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Supporting Information for

A DFT Study on Gold-Catalyzed Domino Cyclization for Post-Ugi Synthesis of Spiroindolines: Insights on the Origin of Remarkable Diastereoselectivity

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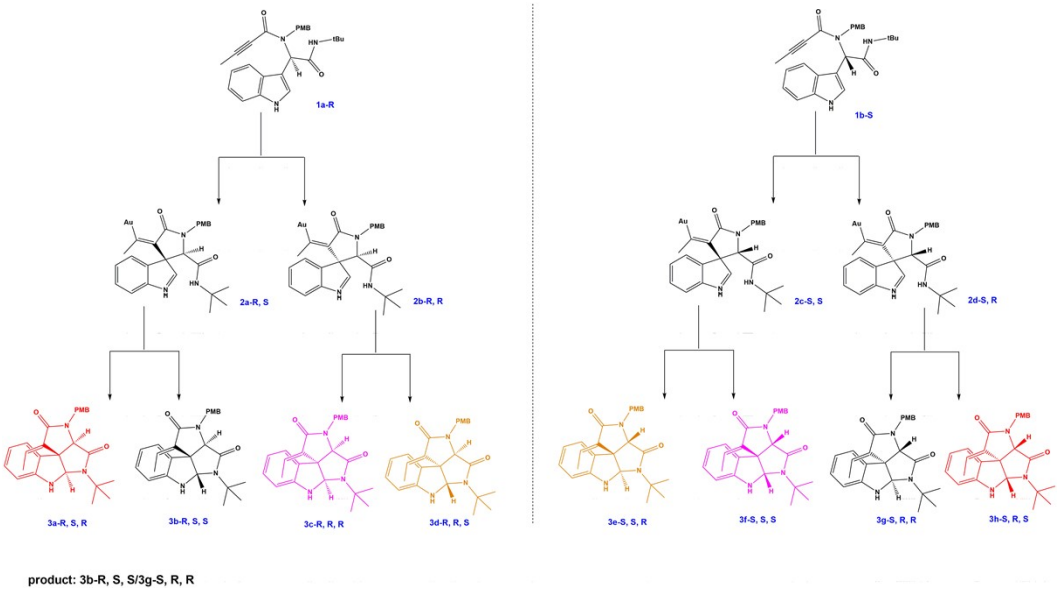


Fig S1. Configuration of spiroindolines.

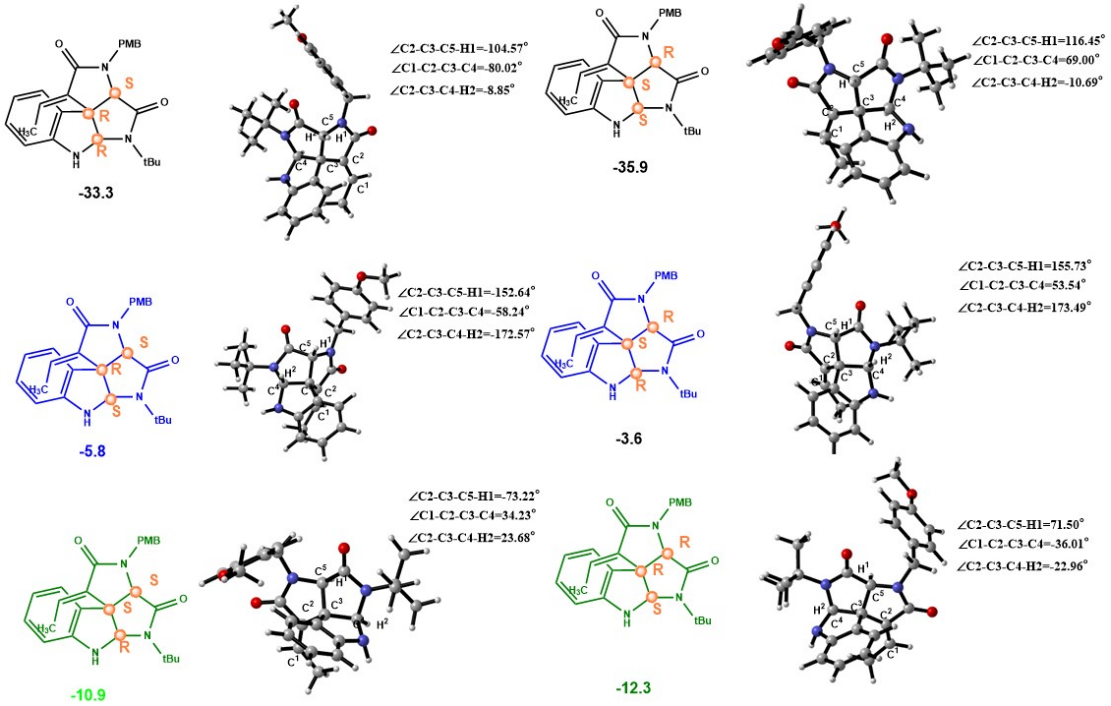


Fig S2. Optimized structures for spiroindolines. The ΔG values are in kcal/mol. The dihetral angles are in degree.

