364936
C	-5.2158662	2.3727903	-1.4989026

C	3.4365288	2.0152223	1.3022704
C	3.9804368	2.2779313	0.0411774
C	3.1655538	2.7991553	-0.9682146
C	1.8235868	3.0562533	-0.6985446
C	1.2701198	2.8030693	0.5552874
C	2.0957558	2.2694173	1.5491754
C	-0.1836742	3.0675093	0.8225114
O	5.2871958	1.9619013	-0.1127816
C	5.8998738	2.2604683	-1.3494236
H	-4.8762362	3.2701673	-0.9801816
H	-5.5342312	2.6436413	-2.5133536
H	-6.1070532	1.9729293	-0.9993116
H	4.0946118	1.6231213	2.0750484
H	3.5651738	3.0202833	-1.9534886
H	1.1921768	3.4709513	-1.4846246
H	1.6770188	2.0605243	2.5334854
H	-0.4703992	4.0971803	0.5750974
H	-0.4099672	2.9131783	1.8864234
H	6.9490168	1.9769963	-1.2521976
H	5.8383208	3.3316063	-1.5816736
H	5.4461158	1.6878943	-2.1724046
P	2.9632038	-2.1733377	0.1844684
C	3.9942188	-3.6700587	0.2277424
H	4.0786988	-4.0953657	-0.7765516
H	4.9942818	-3.4196047	0.6001084

H	3.5408558	-4.4164847	0.8865874
C	2.9463978	-1.5092487	1.8783704
H	3.9698928	-1.3325197	2.2301914
H	2.3942928	-0.5613707	1.8810394
H	2.4432078	-2.2131437	2.5488404
C	3.8621868	-0.9538207	-0.8215956
H	4.8162268	-0.6873727	-0.3490146
H	4.0420478	-1.3606827	-1.8216796
H	3.2533938	-0.0450647	-0.9100666
H	0.2392328	0.5948723	-0.4358046
H	-3.3585542	-1.1864117	-0.8932206
C	-2.8648072	-1.7672647	1.7464444
C	-3.9258002	-0.7579447	2.1634234
C	-3.5106242	-2.9938337	1.1131964
C	-2.0229152	-2.2305457	2.9326094
H	-3.4750542	0.1282473	2.6226214
H	-4.5323042	-0.4394177	1.3059694
H	-4.5983202	-1.2125227	2.8994554
H	-2.7673392	-3.7536067	0.8421504
H	-4.1772092	-3.4461677	1.8547154
H	-4.1259642	-2.7618407	0.2370614
H	-2.6476282	-2.8505857	3.5849124
H	-1.1804402	-2.8471507	2.5897064
H	-1.6300592	-1.3970097	3.5151124
H	-4.4284952	0.4033473	-2.0749706

H	-1.1896882	1.3431003	-3.0514226
H	-0.5743242	-0.6668047	-4.3223846
H	-1.9502062	-3.1722907	-1.1875366
H	-1.0035452	-1.9957387	0.1012054

Zero-point correction= 0.590396 (Hartree/Particle)

Thermal correction to Energy= 0.628268

Thermal correction to Enthalpy= 0.629212

Thermal correction to Gibbs Free Energy= 0.519939

Sum of electronic and zero-point Energies= -1936.529820

Sum of electronic and thermal Energies= -1936.491948

Sum of electronic and thermal Enthalpies= -1936.491003

Sum of electronic and thermal Free Energies= -1936.600277

E-1

C	1.5926263	-2.3383304	2.1785921
C	0.3957783	-2.8914254	2.6751151
C	-0.7758627	-2.1821944	2.5648371
C	-0.7915137	-0.8995224	1.9669241
C	0.4236523	-0.3160234	1.4863351
C	1.6033243	-1.0890864	1.6068931
C	-2.0222067	-0.1893194	1.8361881
C	-2.0304287	1.0828486	1.3084121
C	-0.8308857	1.6467856	0.8544971
C	0.3865323	0.9927296	0.8997501
C	0.2784393	1.1869046	-2.1123099
C	1.7032393	0.8135876	-1.9919309

N	2.3071233	1.0499566	-0.7948189
C	1.5629643	1.7427386	0.2956301
C	-0.7765587	1.6931326	-2.4949119
N	2.9491273	3.5390666	1.3223911
C	2.5534633	2.2323086	1.3579021
O	3.0050273	1.4787586	2.2052491
O	2.2547993	0.3310086	-2.9700429
O	-3.1380307	-0.8152944	2.2361181
H	1.1172773	2.6322586	-0.1610539
Au	-1.0409037	-0.6194544	-1.6128529
C	-2.0110637	2.3387756	-2.8913129
C	2.5908063	4.7215876	0.5068571
C	1.1584763	5.1736746	0.7835981
C	2.8259713	4.4811056	-0.9836979
C	3.5462893	5.8210226	0.9666161
C	5.4081003	-1.9305474	1.1867521
C	5.1473733	-3.0413684	0.3794111
C	4.4516313	-2.8768344	-0.8198279
C	4.0228513	-1.6074334	-1.1977509
C	4.2680503	-0.4941094	-0.3951339
C	4.9724163	-0.6744054	0.7993051
C	3.7802363	0.8715376	-0.7960859
O	5.6050623	-4.2293014	0.8452641
C	5.3704843	-5.3749094	0.0655581
H	2.5283893	-2.8881024	2.2634151

H	0.4008603	-3.8702404	3.1498551
H	-1.7123497	-2.5803224	2.9479911
H	2.5436413	-0.6648534	1.2864131
H	-2.9662097	1.6231776	1.1988301
H	-0.8881287	2.6361356	0.3985251
H	3.5710553	3.7235756	2.1027491
H	-3.9140507	-0.4080904	1.7964831
H	-1.7937317	3.3654666	-3.2078289
H	-2.4787327	1.8146246	-3.7316039
H	-2.7282457	2.3721086	-2.0575459
H	1.0162973	5.3618676	1.8536361
H	0.9440033	6.1011446	0.2388821
H	0.4158173	4.4299876	0.4743381
H	3.8519703	4.1367746	-1.1604589
H	2.6830243	5.4204236	-1.5309339
H	2.1394283	3.7474156	-1.4204629
H	3.3493013	6.7475186	0.4171161
H	3.4171233	6.0320716	2.0357031
H	4.5895853	5.5334096	0.7886241
H	5.9503763	-2.0837264	2.1162411
H	4.2475583	-3.7234464	-1.4691329
H	3.4905623	-1.4744124	-2.1379439
H	5.1442343	0.1797176	1.4525941
H	4.1031083	1.0990776	-1.8185909
H	4.2143663	1.6325296	-0.1406119

H	5.8110103	-6.2152454	0.6059481
H	5.8439973	-5.2985594	-0.9238869
H	4.2950893	-5.5617724	-0.0704079
P	-1.9429427	-2.7517604	-1.3307069
C	-3.3873447	-2.8881614	-0.2496119
H	-4.1732527	-2.2145664	-0.6053609
H	-3.7603217	-3.9192104	-0.2543519
H	-3.1487297	-2.5840194	0.7744091
C	-0.7056157	-3.9402914	-0.7254749
H	-1.1421777	-4.9451244	-0.6792509
H	0.1596843	-3.9425354	-1.3960249
H	-0.3751557	-3.6373564	0.2747891
C	-2.4986517	-3.4215714	-2.9339769
H	-2.8838747	-4.4394614	-2.8002219
H	-3.2958057	-2.7855964	-3.3307449
H	-1.6673047	-3.4339124	-3.6452669
C	-7.1151117	-0.0364874	2.3373391
F	-6.1311417	0.0953446	3.2183941
F	-8.1067227	-0.7148564	2.8903761
F	-7.5419597	1.1602696	1.9800391
S	-6.5071127	-0.9742124	0.8699281
O	-7.6293557	-1.0569604	-0.0467379
O	-5.9178377	-2.1820224	1.4289451
N	-5.2505267	-0.0455794	0.3738581
S	-5.4322737	1.1270626	-0.7180209

O	-6.7494137	1.7238436	-0.8266259
O	-4.2540387	1.9919306	-0.6478749
C	-5.1844257	0.2501486	-2.3260919
F	-3.9430667	-0.2644834	-2.3892199
F	-6.0398297	-0.7386124	-2.4886189
F	-5.3087087	1.1196986	-3.3182989

Zero-point correction= 0.701154 (Hartree/Particle)

Thermal correction to Energy= 0.758671

Thermal correction to Enthalpy= 0.759615

Thermal correction to Gibbs Free Energy= 0.605926

Sum of electronic and zero-point Energies= -3916.901802

Sum of electronic and thermal Energies= -3916.844284

Sum of electronic and thermal Enthalpies= -3916.843340

Sum of electronic and thermal Free Energies= -3916.997030

E-ts1

C	1.2872475	-1.2882848	3.0110010
C	0.0281535	-1.5203688	3.5949700
C	-1.0931485	-0.9658658	3.0303860
C	-0.9944825	-0.1661788	1.8677680
C	0.2831305	0.1251982	1.3069570
C	1.4148565	-0.4822388	1.9051770
C	-2.1880345	0.3054212	1.2265300
C	-2.0997695	1.0166772	0.0364900
C	-0.8459305	1.3480442	-0.4651900
C	0.3447705	0.9448482	0.1244800

C	0.7270435	-1.0216738	-1.4937660
C	2.0808355	-0.5009378	-1.6567410
N	2.5576945	0.5584482	-0.9620730
C	1.6189305	1.5529252	-0.4275060
C	-0.1516615	-1.8797388	-1.7628040
N	2.0600535	3.7555862	0.6690920
C	2.3056665	2.4132032	0.6435780
O	3.0050325	1.9070852	1.5084900
O	2.7120905	-1.1262508	-2.5020410
O	-3.3367745	0.0071422	1.8150280
H	1.3153575	2.2121532	-1.2549840
Au	-1.6964285	-2.2934378	-0.2892630
C	-0.2975525	-2.8770848	-2.8752640
C	1.6673265	4.7684402	-0.3417460
C	0.1968235	4.6629712	-0.7319280
C	2.5677115	4.6941792	-1.5730730
C	1.8857535	6.1117972	0.3513110
C	6.3303915	-0.9000578	0.9192130
C	7.0327915	-1.6838958	-0.0022470
C	6.7154115	-1.6091098	-1.3577950
C	5.6977775	-0.7543338	-1.7745320
C	4.9954965	0.0327522	-0.8689890
C	5.3268645	-0.0509028	0.4893750
C	3.9225845	0.9761492	-1.3416020
O	7.9995005	-2.4796208	0.5178680