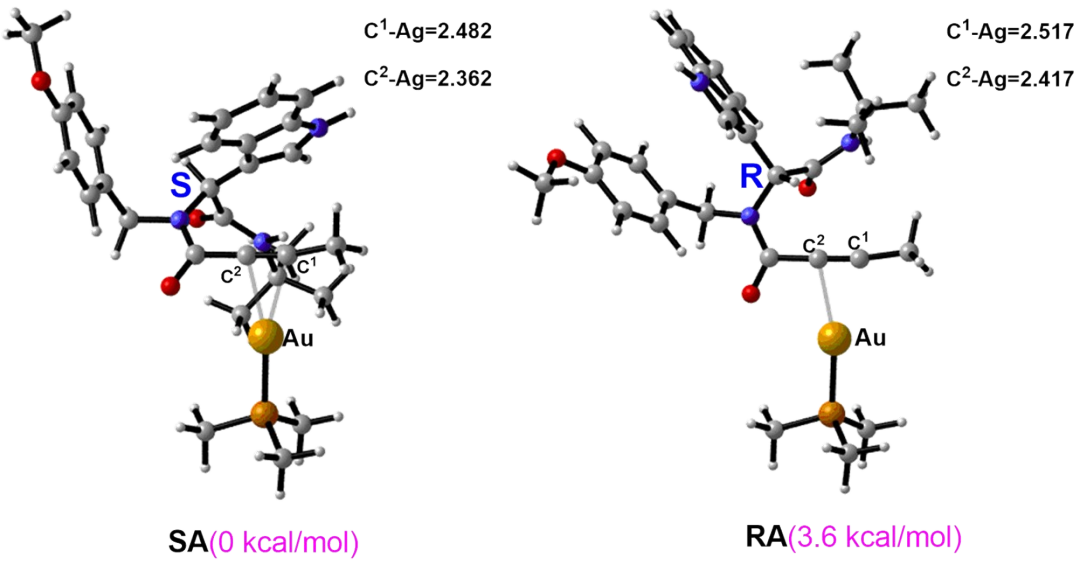
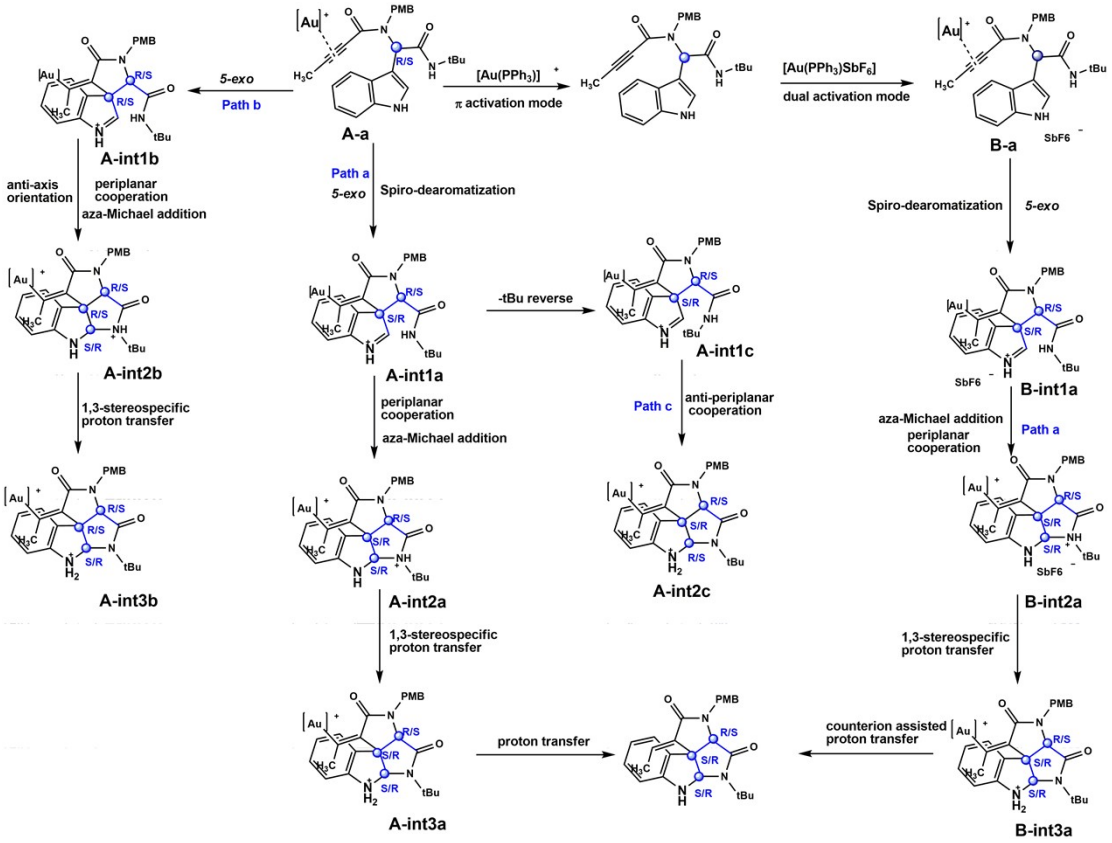