C	8.7344715	-3.2832808	-0.3704290
H	2.1753855	-1.7452908	3.4409090
H	-0.0545165	-2.1378358	4.4865410
H	-2.0777055	-1.1279938	3.4610500
H	2.3965435	-0.3027088	1.4823300
H	-3.0004275	1.3482872	-0.4717560
H	-0.8059295	1.9274152	-1.3855350
H	2.5253415	4.1438362	1.4834300
H	0.5345225	-2.7676638	-3.5779430
H	-0.2971565	-3.8959488	-2.4744530
H	-1.2509205	-2.7332978	-3.3934770
H	-0.4375585	4.5603882	0.1555210
H	-0.1057705	5.5666322	-1.2740020
H	0.0004945	3.8146252	-1.3935950
H	3.6214705	4.8055902	-1.2900540
H	2.3133595	5.5003862	-2.2717790
H	2.4566825	3.7472312	-2.1154380
H	1.6368205	6.9325452	-0.3292750
H	1.2475695	6.2003922	1.2388390
H	2.9329415	6.2337662	0.6562230
H	6.6019915	-0.9744098	1.9693000
H	7.2419215	-2.2105508	-2.0928460
H	5.4351465	-0.7133188	-2.8300430
H	4.7851045	0.5639762	1.2066780
H	3.9675605	1.0754032	-2.4353080

H	4.0802405	1.9708922	-0.9108290
H	9.4541635	-3.8390148	0.2342930
H	9.2800565	-2.6792088	-1.1099290
H	8.0892995	-3.9964668	-0.9037430
P	-3.3215315	-3.5472328	0.8940280
C	-4.5555025	-2.7461778	1.9678060
H	-5.1341245	-2.0177728	1.3942440
H	-5.2256955	-3.5185928	2.3654510
H	-4.0620165	-2.2194778	2.7880530
C	-2.5671265	-4.8113008	1.9788680
H	-3.3393285	-5.4344308	2.4459590
H	-1.8931895	-5.4434678	1.3922820
H	-1.9797245	-4.3140088	2.7577800
C	-4.3262935	-4.5125828	-0.2848700
H	-5.0699675	-5.1157068	0.2498310
H	-4.8310415	-3.8183118	-0.9632360
H	-3.6743635	-5.1694618	-0.8695180
H	-4.1200315	0.2091682	1.2378050
C	-5.3140255	3.0492902	0.1704580
F	-4.3172085	2.9765392	1.0479260
F	-5.9531575	4.1936632	0.3354220
F	-4.8049755	3.0025152	-1.0529230
S	-6.4912285	1.6558032	0.4443630
O	-7.5480175	1.8478852	-0.5306770
O	-6.7563515	1.6909082	1.8700510

N	-5.5356625	0.3557752	0.1618070
S	-5.4450605	-0.3789558	-1.2753460
O	-5.5360375	0.4727992	-2.4462310
O	-4.3420665	-1.3393238	-1.1624370
C	-6.9226235	-1.4910098	-1.3430650
F	-6.9674025	-2.2474008	-0.2478560
F	-8.0446015	-0.8175958	-1.4516040
F	-6.7782605	-2.2889478	-2.3952190

Zero-point correction= 0.699129 (Hartree/Particle)

Thermal correction to Energy= 0.756368

Thermal correction to Enthalpy= 0.757312

Thermal correction to Gibbs Free Energy= 0.603305

Sum of electronic and zero-point Energies= -3916.876172

Sum of electronic and thermal Energies= -3916.818933

Sum of electronic and thermal Enthalpies= -3916.817988

Sum of electronic and thermal Free Energies= -3916.971995

E-int1

C	1.9294502	-0.9693534	2.8927014
C	0.8210062	-0.7361004	3.7119434
C	-0.3859488	-0.4007844	3.1362924
C	-0.4868688	-0.2749294	1.7381624
C	0.6350862	-0.4889834	0.9099274
C	1.8360622	-0.8599604	1.5140904
C	-1.7643158	0.0319746	1.1469694
C	-1.9195768	0.0834426	-0.2719126

C	-0.8522768	-0.1424374	-1.0649716
C	0.5400952	-0.2863504	-0.5843326
C	1.3207652	-1.3425284	-1.3687246
C	2.6651142	-0.7750674	-1.6544846
N	2.6594252	0.5331616	-1.1927196
C	1.3140552	1.0254166	-1.0486766
C	0.8447602	-2.5765154	-1.6404246
N	0.2211382	3.1423266	-0.3823736
C	1.1384572	2.1750746	-0.0678206
O	1.7050112	2.1769316	1.0143214
O	3.6441542	-1.2996344	-2.1567716
O	-2.7638698	0.1983626	1.9393404
H	0.8968482	1.3082996	-2.0276006
Au	-0.9890448	-3.2192104	-0.8855376
C	1.6465652	-3.5763554	-2.4134576
C	-0.1388268	3.7863046	-1.6772546
C	-1.0951288	2.9464006	-2.5195056
C	1.1195752	4.1337236	-2.4696056
C	-0.8625798	5.0738576	-1.2873316
C	5.7845762	0.6493306	1.8800864
C	6.9561412	0.0676726	1.3830184
C	7.1185452	-0.0939484	0.0081914
C	6.1067322	0.3255416	-0.8534036
C	4.9442012	0.9144346	-0.3729486
C	4.7932502	1.0697276	1.0110424

C	3.8545742	1.3587276	-1.3140026
O	7.8687432	-0.3076154	2.3149324
C	9.0618962	-0.8945014	1.8609804
H	2.8862532	-1.2383354	3.3350654
H	0.9080882	-0.8236814	4.7913914
H	-1.2708898	-0.2265644	3.7419764
H	2.7201492	-1.0377084	0.9088174
H	-2.9105308	0.2313206	-0.6870146
H	-0.9827088	-0.1507404	-2.1470646
H	0.1461092	3.7741576	0.4098514
H	2.6163082	-3.1945024	-2.7451266
H	1.8092882	-4.4701514	-1.7958816
H	1.0701372	-3.9207674	-3.2822096
H	-1.9508878	2.6160806	-1.9233556
H	-1.4713348	3.5542686	-3.3508266
H	-0.6159018	2.0681026	-2.9654316
H	1.7963392	4.7546066	-1.8699446
H	0.8528542	4.6929676	-3.3745266
H	1.6675322	3.2382266	-2.7890856
H	-1.1474728	5.6318326	-2.1854356
H	-1.7740418	4.8526916	-0.7190776
H	-0.2171598	5.7227096	-0.6814926
H	5.6865272	0.7679436	2.9568294
H	8.0132742	-0.5522864	-0.4024746
H	6.2192742	0.1694736	-1.9249146

H	3.8784802	1.5184276	1.3975344
H	4.2182092	1.3223176	-2.3517246
H	3.5614112	2.3938896	-1.0968636
H	9.6571822	-1.1189644	2.7486714
H	9.6307062	-0.2121194	1.2126104
H	8.8737942	-1.8281374	1.3110054
P	-2.9527298	-4.0920724	0.2066484
C	-3.4355628	-3.1355544	1.6868064
H	-3.8079818	-2.1561204	1.3713464
H	-4.2296278	-3.6530204	2.2386374
H	-2.5649318	-2.9987644	2.3375664
C	-2.5989608	-5.7549414	0.8896674
H	-3.4546638	-6.1309984	1.4633954
H	-2.3784258	-6.4493424	0.0728034
H	-1.7200978	-5.7016004	1.5402064
C	-4.5288968	-4.3330244	-0.6839356
H	-5.2581698	-4.8115634	-0.0182736
H	-4.9134228	-3.3596944	-1.0041056
H	-4.3685968	-4.9664424	-1.5614526
H	-3.6645558	0.3896826	1.4671814
C	-4.3084828	3.2013326	-0.0733616
F	-3.0462898	2.9482126	0.2854014
F	-4.5102698	4.5047106	-0.0137076
F	-4.4799448	2.7810776	-1.3173446
S	-5.4557448	2.3253736	1.0797384

O	-6.7956088	2.6836596	0.6681174
O	-4.9442018	2.6387526	2.3995534
N	-5.0273848	0.7727256	0.7703964
S	-5.7152548	-0.1547034	-0.3726226
O	-6.4504258	0.5478356	-1.4033666
O	-4.7102828	-1.1564094	-0.7365446
C	-6.9600518	-1.1232324	0.5791414
F	-6.3578278	-1.7971724	1.5518564
F	-7.8695408	-0.3231204	1.0941964
F	-7.5308458	-1.9870814	-0.2473896

Zero-point correction= 0.702720 (Hartree/Particle)

Thermal correction to Energy= 0.758639

Thermal correction to Enthalpy= 0.759583

Thermal correction to Gibbs Free Energy= 0.611670

Sum of electronic and zero-point Energies= -3916.921283

Sum of electronic and thermal Energies= -3916.865364

Sum of electronic and thermal Enthalpies= -3916.864420

Sum of electronic and thermal Free Energies= -3917.012333

E-ts2

C	-2.4165648	1.6912984	2.7037620
C	-1.2772628	1.8366834	3.4965630
C	-0.0482728	1.4291534	3.0084910
C	0.0484172	0.8777044	1.7228970
C	-1.0917508	0.7418464	0.9190550
C	-2.3240738	1.1495144	1.4293970

C	1.3395182	0.4743854	1.1900700
C	1.4880882	0.1092974	-0.1405690
C	0.3773532	-0.1560506	-0.9344370
C	-1.0327318	0.0477064	-0.4302860
C	-1.8408078	0.7718924	-1.5082820
C	-2.9894858	-0.0821446	-1.8769010
N	-2.8432058	-1.3052886	-1.2208990
C	-1.7754568	-1.3134846	-0.2441870
C	-1.5040238	1.9849614	-2.0033930
N	0.3571862	-2.2863466	-1.0664430
C	-0.9066948	-2.5483986	-0.4341860
O	-1.2928908	-3.6430276	-0.1065400
O	-3.9435358	0.1621834	-2.5973340
O	2.3542412	0.5723804	2.0067020
Au	0.2473562	2.9285904	-1.3687480
C	-2.3154338	2.6695174	-3.0572090
C	-5.0865218	-1.8914036	2.6472060
C	-5.8791028	-0.7406176	2.6246800
C	-6.1116858	-0.0823766	1.4146430
C	-5.5414728	-0.5763556	0.2441860
C	-4.7408188	-1.7186916	0.2545430
C	-4.5270608	-2.3709096	1.4735790
C	-4.0209128	-2.1466066	-0.9957370
O	-6.3743938	-0.3421156	3.8218610
C	-7.1901878	0.8023094	3.8474620

H	-3.3900018	1.9965814	3.0817270
H	-1.3542058	2.2609924	4.4940860
H	0.8534192	1.5224394	3.6076770
H	-3.2232788	1.0355744	0.8244600
H	2.4875432	-0.0343776	-0.5414890
H	3.1863282	0.1789234	1.5902130
H	-3.1851788	2.0945834	-3.3866150
H	-2.6527298	3.6435364	-2.6775540
H	-1.6792208	2.9006064	-3.9220370
H	-4.9251658	-2.3874366	3.6008190
H	-6.7360568	0.8053614	1.3703050
H	-5.7079898	-0.0570066	-0.6990590
H	-3.9017068	-3.2638636	1.4975630
H	-4.6469058	-2.0226476	-1.8853880
H	-3.6998578	-3.1934666	-0.9347360
H	-7.4852528	0.9515024	4.8880410
H	-8.0936608	0.6731744	3.2344800
H	-6.6516188	1.6956344	3.4972760
P	2.3706072	3.8510324	-0.7139530
C	2.7115012	3.9163934	1.0795730
H	2.7505992	2.8995604	1.4854560
H	3.6847752	4.3873874	1.2609100
H	1.9218342	4.4772004	1.5893590
C	2.6969492	5.5600864	-1.2807210
H	3.7011522	5.8809114	-0.9792510

H	2.6138382	5.6065494	-2.3710490
H	1.9547412	6.2390964	-0.8498080
C	3.7803902	2.8992104	-1.3803880
H	4.7311182	3.3620834	-1.0925490
H	3.7665222	1.8879634	-0.9580820
H	3.7033852	2.8380474	-2.4704450
C	5.2454482	-1.9785366	-1.3195020
F	4.7414152	-0.9282966	-1.9644120
F	4.8375942	-3.0871166	-1.9280740
F	6.5545622	-1.9271026	-1.3472770
S	4.5844012	-2.0215546	0.4169040
O	5.4931972	-2.8763266	1.1536090
O	3.1855902	-2.4169636	0.2347670
H	-2.2018388	-1.3953786	0.7695810
H	0.4933572	-0.1389766	-2.0136310
H	1.1360482	-2.4718336	-0.4198590
C	0.6292032	-3.0349996	-2.3517450
C	-0.6197508	-3.0136316	-3.2193010
C	1.7659142	-2.3035936	-3.0534580
C	1.0631452	-4.4590746	-2.0206170
H	-1.4364848	-3.6042036	-2.7886880
H	-0.9787718	-1.9882276	-3.3783190
H	-0.3805948	-3.4422606	-4.1988330
H	2.6152302	-2.1641456	-2.3790740
H	2.1098702	-2.9000626	-3.9065280

H	1.4523832	-1.3267236	-3.4401790
H	1.2461262	-5.0140026	-2.9490620
H	1.9968532	-4.4472606	-1.4429480
H	0.2963562	-4.9838296	-1.4430800
N	4.5289212	-0.4679296	0.8833100
S	5.8274682	0.4562394	1.2269370
O	7.0374722	0.0589694	0.5320280
O	5.3491592	1.8323944	1.1916270
C	6.1252522	0.1422364	3.0216460
F	5.0014512	0.3590184	3.6923740
F	6.5272622	-1.0946586	3.2230740
F	7.0540792	0.9865944	3.4399650

Zero-point correction= 0.701269 (Hartree/Particle)

Thermal correction to Energy= 0.756895

Thermal correction to Enthalpy= 0.757840

Thermal correction to Gibbs Free Energy= 0.609874

Sum of electronic and zero-point Energies= -3916.905245

Sum of electronic and thermal Energies= -3916.849619

Sum of electronic and thermal Enthalpies= -3916.848675

Sum of electronic and thermal Free Energies= -3916.996640

E-int2

C	-2.6741061	-0.7736924	-3.0183513
C	-1.5750251	-0.7873144	-3.8720633
C	-0.3030651	-0.5844044	-3.3565673
C	-0.1211191	-0.3718504	-1.9869623

C	-1.2221831	-0.3765804	-1.1214113
C	-2.4954531	-0.5725054	-1.6549373
C	1.2187329	-0.1569114	-1.4403873
C	1.4446169	-0.0557374	-0.1167323
C	0.3670159	0.0472756	0.8816217
C	-1.0915071	-0.0754434	0.3659567
C	-1.8894501	-1.0635014	1.2202217
C	-3.0364041	-0.3370714	1.8074077
N	-2.8476451	1.0285046	1.5597157
C	-1.7631021	1.2852006	0.6432037
C	-1.5549891	-2.3633544	1.3887487
N	0.5070719	1.4250436	1.5881917
C	-0.7466761	2.2017546	1.2728077
O	-0.8441561	3.3669496	1.5050117
O	-4.0096911	-0.7534374	2.4126567
O	2.2026619	-0.1273324	-2.3472223
Au	0.2091379	-3.1217354	0.5519487
C	-2.3780571	-3.2973354	2.2193677
C	-5.0080751	2.9462256	-1.9017323
C	-5.8645831	1.8963386	-2.2448043
C	-6.1499971	0.8991906	-1.3085503
C	-5.5674181	0.9566106	-0.0459553
C	-4.7038351	1.9940406	0.3058807
C	-4.4381201	2.9897976	-0.6396073
C	-3.9789481	1.9548556	1.6220147

O	-6.3673681	1.9339596	-3.5015043
C	-7.2301011	0.8964576	-3.8975173
H	-3.6785841	-0.9185134	-3.4106263
H	-1.7099251	-0.9474624	-4.9388373
H	0.5686529	-0.5757624	-4.0051383
H	-3.3660621	-0.5629244	-0.9989443
H	2.4654969	0.0363596	0.2410787
H	3.0194479	0.1931086	-1.9051323
H	-3.2435211	-2.8244224	2.6920507
H	-2.7294561	-4.1235794	1.5862547
H	-1.7493341	-3.7691374	2.9860917
H	-4.8070351	3.7116236	-2.6466613
H	-6.8226981	0.0810976	-1.5492083
H	-5.7730741	0.1714376	0.6811067
H	-3.7677431	3.8100116	-0.3776463
H	-4.6210641	1.5833516	2.4274717
H	-3.6068551	2.9479416	1.9051467
H	-7.5150801	1.1062366	-4.9303283
H	-8.1367351	0.8606426	-3.2767693
H	-6.7333901	-0.0840954	-3.8557563
P	2.3520329	-3.7785094	-0.3175593
C	2.6143279	-3.4865984	-2.1000513
H	2.4568719	-2.4269884	-2.3308983
H	3.6421359	-3.7514384	-2.3760353
H	1.9057159	-4.0861864	-2.6802363

C	2.8104419	-5.5366384	-0.0931403
H	3.8142399	-5.7262654	-0.4916063
H	2.7906879	-5.7880554	0.9719227
H	2.0886359	-6.1754214	-0.6114223
C	3.7326379	-2.8780584	0.4727497
H	4.6950679	-3.2349214	0.0882077
H	3.6581259	-1.8121234	0.2300027
H	3.6887179	-3.0087154	1.5589727
C	5.3329799	1.6556826	1.7221807
F	5.1047159	0.3627396	1.9449587
F	4.8124859	2.3487306	2.7326607
F	6.6215929	1.8801736	1.6705637
S	4.4652219	2.1956386	0.1562747
O	5.2288989	3.3265116	-0.3316553
O	3.0863189	2.4175576	0.6187407
H	-2.1280551	1.7768256	-0.2741223
H	0.4980999	-0.6836164	1.6817717
H	1.3119899	1.9171666	1.1448907
C	0.8609939	1.3815626	3.1137327
C	-0.3561961	0.9064466	3.8834977
C	2.0354279	0.4274946	3.2880707
C	1.2885309	2.7853986	3.5177097
H	-1.2043341	1.5953096	3.7906767
H	-0.6806151	-0.0936464	3.5687147
H	-0.0891781	0.8504276	4.9445157

H	2.8566429	0.6724906	2.6101627
H	2.4093859	0.5427546	4.3113987
H	1.7654049	-0.6266314	3.1595407
H	1.5905669	2.7578276	4.5705367
H	2.1509309	3.1170156	2.9271917
H	0.4834969	3.5156586	3.4124697
N	4.4084829	0.8938626	-0.7966433
S	5.7354109	0.1794206	-1.4144083
O	6.9522049	0.4317636	-0.6612513
O	5.3366069	-1.1763704	-1.7687803
C	5.9577079	1.0176756	-3.0432433
F	4.8366339	0.9178016	-3.7444693
F	6.2614169	2.2883856	-2.8769843
F	6.9353859	0.4079506	-3.6942143

Zero-point correction= 0.704801 (Hartree/Particle)

Thermal correction to Energy= 0.760161

Thermal correction to Enthalpy= 0.761105

Thermal correction to Gibbs Free Energy= 0.614012

Sum of electronic and zero-point Energies= -3916.917201

Sum of electronic and thermal Energies= -3916.861840

Sum of electronic and thermal Enthalpies= -3916.860896

Sum of electronic and thermal Free Energies= -3917.007989

E-ts3

C	1.8327328	-2.3176629	2.5689504
C	0.6292778	-2.3272679	3.2751614

C	-0.4403082	-1.5879639	2.8052574
C	-0.3214972	-0.8414449	1.6225494
C	0.8812638	-0.8407579	0.9021284
C	1.9547968	-1.5803009	1.4007694
C	-1.4767392	-0.1165169	1.1097254
C	-1.4066012	0.6495391	-0.0485746
C	-0.1519992	0.7227341	-0.8840036
C	1.0958048	-0.0402399	-0.3655006
C	1.7032608	-0.8724059	-1.4931316
C	2.9494578	-0.2024949	-1.9297126
N	3.0615948	0.9885051	-1.2092596
C	2.1454878	1.0585591	-0.0938106
C	1.1274848	-1.9797839	-2.0102586
N	0.1190678	2.2170481	-0.6983516
C	1.4366998	2.3906501	-0.1310966
O	1.8970108	3.4456401	0.2189384
O	3.7791978	-0.5460129	-2.7551846
O	-2.5605412	-0.2171159	1.8239724
Au	-0.7140352	-2.6785599	-1.3176906
C	1.7443968	-2.7433789	-3.1409776
C	6.0104498	1.6629881	2.2467934
C	6.6718918	0.4325361	2.2110434
C	6.5782578	-0.3734029	1.0738034
C	5.8300368	0.0629701	-0.0158456
C	5.1732908	1.2926531	0.0049654

C	5.2690698	2.0828051	1.1543354
C	4.3252748	1.7164531	-1.1625356
O	7.3738128	0.1084731	3.3241814
C	8.0744358	-1.1103479	3.3279304
H	2.6824808	-2.8903279	2.9326304
H	0.5342258	-2.9041109	4.1911454
H	-1.3857562	-1.5706499	3.3403604
H	2.8971198	-1.5828759	0.8533814
H	-2.3446292	0.9092851	-0.5353936
H	-3.3794252	0.2074921	1.4017074
H	2.6806428	-2.3117869	-3.5055916
H	1.9270668	-3.7789169	-2.8230046
H	1.0287868	-2.8176459	-3.9708456
H	6.0965938	2.2681491	3.1456184
H	7.0882668	-1.3310359	1.0229844
H	5.7555908	-0.5602079	-0.9071536
H	4.7459998	3.0388211	1.1886684
H	4.8197108	1.5003381	-2.1160256
H	4.1155168	2.7930421	-1.1167656
H	8.5756388	-1.1784069	4.2955724
H	8.8300638	-1.1479739	2.5301464
H	7.3979388	-1.9701079	3.2149874
P	-2.8827432	-3.4489619	-0.6319776
C	-3.1497032	-3.6390909	1.1630444
H	-3.1107912	-2.6554509	1.6430384