Fig S3. Optimized structures for SA and RA. The Gibbs relative free energy are in kcal/mol. The distances are in Å.



Scheme S1 . General catalytic cycle induced by π coordination mode and dual coordination mode.

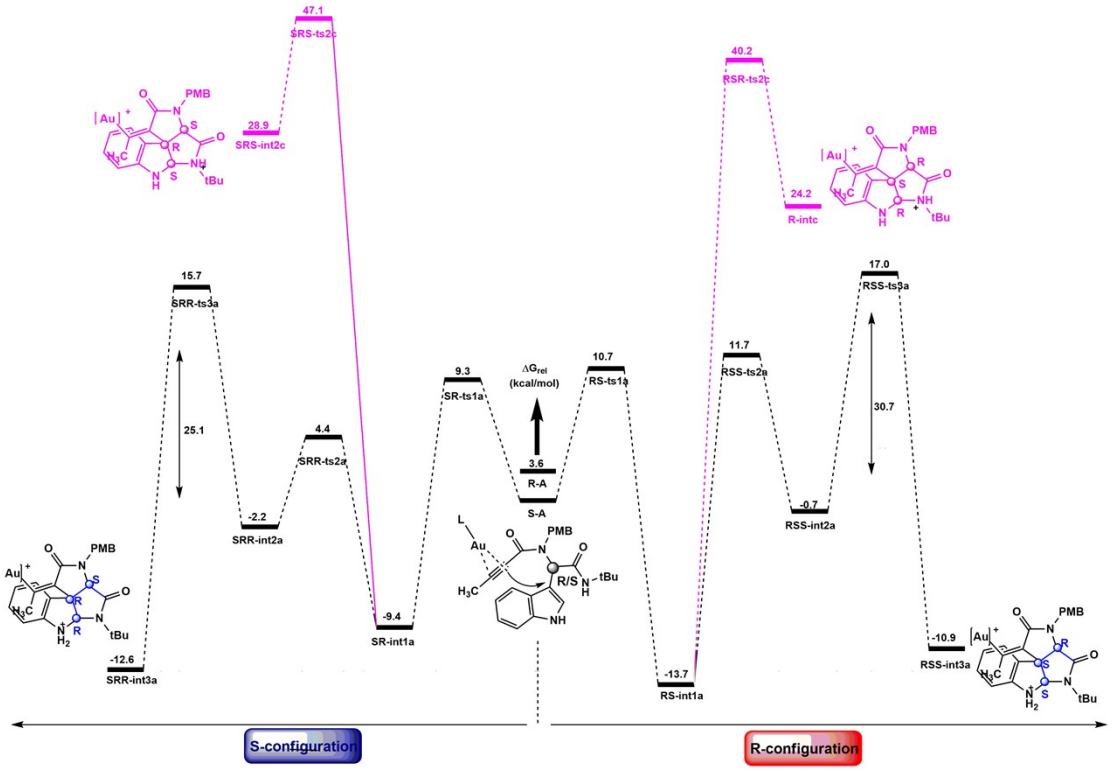


Fig. S4. Gibbs free-energy profiles for [PMe_3Au]+catalyzed domino cyclization