H	-4.1413522	-4.0635739	1.3560614
H	-2.3705722	-4.2848079	1.5811574
C	-3.3203062	-5.0911589	-1.3108926
H	-4.3318582	-5.3770469	-0.9989076
H	-3.2730312	-5.0612389	-2.4039596
H	-2.6058642	-5.8398619	-0.9547336
C	-4.2448342	-2.3715299	-1.1919806
H	-5.2138632	-2.7712649	-0.8714366
H	-4.1217662	-1.3784589	-0.7470526
H	-4.2120202	-2.2782929	-2.2823776
C	-5.2183952	1.4240901	-1.7747836
F	-4.0930942	0.7878811	-2.1205186
F	-5.3553552	2.4805021	-2.5586436
F	-6.2336242	0.6022041	-1.9420456
S	-5.1071512	1.9952621	-0.0213606
O	-6.3619322	2.6661961	0.2458174
O	-3.8428202	2.7255011	0.0217304
H	2.6759178	0.9519931	0.8659114
H	-0.3072842	0.4901841	-1.9406496
H	-0.8481982	1.9745021	0.1577674
C	-0.2962852	3.2253631	-1.7841916
C	0.8252858	3.2952011	-2.8120136
C	-1.5891952	2.7778531	-2.4518546
C	-0.5464652	4.5634971	-1.1010226
H	1.7523578	3.6924291	-2.3857656

H	1.0328058	2.3085751	-3.2463916
H	0.5214688	3.9619781	-3.6267366
H	-2.4285672	2.7577701	-1.7503376
H	-1.8292032	3.5209921	-3.2205966
H	-1.5085272	1.8109591	-2.9602236
H	-0.8495422	5.2922471	-1.8616826
H	-1.3688772	4.4716471	-0.3803196
H	0.3411448	4.9397521	-0.5891536
N	-4.8554552	0.6025221	0.7740284
S	-6.0545542	-0.3331189	1.3771764
O	-7.3232122	-0.2221919	0.6848624
O	-5.4544722	-1.6360899	1.6321034
C	-6.2983022	0.3817861	3.0602454
F	-5.1467592	0.3462121	3.7172604
F	-6.7195342	1.6283951	2.9821094
F	-7.1916362	-0.3523369	3.7023054

Zero-point correction= 0.698665 (Hartree/Particle)

Thermal correction to Energy= 0.753855

Thermal correction to Enthalpy= 0.754799

Thermal correction to Gibbs Free Energy= 0.606340

Sum of electronic and zero-point Energies= -3916.886753

Sum of electronic and thermal Energies= -3916.831564

Sum of electronic and thermal Enthalpies= -3916.830620

Sum of electronic and thermal Free Energies= -3916.979078

E-int3

C	-2.3030688	2.5741769	-1.7996096
C	-1.0755838	3.1394319	-2.1569046
C	0.0898712	2.5697379	-1.6837606
C	0.0376892	1.4358509	-0.8566086
C	-1.1899568	0.8317749	-0.5381326
C	-2.3589718	1.4326039	-1.0152506
C	1.2742292	0.9503859	-0.2483906
C	1.1242572	0.0672509	0.9524924
C	0.0558592	-1.0114931	0.7609044
C	-1.2867658	-0.4612171	0.2408294
C	-2.0666248	-1.5047541	-0.5758056
C	-3.4216878	-1.6196921	0.0337914
N	-3.4004568	-0.9168611	1.2195534
C	-2.1292348	-0.3063931	1.5196134
C	-1.6203178	-2.1129921	-1.6930306
N	-0.2915848	-1.6726581	2.0134464
C	-1.4084688	-1.1268211	2.5856774
O	-1.8245278	-1.2899791	3.7192934
O	-4.4253528	-2.1729591	-0.3937956
O	2.3828602	1.3175769	-0.6572526
Au	0.2775182	-1.7367611	-2.4760026
C	-2.4493418	-3.1076651	-2.4493536
C	-5.1771178	3.1772289	1.6099224
C	-5.8530608	3.2446069	0.3892494
C	-6.1775038	2.0676359	-0.2895236

C	-5.8138398	0.8390319	0.2560734
C	-5.1296068	0.7581469	1.4688584
C	-4.8232658	1.9458429	2.1391834
C	-4.6110298	-0.5714811	1.9473564
O	-6.1515258	4.4928539	-0.0526876
C	-6.8583868	4.6082829	-1.2611396
H	-3.2330878	3.0259379	-2.1392416
H	-1.0405258	4.0278469	-2.7818986
H	1.0635702	3.0022329	-1.9031386
H	-3.3303478	1.0032969	-0.7720646
H	2.0999922	-0.3617971	1.2116874
H	3.8612472	1.1425679	0.0451834
H	-3.4255698	-3.2941661	-1.9936786
H	-2.6023048	-2.7522361	-3.4777506
H	-1.9012288	-4.0545741	-2.5445966
H	-4.9442818	4.1076999	2.1215734
H	-6.7141728	2.0944059	-1.2336506
H	-6.0418558	-0.0819621	-0.2799826
H	-4.2975508	1.9006139	3.0934504
H	-5.3301898	-1.3746751	1.7533564
H	-4.3766158	-0.5620571	3.0187324
H	-7.0091518	5.6759549	-1.4339916
H	-7.8384698	4.1123549	-1.2101866
H	-6.2953108	4.1864269	-2.1073506
P	2.5267432	-1.3361031	-3.2153176

C	2.9103682	0.3486369	-3.8042256
H	2.6744442	1.0613329	-3.0066436
H	3.9749782	0.4386229	-4.0489036
H	2.2997422	0.5746049	-4.6839106
C	3.1616952	-2.4195201	-4.5465976
H	4.2151402	-2.1976281	-4.7548676
H	3.0635962	-3.4668731	-4.2444986
H	2.5734152	-2.2679001	-5.4567736
C	3.7114062	-1.6137121	-1.8480396
H	4.7386862	-1.4014741	-2.1669826
H	3.4556512	-0.9416451	-1.0207376
H	3.6284072	-2.6495461	-1.5011826
C	5.4456972	-0.9127481	2.0914274
F	4.4824172	-1.5860951	1.4763714
F	5.5044022	-1.2792581	3.3550704
F	6.5932172	-1.1363341	1.4913774
S	5.0434742	0.8892489	2.0385014
O	6.1911652	1.6015919	2.5383244
O	3.7103912	1.0133149	2.5897604
H	-2.2584398	0.7372049	1.8477784
H	0.4371062	-1.7447661	0.0419834
C	0.5838762	-2.6612921	2.6954704
C	-0.2833798	-3.7641891	3.3026914
C	1.5031842	-3.3121851	1.6652134
C	1.3954942	-1.9688671	3.7894044

H	-0.9407798	-3.3741491	4.0817264
H	-0.9006338	-4.2326081	2.5267294
H	0.3660342	-4.5333241	3.7376874
H	2.1878612	-2.6025581	1.1870264
H	2.1169902	-4.0661621	2.1707854
H	0.9225602	-3.8168981	0.8815044
H	2.0194932	-2.7020381	4.3159864
H	2.0572222	-1.1932081	3.3835754
H	0.7236872	-1.5039661	4.5186574
N	4.8598482	1.1015949	0.3888714
S	6.0279982	1.5273589	-0.7312496
O	7.3335422	1.1470139	-0.2538816
O	5.5026652	1.1390419	-2.0230426
C	5.9117352	3.3700539	-0.6737606
F	4.6760842	3.7224329	-0.9782696
F	6.2178732	3.7958159	0.5321864
F	6.7546292	3.8591139	-1.5611546
H	0.8411592	0.7195039	1.7964844

Zero-point correction= 0.703422 (Hartree/Particle)

Thermal correction to Energy= 0.759208

Thermal correction to Enthalpy= 0.760152

Thermal correction to Gibbs Free Energy= 0.610668

Sum of electronic and zero-point Energies= -3916.957492

Sum of electronic and thermal Energies= -3916.901707

Sum of electronic and thermal Enthalpies= -3916.900763

Sum of electronic and thermal Free Energies= -3917.050246

E-int4

C	0.6801995	2.4683091	-2.0101624
C	0.2880435	1.9240161	-3.2341844
C	0.1694345	0.5511461	-3.3542874
C	0.4771575	-0.2803719	-2.2704294
C	0.8768565	0.2579721	-1.0367104
C	0.9551045	1.6494251	-0.9238544
C	0.4345085	-1.7404959	-2.4645884
C	1.3444415	-2.5159729	-1.5527544
C	1.1224295	-2.1302379	-0.0888424
C	1.2142145	-0.6092289	0.1619416
C	0.4301105	-0.1815929	1.4099106
C	1.3655995	0.5620741	2.2987046
N	2.6299055	0.4208491	1.7746746
C	2.6810175	-0.4214669	0.6051546
C	-0.8842835	-0.3698679	1.6381956
N	2.1394365	-2.6939559	0.7904366
C	3.1615635	-1.8126169	1.0144336
O	4.2492395	-2.0428179	1.5141696
O	1.1104935	1.2351191	3.2872676
O	-0.2511945	-2.2778779	-3.3242334
Au	-2.0717745	-1.3095929	0.1970906
C	-1.5268675	0.0835181	2.9220186
C	4.5784805	3.6777311	-0.6210264

C	3.6531265	4.6963121	-0.3810924
C	2.8128165	4.6218191	0.7322916
C	2.8993505	3.5239251	1.5834336
C	3.8073865	2.4917981	1.3463986
C	4.6498925	2.5900541	0.2357636
C	3.7520715	1.2471421	2.1913906
O	3.6446425	5.7113151	-1.2822944
C	2.7292935	6.7581291	-1.0799534
H	0.7692375	3.5471111	-1.8918874
H	0.0716865	2.5729561	-4.0794714
H	-0.1334085	0.0838231	-4.2893654
H	1.2407825	2.1077611	0.0221806
H	1.1929605	-3.5886839	-1.7206994
H	-3.0071715	0.8197351	0.8684346
H	-0.8389085	0.0462781	3.7721136
H	-1.8334475	1.1383111	2.8445886
H	-2.4244985	-0.5037149	3.1503966
H	5.2263055	3.7645971	-1.4896704
H	2.0918845	5.4058151	0.9452706
H	2.2274435	3.4471491	2.4379246
H	5.3724325	1.7971181	0.0402176
H	3.5851315	1.4881291	3.2470696
H	4.6679135	0.6491621	2.1115446
H	2.8760165	7.4638661	-1.9003124
H	2.9056335	7.2768801	-0.1266334

H	1.6888075	6.4004491	-1.0978424
P	-3.3564755	-2.4181019	-1.5001994
C	-3.4570455	-1.5209869	-3.0881064
H	-2.4382725	-1.3965369	-3.4777124
H	-4.0578665	-2.0865889	-3.8104194
H	-3.9093205	-0.5369949	-2.9269914
C	-5.0941085	-2.7769499	-1.0660644
H	-5.5983425	-3.3009469	-1.8867824
H	-5.1211755	-3.3968859	-0.1642474
H	-5.6166175	-1.8421379	-0.8422194
C	-2.6658775	-4.0461599	-1.9635914
H	-3.3086935	-4.5454239	-2.6986334
H	-1.6723345	-3.8906229	-2.4009484
H	-2.5774245	-4.6743829	-1.0709284
C	-5.5256325	1.8641811	2.7192836
F	-4.6658045	1.3025281	3.5443846
F	-6.7598225	1.5967501	3.0966926
F	-5.3305985	3.1633551	2.6731986
S	-5.2940465	1.1530741	1.0279196
O	-6.1779995	1.8609761	0.1364436
O	-5.2911895	-0.2878099	1.1729786
H	3.3295115	0.0144641	-0.1704084
H	0.1301945	-2.4847549	0.2119686
C	2.1714305	-4.1112329	1.2341866
C	2.5091325	-4.1502609	2.7243436

C	0.7917805	-4.7383019	1.0504336
C	3.2178945	-4.8798759	0.4299996
H	3.5026775	-3.7406959	2.9172746
H	1.7732315	-3.5687559	3.2932166
H	2.4795205	-5.1876719	3.0786556
H	0.4731125	-4.7793329	0.0010816
H	0.8275865	-5.7693879	1.4196756
H	0.0284125	-4.2009239	1.6291176
H	3.2728835	-5.9189779	0.7778476
H	2.9683555	-4.8939839	-0.6383504
H	4.2031855	-4.4201649	0.5550656
N	-3.6956515	1.5831731	0.7400666
S	-3.0954185	2.9662891	-0.0087694
O	-4.0530075	4.0341531	0.1232626
O	-1.7083435	3.0573591	0.3780726
C	-3.1023775	2.4088781	-1.7723934
F	-2.4006595	1.2946341	-1.8640214
F	-4.3382815	2.1828921	-2.1730764
F	-2.5523325	3.3572931	-2.5037844
H	2.3843145	-2.2764499	-1.8302434

Zero-point correction= 0.703069 (Hartree/Particle)

Thermal correction to Energy= 0.758744

Thermal correction to Enthalpy= 0.759688

Thermal correction to Gibbs Free Energy= 0.611341

Sum of electronic and zero-point Energies= -3916.951998

Sum of electronic and thermal Energies= -3916.896323

Sum of electronic and thermal Enthalpies= -3916.895379

Sum of electronic and thermal Free Energies= -3917.043726

E-ts4

C	-0.0185577	-2.4349889	2.3017001
C	-0.3358827	-1.6991029	3.4425971
C	-0.1478367	-0.3279669	3.4375651
C	0.3947353	0.3052831	2.3128621
C	0.7073623	-0.4290629	1.1571631
C	0.4694883	-1.8035699	1.1657571
C	0.7522863	1.7302931	2.4121021
C	1.8988933	2.1412161	1.5292641
C	1.7113303	1.7010391	0.0773671
C	1.3311823	0.1992951	-0.0764359
C	0.5107203	-0.0098679	-1.3537389
C	1.3150433	-0.8579079	-2.2947949
N	2.4836323	-1.1822929	-1.6561609
C	2.6884383	-0.4640579	-0.4197139
C	-0.7583267	0.3856821	-1.6276039
N	2.9365733	1.8442371	-0.7010659
C	3.6523443	0.6788091	-0.7282359
O	4.8195003	0.5224901	-1.0375619
O	0.9713713	-1.3007959	-3.3776239
O	0.2253723	2.5015301	3.2023831
Au	-1.5213687	1.9591891	-0.2396229

C	-1.3046707	0.2934871	-3.0350929
C	2.5653153	-4.8362409	0.8343951
C	1.2810533	-5.2746519	0.5007431
C	0.7145023	-4.9004169	-0.7193589
C	1.4090293	-4.0377859	-1.5589969
C	2.6634653	-3.5359369	-1.2075309
C	3.2423853	-3.9699739	-0.0119679
C	3.2384503	-2.3875539	-1.9940009
O	0.6483853	-6.0335359	1.4317351
C	-0.6975107	-6.3726009	1.1834941
H	-0.1475227	-3.5166699	2.2859951
H	-0.7279927	-2.1980029	4.3254321
H	-0.3690397	0.2813051	4.3115311
H	0.6649313	-2.4004239	0.2772791
H	2.0349123	3.2264331	1.6054301
H	-1.8700457	-0.0370589	-0.9595659
H	-0.6002577	0.6936691	-3.7699409
H	-1.4884187	-0.7503389	-3.3174519
H	-2.2502447	0.8411911	-3.1050189
H	2.9918353	-5.1588659	1.7809241
H	-0.2795537	-5.2298569	-1.0046139
H	0.9387153	-3.6986149	-2.4811009
H	4.2278853	-3.6000119	0.2725521
H	3.1293503	-2.5303349	-3.0743139
H	4.2958613	-2.2069009	-1.7687779

H	-1.0487807	-6.9126489	2.0650571
H	-0.7989447	-7.0227069	0.3033581
H	-1.3167907	-5.4746739	1.0339221
P	-2.4964897	3.4769841	1.2584821
C	-3.0147557	2.6129581	2.7764141
H	-2.1176077	2.2525651	3.2921961
H	-3.5727137	3.2918941	3.4325471
H	-3.6484647	1.7622651	2.5022491
C	-4.0357317	4.1829641	0.5846621
H	-4.5238617	4.8221481	1.3298831
H	-3.8163327	4.7657951	-0.3150549
H	-4.7003887	3.3602311	0.3003941
C	-1.5055867	4.8967561	1.8264101
H	-2.0897587	5.5164721	2.5171351
H	-0.6183887	4.5128751	2.3425471
H	-1.1993677	5.5011231	0.9669211
C	-5.4106747	-0.5093899	-2.4831839
F	-4.5418547	-0.9531389	-3.3718509
F	-6.1110617	0.4838471	-3.0061889
F	-6.2256487	-1.4696349	-2.1170389
S	-4.4996387	0.1970851	-1.0108539
O	-5.3875007	0.0692561	0.1324921
O	-4.0803627	1.5213801	-1.4597639
H	3.0754713	-1.1279209	0.3653321
H	0.9196423	2.3152211	-0.3636999

C	3.4819713	3.1463071	-1.1681619
C	4.0387663	2.9598211	-2.5794719
C	2.3555363	4.1738431	-1.2394359
C	4.5841853	3.6210901	-0.2234219
H	4.8717853	2.2537631	-2.5886039
H	3.2556483	2.5873771	-3.2510969
H	4.3908393	3.9250521	-2.9622399
H	1.9115273	4.3981521	-0.2611519
H	2.7642583	5.1112651	-1.6326399
H	1.5581333	3.8456021	-1.9193199
H	5.0187263	4.5575041	-0.5945349
H	4.1972393	3.8070801	0.7858271
H	5.3793953	2.8714291	-0.1631259
N	-3.1227997	-0.6836609	-0.8525719
S	-3.1417717	-2.2488499	-0.3563329
O	-4.2771217	-2.9814159	-0.8825349
O	-1.7825537	-2.7360469	-0.5107539
C	-3.4374797	-2.1286689	1.4807031
F	-2.8892527	-1.0178279	1.9507691
F	-4.7237977	-2.1353229	1.7477161
F	-2.8723527	-3.1809299	2.0589221
H	2.8075923	1.6629711	1.9311121

Zero-point correction= 0.698141 (Hartree/Particle)

Thermal correction to Energy= 0.752881

Thermal correction to Enthalpy= 0.753825

Thermal correction to Gibbs Free Energy= 0.611021

Sum of electronic and zero-point Energies= -3916.929908

Sum of electronic and thermal Energies= -3916.875169

Sum of electronic and thermal Enthalpies= -3916.874224

Sum of electronic and thermal Free Energies= -3917.017028

E-2

C	-2.7289296	-3.2669547	-1.2519244
C	-1.5979816	-3.7351497	-1.9247604
C	-0.4460276	-2.9719087	-1.9236734
C	-0.4210566	-1.7385607	-1.2549924
C	-1.5381136	-1.2892487	-0.5258254
C	-2.6947766	-2.0715707	-0.5479604
C	0.7362324	-0.8636907	-1.4114184
C	0.4841374	0.5811243	-1.1251514
C	-0.2028286	0.7792493	0.2263516
C	-1.5036266	-0.0428187	0.3369406
C	-1.8224206	-0.4025367	1.7837816
C	-3.1831706	0.0993403	2.1105616
N	-3.5886646	0.8615553	1.0415116
C	-2.6064356	0.9745243	-0.0128894
C	-1.0250416	-1.1291297	2.5744586
N	-0.6259046	2.1596243	0.4135036
C	-1.9358016	2.3453873	0.0644146
O	-2.5235946	3.3991093	-0.1042984
O	-3.8677536	-0.1309307	3.0949816

O	1.8246834	-1.2904937	-1.8222854
Au	3.6531254	-0.0256557	-1.8178104
C	-1.2629176	-1.5078257	3.9909686
C	-6.3729936	-0.5597307	-2.1556354
C	-6.7817206	-1.7627977	-1.5739934
C	-6.6587726	-1.9428037	-0.1937884
C	-6.1177716	-0.9230367	0.5847226
C	-5.6963166	0.2779393	0.0146706
C	-5.8386396	0.4458473	-1.3656474
C	-4.9677786	1.2894883	0.8569166
O	-7.2845766	-2.6891697	-2.4265014
C	-7.7186996	-3.9122427	-1.8864104
H	-3.6498716	-3.8464647	-1.2653484
H	-1.6273366	-4.6830307	-2.4549564
H	0.4473634	-3.2880787	-2.4564604
H	-3.5826646	-1.7463067	-0.0052174
H	1.4248934	1.1418733	-1.1866094
H	-2.1989186	-1.0955147	4.3713126
H	-1.2862776	-2.6005617	4.0907396
H	-0.4229436	-1.1643057	4.6088036
H	-6.4887476	-0.4422097	-3.2300634
H	-6.9835026	-2.8635327	0.2823136
H	-5.9993296	-1.0662347	1.6587646
H	-5.5229256	1.3830083	-1.8252064
H	-5.4029266	1.3697183	1.8590336

H	-4.9605296	2.2848573	0.3967146
H	-8.0845436	-4.5102887	-2.7234224
H	-8.5347316	-3.7723157	-1.1631104
H	-6.8985906	-4.4542127	-1.3919434
P	5.3624114	1.5097363	-1.8049884
C	6.9282174	0.8214113	-1.1947184
H	7.2085224	-0.0477887	-1.7975214
H	7.7176794	1.5811063	-1.2354864
H	6.7734054	0.4798033	-0.1667084
C	5.0127394	2.9265093	-0.7181414
H	5.8643434	3.6176723	-0.7131394
H	4.1162974	3.4499303	-1.0680764
H	4.8344924	2.5430393	0.2937906
C	5.7624904	2.2426403	-3.4274934
H	6.5823434	2.9639503	-3.3268824
H	6.0581944	1.4529343	-4.1247084
H	4.8797514	2.7488803	-3.8295204
H	-3.0688496	0.8158343	-0.9992684
H	0.4884734	0.4888233	1.0202216
C	0.3215814	3.2791923	0.6826026
C	-0.3035746	4.2098963	1.7211636
C	1.6216804	2.7295953	1.2622286
C	0.5944584	4.0420113	-0.6133204
H	-1.2256146	4.6627333	1.3504586
H	-0.5280076	3.6557093	2.6399826

H	0.4083064	5.0063573	1.9678286
H	2.1712024	2.0576993	0.5882556
H	2.2899294	3.5712823	1.4787946
H	1.4562654	2.1972353	2.2055496
H	1.2482234	4.8994323	-0.4090354
H	1.0954894	3.4073633	-1.3565904
H	-0.3401996	4.4171633	-1.0427664
H	-0.1817056	0.9603603	-1.9184644
H	-0.0855396	-1.4805537	2.1375496
C	2.7248884	-0.9963557	2.3036546
F	2.0858154	-1.0878377	1.1269786
F	2.1032644	-0.0724927	3.0328486
F	2.6360664	-2.1481547	2.9240276
S	4.4881254	-0.4603857	2.0145896
O	5.2255674	-1.0097257	3.1378526
O	4.3726364	0.9878993	1.8521186
N	4.8776234	-1.0225837	0.5580436
S	5.0026804	-2.5864797	0.1751466
O	4.2364864	-3.4864907	1.0237426
O	4.8873784	-2.6641797	-1.2798114
C	6.7736754	-2.9907567	0.4994066
F	7.5576454	-2.1564567	-0.1775924
F	7.0454674	-2.8922267	1.7848846
F	7.0053954	-4.2270707	0.0883516

Zero-point correction= 0.703198 (Hartree/Particle)

Thermal correction to Energy= 0.759354

Thermal correction to Enthalpy= 0.760298

Thermal correction to Gibbs Free Energy= 0.608475

Sum of electronic and zero-point Energies= -3916.974915

Sum of electronic and thermal Energies= -3916.918760

Sum of electronic and thermal Enthalpies= -3916.917815

Sum of electronic and thermal Free Energies= -3917.069638

E-int5

C	0.1971766	0.0326606	2.8997826
C	0.6176776	-1.1649494	3.4813496
C	0.6499406	-2.3162694	2.7154206
C	0.2428956	-2.2883304	1.3756546
C	-0.2164674	-1.0922164	0.7987556
C	-0.2142014	0.0683836	1.5763346
C	0.4064856	-3.5203744	0.5714756
C	0.0284956	-3.4406524	-0.8409014
C	-0.4467304	-2.3121974	-1.3801844
C	-0.6981384	-1.0407864	-0.6373904
C	-0.0751944	0.1325996	-1.4087744
C	-1.1371014	1.1243206	-1.6952714
N	-2.2897614	0.6881636	-1.0659704
C	-2.2528004	-0.7204054	-0.7683234
C	1.2358006	0.2585736	-1.6968124
N	-3.5997374	-2.3392644	0.5599836
C	-3.0422374	-1.0831464	0.4821556

O	-3.0988234	-0.3260724	1.4366166
O	-1.0724874	2.1604906	-2.3352794
O	0.8948826	-4.5498474	1.0340136
H	-2.6391544	-1.3055494	-1.6213274
Au	2.5924566	-1.1354064	-0.9370084
C	1.7424266	1.4446496	-2.4692474
C	-4.3579454	-3.1287494	-0.4480364
C	-3.4438134	-3.9512984	-1.3478584
C	-5.2766544	-2.2326054	-1.2770554
C	-5.2155474	-4.0917354	0.3700206
C	-3.3791404	4.1195556	1.4151886
C	-3.5240124	5.2844656	0.6549476
C	-3.6568834	5.1953476	-0.7294004
C	-3.6438304	3.9408536	-1.3358874
C	-3.5135984	2.7771906	-0.5903124
C	-3.3738004	2.8812676	0.7983996
C	-3.5296734	1.4271246	-1.2566174
O	-3.5189764	6.4497826	1.3538616
C	-3.6332054	7.6453466	0.6273106
H	0.1958736	0.9525116	3.4806636
H	0.9315356	-1.1870384	4.5226996
H	0.9908546	-3.2662704	3.1216036
H	-0.5403914	1.0093066	1.1393466
H	0.1870776	-4.3406684	-1.4321664
H	-0.6836184	-2.2734394	-2.4454394

H	-3.9883264	-2.4312294	1.4943056
H	1.0312896	1.7835216	-3.2282044
H	1.8715436	2.3005666	-1.7883294
H	2.7129586	1.2432236	-2.9374224
H	-2.7727974	-4.5765014	-0.7480924
H	-4.0503734	-4.6032164	-1.9885734
H	-2.8261104	-3.3282224	-2.0029084
H	-5.9265814	-1.6361044	-0.6249264
H	-5.9136864	-2.8455534	-1.9263724
H	-4.7170354	-1.5467404	-1.9244494
H	-5.7982054	-4.7390794	-0.2941284
H	-4.5867134	-4.7298464	1.0027876
H	-5.9198574	-3.5459204	1.0108556
H	-3.2717354	4.2199226	2.4925366
H	-3.7549124	6.0851536	-1.3443054
H	-3.7158914	3.8720846	-2.4204824
H	-3.2522614	1.9716776	1.3858116
H	-3.7249024	1.5489856	-2.3338894
H	-4.3389014	0.8128636	-0.8392344
H	-3.5995424	8.4588456	1.3555366
H	-4.5836244	7.6998956	0.0757036
H	-2.8053744	7.7704236	-0.0861404
P	4.1981496	-2.6873884	-0.0315594
C	3.8919476	-3.3905044	1.6273026
H	2.9760056	-3.9935894	1.6049716

H	4.7405086	-4.0192604	1.9238146
H	3.7599236	-2.5860984	2.3562286
C	5.8848256	-1.9931704	0.1077406
H	6.5948166	-2.7628204	0.4337506
H	6.1986106	-1.5746244	-0.8533064
H	5.8808426	-1.1801844	0.8435356
C	4.4078716	-4.1823884	-1.0633874
H	5.1920356	-4.8318034	-0.6561764
H	3.4595966	-4.7311754	-1.0766224
H	4.6638346	-3.8966494	-2.0881194
C	5.4528296	3.4366506	-1.6664304
F	4.4891776	3.3003926	-2.5537494
F	6.6050796	3.6395556	-2.2749134
F	5.1838406	4.4314206	-0.8516684
S	5.6186616	1.8651256	-0.7026374
O	6.6035086	2.0915726	0.3257416
O	5.7017496	0.7950746	-1.6736314
N	4.0870776	1.7307776	-0.0230264
S	3.5136396	2.3584106	1.4294316
O	4.2959196	3.5116106	1.7937146
O	2.0747506	2.3362576	1.3285996
C	3.9659956	0.9961956	2.5957666
F	3.4467086	-0.1371484	2.1506476
F	5.2765126	0.8785286	2.6689016
F	3.4654876	1.2845546	3.7793296

H	3.4614806	1.0406036	-0.4806504

Zero-point correction= 0.701062 (Hartree/Particle)

Thermal correction to Energy= 0.757806

Thermal correction to Enthalpy= 0.758750

Thermal correction to Gibbs Free Energy= 0.607060

Sum of electronic and zero-point Energies= -3916.913058

Sum of electronic and thermal Energies= -3916.856315

Sum of electronic and thermal Enthalpies= -3916.855371

Sum of electronic and thermal Free Energies= -3917.007061

E-ts5

C	1.4121954	-1.4394930	2.8862559
C	2.2555414	-2.5168810	2.6222779
C	2.3473404	-3.0010990	1.3285479
C	1.5645714	-2.4504510	0.3086369
C	0.6733694	-1.3948980	0.5820719
C	0.6479624	-0.8721460	1.8756319
C	1.7377544	-2.9837380	-1.0593741
C	0.7976554	-2.5035610	-2.0731761
C	-0.0776426	-1.5257160	-1.8123731
C	-0.2490616	-0.8425070	-0.4796801
C	-0.1433016	0.6648980	-0.7693031
C	-1.5139926	1.0861990	-1.2201801
N	-2.3880076	0.0797390	-0.8857901
C	-1.7958626	-1.0279350	-0.1829131
C	0.9536814	1.4615950	-0.8279361

N	-2.4982166	-2.1414320	1.9464809
C	-2.1989456	-0.9862810	1.2934499
O	-2.2471096	0.0878030	1.8757049
O	-1.8288306	2.0898870	-1.8298091
O	2.6394894	-3.7690700	-1.3481961
H	-2.1254156	-1.9743050	-0.6332341
Au	2.7159604	0.2443920	-1.4397811
C	0.8092614	2.8779090	-1.3375981
C	-2.6736496	-3.5525260	1.5375139
C	-1.3976926	-4.1369670	0.9385579
C	-3.8568316	-3.7095090	0.5830419
C	-2.9862386	-4.3009760	2.8311459
C	-5.0939306	3.1461920	0.7224639
C	-6.0047336	3.6853510	-0.1917321
C	-6.1744786	3.0794110	-1.4344591
C	-5.4290306	1.9433680	-1.7442221
C	-4.5307406	1.3931420	-0.8394881
C	-4.3682946	2.0130300	0.4042879
C	-3.8096956	0.1195940	-1.1974791
O	-6.6683396	4.7959530	0.2205419
C	-7.5695516	5.3876900	-0.6785511
H	1.3618844	-1.0106070	3.8835499
H	2.8555824	-2.9521950	3.4180439
H	3.0151174	-3.8198800	1.0695579
H	0.0264554	-0.0110700	2.1005459

H	0.8842354	-2.9460900	-3.0637181
H	-0.7413046	-1.1678210	-2.6010861
H	-2.7352396	-1.9342340	2.9110179
H	0.3957064	2.8885940	-2.3512711
H	0.1094644	3.4536730	-0.7209131
H	1.7706964	3.3945070	-1.3464331
H	-0.5488166	-3.9899760	1.6173409
H	-1.5299816	-5.2134500	0.7753679
H	-1.1396786	-3.6931920	-0.0298801
H	-4.7632426	-3.2734950	1.0194909
H	-4.0445396	-4.7729320	0.3908839
H	-3.6815126	-3.2313990	-0.3878081
H	-3.1349656	-5.3662440	2.6257239
H	-2.1599686	-4.2036030	3.5457869
H	-3.9024906	-3.9165950	3.2971109
H	-4.9722526	3.6453580	1.6805939
H	-6.8644406	3.4833130	-2.1694731
H	-5.5529586	1.4830690	-2.7243831
H	-3.6510946	1.6078040	1.1165569
H	-3.9536786	-0.0815770	-2.2708371
H	-4.2609666	-0.7282020	-0.6578451
H	-7.9890616	6.2601110	-0.1727541
H	-8.3880986	4.7032200	-0.9470131
H	-7.0687336	5.7161690	-1.6011631
P	4.6430734	-0.8940910	-2.1250081

C	5.3797084	-1.9148090	-0.8070771
H	4.7013114	-2.7500020	-0.6015001
H	6.3547994	-2.3023320	-1.1259471
H	5.4980984	-1.3113160	0.0981639
C	5.9591974	0.2788160	-2.5908051
H	6.8664154	-0.2584390	-2.8920491
H	5.6136484	0.9164960	-3.4100331
H	6.1759454	0.9254520	-1.7335771
C	4.4786264	-2.0400150	-3.5340201
H	5.4577544	-2.4552350	-3.8013171
H	3.8069844	-2.8544460	-3.2372071
H	4.0579694	-1.5139650	-4.3962551
C	4.1831894	4.8525840	0.3522469
F	2.9169174	5.2059640	0.4588299
F	4.7205804	5.4419720	-0.7026671
F	4.8481674	5.1954080	1.4297609
S	4.2981444	3.0074910	0.0527159
O	5.5467244	2.5573490	0.6442289
O	4.0772864	2.8570510	-1.3784981
N	2.9793644	2.3556480	0.8068349
S	2.9282374	2.2432000	2.4526619
O	3.5177904	3.4054720	3.0853059
O	1.5985924	1.7733970	2.7818949
C	4.0724684	0.8191740	2.8485699
F	4.0559484	-0.0583810	1.8520039

F	5.3006434	1.2351150	3.0528629
F	3.6280074	0.2341730	3.9517829
H	2.0731034	1.6983470	0.0897669

Zero-point correction= 0.695657 (Hartree/Particle)

Thermal correction to Energy= 0.751945

Thermal correction to Enthalpy= 0.752890

Thermal correction to Gibbs Free Energy= 0.603532

Sum of electronic and zero-point Energies= -3916.894470

Sum of electronic and thermal Energies= -3916.838182

Sum of electronic and thermal Enthalpies= -3916.837238

Sum of electronic and thermal Free Energies= -3916.986596

H-int6

C	2.1046064	2.8812201	-1.0035984
C	1.6171064	3.2493171	-2.2575744
C	0.6004784	2.5065321	-2.8305094
C	0.0809524	1.3855551	-2.1725564
C	0.5912524	0.9904791	-0.9244364
C	1.5930274	1.7735411	-0.3428754
C	-1.0647136	0.6859451	-2.7995514
C	-1.6680356	-0.4071769	-2.0344184
C	-1.1653836	-0.8033319	-0.8588074
C	0.0867294	-0.2729989	-0.2466064
C	-0.0190686	-0.1004179	1.2638446
C	1.2622884	-0.5544879	1.8687356
N	1.9933794	-1.1337319	0.8543236

C	1.1631414	-1.4369539	-0.2899374
C	-1.0933066	0.3551381	1.9188516
N	1.5509134	-2.4786509	-2.5031094
C	1.9117514	-1.5062539	-1.6108674
O	2.7498094	-0.6687509	-1.9090804
O	1.6476254	-0.4508129	3.0203236
O	-1.5404856	1.0485761	-3.8718204
H	0.6111934	-2.3756109	-0.1254824
Au	-3.9426466	1.1298251	-0.3745524
C	-1.2602546	0.4936341	3.3881246
C	1.0408414	-3.8653959	-2.3305764
C	-0.4585126	-3.9125519	-2.0489854
C	1.8285454	-4.6050669	-1.2503144
C	1.2936524	-4.5426329	-3.6758894
C	5.6485144	1.2841261	0.7721836
C	6.1933684	1.3736721	2.0576786
C	5.7988514	0.4679821	3.0408456
C	4.8631484	-0.5157449	2.7266476
C	4.3250314	-0.6228849	1.4506306
C	4.7278084	0.2954891	0.4728066
C	3.3128884	-1.6911269	1.1256896
O	7.0907744	2.3743871	2.2491856
C	7.6641174	2.5016371	3.5252666
H	2.8996744	3.4558101	-0.5330814
H	2.0282384	4.1124721	-2.7753454

H	0.1781264	2.7634391	-3.7997074
H	2.0084074	1.5086641	0.6258346
H	-2.5646626	-0.8672319	-2.4451804
H	-1.6650826	-1.5999759	-0.3080604
H	2.0887354	-2.3435489	-3.3537504
H	-0.3500606	0.2301421	3.9291406
H	-1.5562766	1.5202191	3.6382866
H	-2.0937206	-0.1391629	3.7225326
H	-1.0140696	-3.3258909	-2.7889074
H	-0.8057926	-4.9514239	-2.1010444
H	-0.7217826	-3.5399389	-1.0541214
H	2.9015104	-4.5911109	-1.4781424
H	1.5029544	-5.6510769	-1.1996034
H	1.6845184	-4.1707799	-0.2536124
H	0.9490384	-5.5815759	-3.6468204
H	0.7519614	-4.0276029	-4.4786044
H	2.3636394	-4.5493269	-3.9202384
H	5.9759044	2.0023201	0.0238356
H	6.1964554	0.5236751	4.0498666
H	4.5292484	-1.2020259	3.5032636
H	4.2978774	0.2291981	-0.5261824
H	3.2407994	-2.4027689	1.9615696
H	3.6191354	-2.2527539	0.2340636
H	8.3538914	3.3469791	3.4751836
H	8.2247834	1.5999841	3.8123726

H	6.9056374	2.7046251	4.2954286
P	-3.3887376	3.2530201	-1.0951994
C	-4.6568856	4.4297131	-0.5117054
H	-4.7824866	4.3132471	0.5699336
H	-4.3624276	5.4608601	-0.7411464
H	-5.6136956	4.2076621	-0.9945594
C	-3.2189966	3.6118971	-2.8700854
H	-2.9538006	4.6676221	-3.0041974
H	-2.4598486	2.9684571	-3.3287254
H	-4.1747596	3.4118871	-3.3644834
C	-1.8549136	3.8314241	-0.2981604
H	-1.6121526	4.8510441	-0.6204474
H	-2.0015796	3.8128191	0.7874996
H	-1.0256926	3.1603941	-0.5458024
H	-1.9682616	0.6319661	1.3169726
C	-6.9265416	0.4978721	1.9239946
F	-6.8585366	1.5215781	1.0779706
F	-7.4551456	0.9106781	3.0623356
F	-7.6688546	-0.4528339	1.4017366
S	-5.2202756	-0.1216399	2.2779886
O	-5.3674836	-1.2738209	3.1454126
O	-4.4901376	1.0641431	2.6986676
N	-4.6545626	-0.5464219	0.7900086
S	-4.7593336	-2.0959059	0.2198366
O	-6.0600096	-2.7003289	0.4118446

O	-4.1223326	-2.0623599	-1.0874864
C	-3.5747426	-3.0735499	1.3004246
F	-2.6571316	-2.2725469	1.8286206
F	-4.2162046	-3.7079929	2.2493636
F	-2.9629496	-3.9526889	0.5168266

Zero-point correction= 0.701529 (Hartree/Particle)

Thermal correction to Energy= 0.758668

Thermal correction to Enthalpy= 0.759613

Thermal correction to Gibbs Free Energy= 0.606364

Sum of electronic and zero-point Energies= -3916.952702

Sum of electronic and thermal Energies= -3916.895563

Sum of electronic and thermal Enthalpies= -3916.894618

Sum of electronic and thermal Free Energies= -3917.047867

H-ts6

C	-1.3195133	0.4843175	3.0304735
C	-1.8110873	1.3024115	2.0077375
C	0.1375937	0.2266675	3.1878105
C	1.0541077	0.8070905	2.1641225
C	0.5566997	1.8096645	1.3047715
C	-0.8925583	1.7941125	0.8847215
C	-1.3848903	3.1038815	0.3025345
C	-2.2443383	2.7927895	-0.8738435
N	-2.1020393	1.4438765	-1.1168555
C	-1.0694253	0.8173685	-0.3192065
C	-1.1143533	4.3207305	0.7871275

N	1.2753877	1.5161035	-0.7407695
C	0.1930057	0.6803915	-1.1741555
O	0.1924017	-0.0020715	-2.1711695
O	-2.9745213	3.5337805	-1.5085525
O	0.5747917	-0.3737065	4.1573415
Au	1.1735127	-1.1822765	1.1046425
C	-1.5464643	5.6241155	0.2159445
C	-3.0932053	-3.0288755	-2.0918725
C	-3.8408743	-3.2274655	-0.9281825
C	-4.2862833	-2.1237065	-0.1959875
C	-3.9743303	-0.8405435	-0.6371565
C	-3.2095973	-0.6288985	-1.7825495
C	-2.7735663	-1.7441655	-2.5017685
C	-2.8016683	0.7584815	-2.1920645
O	-4.0551073	-4.5191685	-0.5786635
C	-4.7360633	-4.7671995	0.6278785
H	-2.2005853	5.4909955	-0.6475245
H	-2.0679023	6.2211835	0.9740445
H	-0.6651583	6.2087165	-0.0819925
H	-2.7511193	-3.9036915	-2.6406105
H	-4.8681113	-2.2477335	0.7128735
H	-4.3117983	0.0169805	-0.0548915
H	-2.1554543	-1.5981845	-3.3874065
H	-3.6612693	1.3979225	-2.4319275
H	-2.1689323	0.7112035	-3.0905855

H	-4.7883433	-5.8519825	0.7386125
H	-5.7571343	-4.3608955	0.6110435
H	-4.1980013	-4.3427525	1.4889175
P	0.7674957	-3.2545055	0.0909485
C	1.9899107	-4.5647455	0.4010805
H	2.0653747	-4.7456545	1.4777945
H	1.6897737	-5.4878925	-0.1087305
H	2.9680247	-4.2274745	0.0412665
C	0.5644217	-3.1787045	-1.7115085
H	0.2951077	-4.1709195	-2.0945785
H	-0.2262043	-2.4582505	-1.9483505
H	1.4969537	-2.8238415	-2.1589535
C	-0.8254753	-3.9171175	0.6962775
H	-1.0992963	-4.8363365	0.1627715
H	-0.7584203	-4.1167455	1.7706885
H	-1.6065823	-3.1643775	0.5262355
H	-1.3899773	-0.1867935	-0.0014545
H	1.1013287	2.7484425	1.2341325
C	1.7862547	2.5340215	-1.7524335
C	0.6373147	3.1839915	-2.5093695
C	2.5368497	3.5863815	-0.9473945
C	2.7320537	1.8380845	-2.7267635
H	0.0546487	2.4608645	-3.0924885
H	-0.0347953	3.7363225	-1.8427905
H	1.0576907	3.9062265	-3.2181875

H	3.2852677	3.1304195	-0.2886345
H	3.0501927	4.2726185	-1.6313735
H	1.8479807	4.1813795	-0.3324565
H	3.0913067	2.5668395	-3.4640715
H	3.6016997	1.4275495	-2.2025595
H	2.2309127	1.0194495	-3.2519975
H	-0.4869673	4.3718885	1.6828055
H	2.0592397	0.9780425	2.5507855
C	-2.1824703	-0.0495465	3.9891365
C	-3.1773563	1.5923065	1.9845345
H	-1.7426003	-0.6585235	4.7754295
H	-3.5847903	2.2638705	1.2319805
C	-4.0340933	1.0490865	2.9356895
C	-3.5415393	0.2156615	3.9367945
H	-5.0935163	1.2935825	2.8997845
H	-4.2126223	-0.2023475	4.6830285
H	2.0941157	0.9343155	-0.4849595
C	5.7887677	-1.0100285	-1.6390065
F	5.8003657	0.2013195	-2.1687955
F	5.8515317	-1.9110555	-2.6088735
F	6.8204407	-1.1660445	-0.8376915
S	4.1943887	-1.2994295	-0.7278775
O	4.4608127	-2.4561965	0.1231275
O	3.1912317	-1.4214095	-1.7821505
N	3.8182167	0.0433675	0.0864385

S	4.7628377	0.7890135	1.1717465
O	6.1228817	1.0177735	0.7148085
O	3.9662467	1.8982425	1.6884745
C	4.9389777	-0.3650145	2.6153555
F	3.7679147	-0.9186905	2.9128885
F	5.8167527	-1.3090845	2.3439655
F	5.3576207	0.3401985	3.6526215

Zero-point correction= 0.700401 (Hartree/Particle)

Thermal correction to Energy= 0.755850

Thermal correction to Enthalpy= 0.756795

Thermal correction to Gibbs Free Energy= 0.610197

Sum of electronic and zero-point Energies= -3916.921123

Sum of electronic and thermal Energies= -3916.865674

Sum of electronic and thermal Enthalpies= -3916.864729

Sum of electronic and thermal Free Energies= -3917.011327

H-int7

C	-1.1409083	1.0723612	3.0284633
C	-1.8247833	1.3084792	1.8323823
C	0.3515397	1.1291152	3.1044653
C	1.0573097	1.1698702	1.8122123
C	0.3970627	2.0287212	0.7616063
C	-1.1127353	1.7607652	0.5635493
C	-1.8690283	2.9386242	-0.0402587
C	-2.6052673	2.4695782	-1.2466927
N	-2.2559033	1.1460342	-1.4275467

C	-1.1817973	0.7172102	-0.5635597
C	-1.9134853	4.1687522	0.4841093
N	1.0765097	1.7437692	-0.5921717
C	0.1252567	0.8145102	-1.3268587
O	0.3680337	0.3602572	-2.3990667
O	-3.3887633	3.0742562	-1.9566647
O	0.9198557	1.0514702	4.1848583
Au	1.1163997	-0.9394258	1.3099133
C	-2.6319413	5.3495672	-0.0636697
C	-2.2793183	-3.4194798	-2.1031637
C	-3.2155573	-3.7194348	-1.1097167
C	-4.0275903	-2.7049808	-0.5957167
C	-3.8922963	-1.4089178	-1.0848997
C	-2.9578443	-1.0949338	-2.0695127
C	-2.1472663	-2.1195358	-2.5658817
C	-2.7677843	0.3264972	-2.5170327
O	-3.2468363	-5.0102958	-0.7004217
C	-4.1416423	-5.3511158	0.3315343
H	-3.1850763	5.1013222	-0.9711597
H	-3.3268123	5.7521402	0.6838463
H	-1.9182953	6.1558032	-0.2811217
H	-1.6592093	-4.2264678	-2.4868877
H	-4.7637723	-2.9114778	0.1753643
H	-4.5252253	-0.6189498	-0.6802627
H	-1.3949943	-1.8892798	-3.3199657

H	-3.7084373	0.8016522	-2.8230067
H	-2.0856493	0.3658522	-3.3785637
H	-4.0068783	-6.4179158	0.5200473
H	-5.1859413	-5.1691068	0.0414163
H	-3.9254823	-4.7929328	1.2547763
P	1.0171287	-3.2440908	0.7863893
C	2.2758397	-4.2902778	1.5878133
H	2.2080527	-4.1837798	2.6749543
H	2.1406457	-5.3426078	1.3111633
H	3.2597357	-3.9411638	1.2563153
C	1.1191487	-3.6778708	-0.9796257
H	0.8496867	-4.7324038	-1.1190827
H	0.4354767	-3.0374788	-1.5470777
H	2.1340747	-3.4901558	-1.3376127
C	-0.5958963	-3.9372618	1.3043663
H	-0.6993363	-4.9844988	0.9936723
H	-0.6990433	-3.8583178	2.3915243
H	-1.3934583	-3.3459088	0.8357833
H	-1.3262883	-0.3157888	-0.2114717
H	0.5550117	3.0932092	0.9641003
C	1.6210447	2.9362412	-1.4766937
C	0.5021087	3.5635102	-2.2888057
C	2.2606467	3.9483272	-0.5388487
C	2.6926297	2.3466522	-2.3843517
H	0.0469837	2.8603492	-2.9956757

H	-0.2792463	4.0030892	-1.6610347
H	0.9418717	4.3740482	-2.8805847
H	2.9392057	3.4678832	0.1788763
H	2.8626807	4.6297442	-1.1507447
H	1.5246187	4.5608382	-0.0054557
H	3.0155527	3.1310422	-3.0779277
H	3.5624477	2.0296542	-1.8013787
H	2.3301877	1.4943132	-2.9655717
H	-1.3506573	4.3307882	1.4100793
H	2.0942387	1.4857602	1.9687923
C	-1.8424673	0.7154962	4.1821583
C	-3.2141863	1.1494012	1.8136533
H	-1.2603983	0.5600232	5.0876533
H	-3.7729173	1.3483302	0.9008333
C	-3.9029183	0.7655512	2.9563133
C	-3.2178133	0.5565822	4.1521483
H	-4.9835733	0.6474472	2.9165353
H	-3.7588563	0.2725202	5.0516023
H	1.9399847	1.1790802	-0.3908347
C	5.2556427	-0.8139638	-2.2552217
F	5.2729277	0.4627372	-2.6138927
F	5.0048777	-1.5564238	-3.3248877
F	6.4210367	-1.1581988	-1.7598767
S	3.8659927	-1.1276758	-1.0504817
O	4.2444937	-2.3669398	-0.3768197

O	2.6721517	-1.1249568	-1.8903467
N	3.7074927	0.1708752	-0.0943147
S	4.8668017	0.7129732	0.9057523
O	6.2155707	0.4415102	0.4369693
O	4.4620137	2.0604052	1.2905903
C	4.7284937	-0.2725378	2.4722663
F	3.5808017	-0.0337518	3.0864923
F	4.8198977	-1.5667608	2.2153473
F	5.7244107	0.0920702	3.2617323

Zero-point correction= 0.703839 (Hartree/Particle)

Thermal correction to Energy= 0.759133

Thermal correction to Enthalpy= 0.760078

Thermal correction to Gibbs Free Energy= 0.613853

Sum of electronic and zero-point Energies= -3916.943894

Sum of electronic and thermal Energies= -3916.888599

Sum of electronic and thermal Enthalpies= -3916.887655

Sum of electronic and thermal Free Energies= -3917.033879

H-ts7

C	1.0051856	-0.7601719	2.8407415
C	1.8092096	-1.0037029	1.7194025
C	-0.4262404	-1.1703199	2.8983595
C	-1.0210864	-1.6499209	1.6124415
C	-0.0901794	-2.3957949	0.6687245
C	1.3114256	-1.7720489	0.5039085
C	2.3556576	-2.7866349	0.0450705

C	3.0832746	-2.2218609	-1.1285425
N	2.4234836	-1.0641359	-1.4719325
C	1.1921356	-0.8805479	-0.7484805
C	2.6128776	-3.9542479	0.6449765
N	-0.7990644	-2.2101669	-0.6462745
C	0.0251026	-1.4544879	-1.5345115
O	-0.1490354	-1.3084989	-2.7153995
O	4.0853126	-2.6393009	-1.6824155
O	-1.0766314	-1.0792479	3.9263675
Au	-1.4168164	0.5718661	1.0580965
C	3.6361736	-4.9588059	0.2522275
C	1.7658806	3.4191311	-2.2721545
C	2.6883456	3.8965791	-1.3377595
C	3.6764396	3.0432851	-0.8398325
C	3.7161706	1.7214991	-1.2753735
C	2.7904626	1.2280001	-2.1921775
C	1.8069116	2.0939841	-2.6774985
C	2.8097956	-0.2200489	-2.5908415
O	2.5280566	5.1899081	-0.9597875
C	3.4604016	5.7284001	-0.0536485
H	4.2042346	-4.6354739	-0.6211565
H	4.3286666	-5.1342019	1.0852905
H	3.1590256	-5.9248059	0.0430555
H	1.0170616	4.1079661	-2.6554605
H	4.4104196	3.3930631	-0.1195155

H	4.4886876	1.0545631	-0.8907125
H	1.0605666	1.7172321	-3.3775385
H	3.8130626	-0.5586949	-2.8778625
H	2.1356496	-0.3960299	-3.4394375
H	3.1790586	6.7721051	0.0997065
H	4.4839036	5.6886171	-0.4520245
H	3.4360106	5.2044881	0.9140875
P	-1.0209224	2.8861811	0.9992175
C	-2.0244884	3.8857811	2.1446745
H	-1.9303974	3.4990091	3.1638725
H	-1.7025534	4.9334861	2.1147925
H	-3.0719954	3.8173951	1.8351515
C	-1.2107024	3.7029211	-0.6127655
H	-0.7206624	4.6846341	-0.5873895
H	-0.7634784	3.0736961	-1.3873425
H	-2.2782114	3.8000701	-0.8331565
C	0.7157326	3.1908281	1.4802445
H	0.9407766	4.2652041	1.4637905
H	0.8985446	2.7812311	2.4801135
H	1.3774686	2.6759631	0.7709725
H	1.0062346	0.1836601	-0.5237955
H	-0.0085104	-3.4623969	0.9065705
C	-1.6622034	-3.3324039	-1.2171605
C	-0.7319564	-4.3386569	-1.8851155
C	-2.4482164	-3.9983649	-0.0942305

C	-2.6640764	-2.7367979	-2.1984505
H	-0.1755984	-3.8874169	-2.7132095
H	-0.0158164	-4.7639059	-1.1690135
H	-1.3273594	-5.1644229	-2.2911755
H	-3.1650604	-3.3096539	0.3686695
H	-3.0323044	-4.8109299	-0.5402195
H	-1.8137634	-4.4529299	0.6757025
H	-3.3233004	-3.5415499	-2.5445665
H	-3.2783624	-1.9866709	-1.6901965
H	-2.1831944	-2.2790179	-3.0637755
H	2.0081406	-4.2033659	1.5239535
H	-1.9396354	-2.2071769	1.8265935
C	1.5111446	-0.0544769	3.9372165
C	3.1142526	-0.5001109	1.7209215
H	0.8478786	0.0902521	4.7870705
H	3.7681806	-0.6870889	0.8721395
C	3.6001816	0.2288481	2.7977265
C	2.8010886	0.4476661	3.9192815
H	4.6173666	0.6133481	2.7670955
H	3.1878536	1.0024111	4.7706385
H	-1.4371474	-1.2598969	0.2195205
C	-4.9393004	0.7736921	-2.6445765
F	-5.0232974	-0.5304399	-2.8579595
F	-4.4814754	1.3651471	-3.7379315
F	-6.1261874	1.2572511	-2.3583475

S	-3.7190214	1.1198511	-1.2761175
O	-4.1355884	2.4026001	-0.7103645
O	-2.4114344	1.0375361	-1.9271775
N	-3.7706644	-0.1341759	-0.2584205
S	-5.0689704	-0.5481889	0.6139905
O	-6.3236404	-0.0180139	0.1064095
O	-4.9315524	-1.9588869	0.9479065
C	-4.8107964	0.2987911	2.2375505
F	-3.7053844	-0.1560789	2.8257875
F	-4.6918814	1.6087731	2.0751385
F	-5.8453264	0.0452591	3.0176225

Zero-point correction= 0.697470 (Hartree/Particle)

Thermal correction to Energy= 0.752489

Thermal correction to Enthalpy= 0.753434

Thermal correction to Gibbs Free Energy= 0.608532

Sum of electronic and zero-point Energies= -3916.901854

Sum of electronic and thermal Energies= -3916.846834

Sum of electronic and thermal Enthalpies= -3916.845890

Sum of electronic and thermal Free Energies= -3916.990792