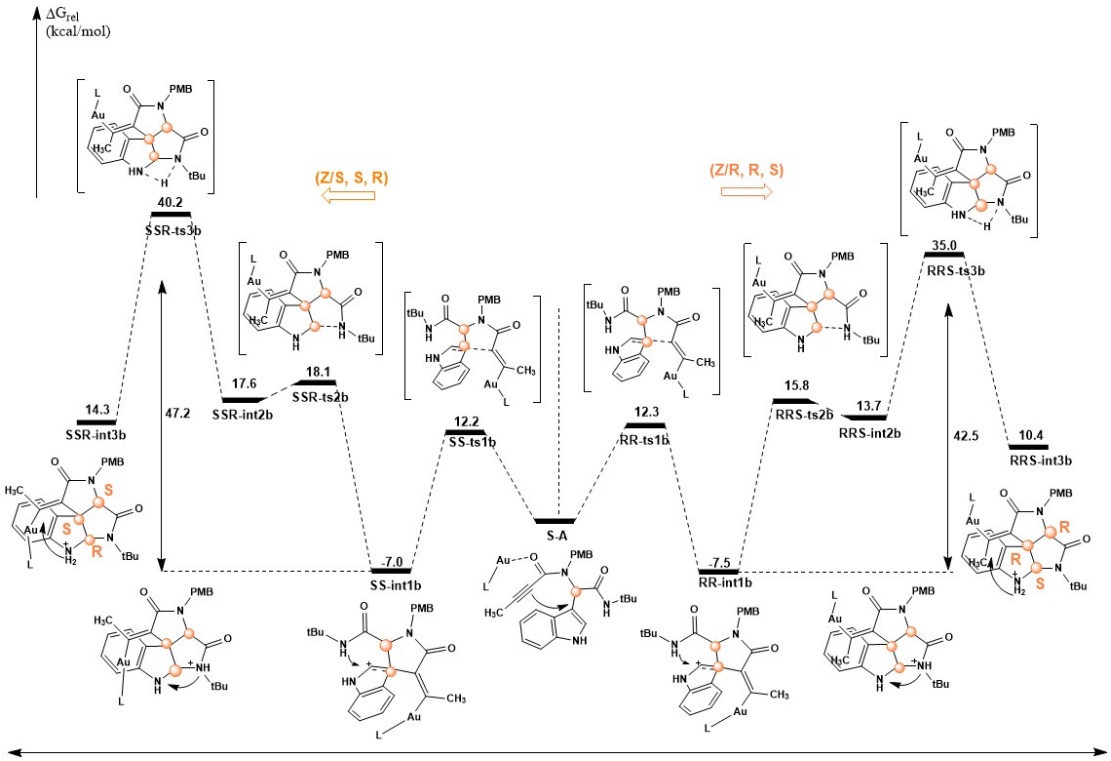


Fig S5. Energy profiles for the formation of spiroindolines intermediate catalyzed by[Au(PMe3)]+.

(path i for product (Z/S, S, R); path j for product (Z/R, R, S).).

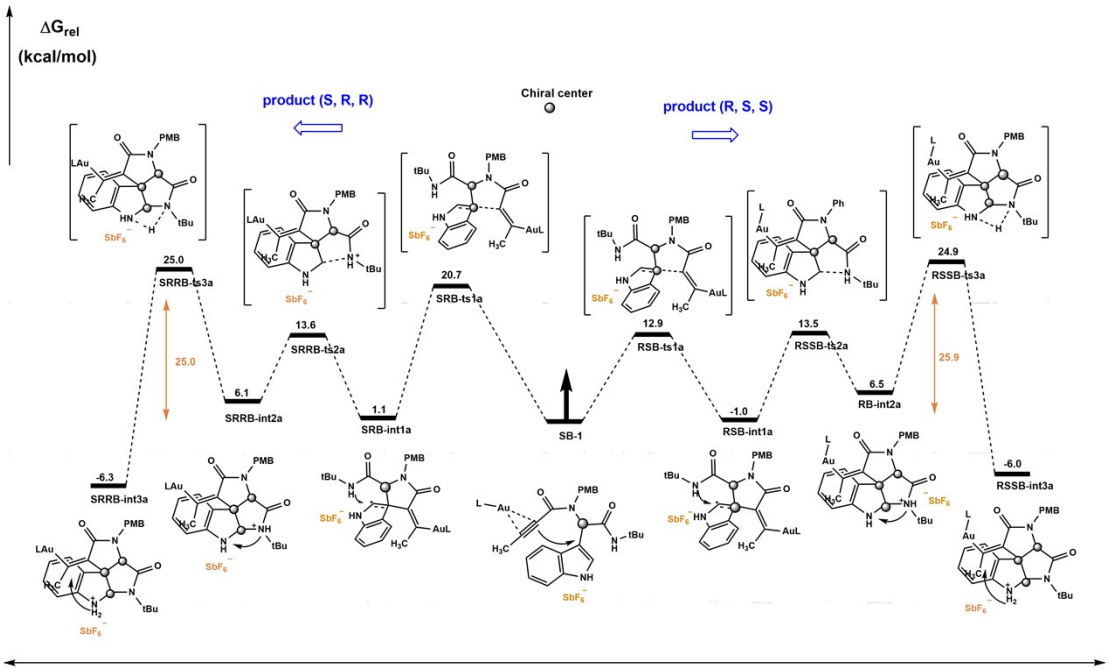


Fig. S6. Energy profiles for the formation of spiroindolines intermediate catalyzed by[Au(PMe_3)SbF_6].

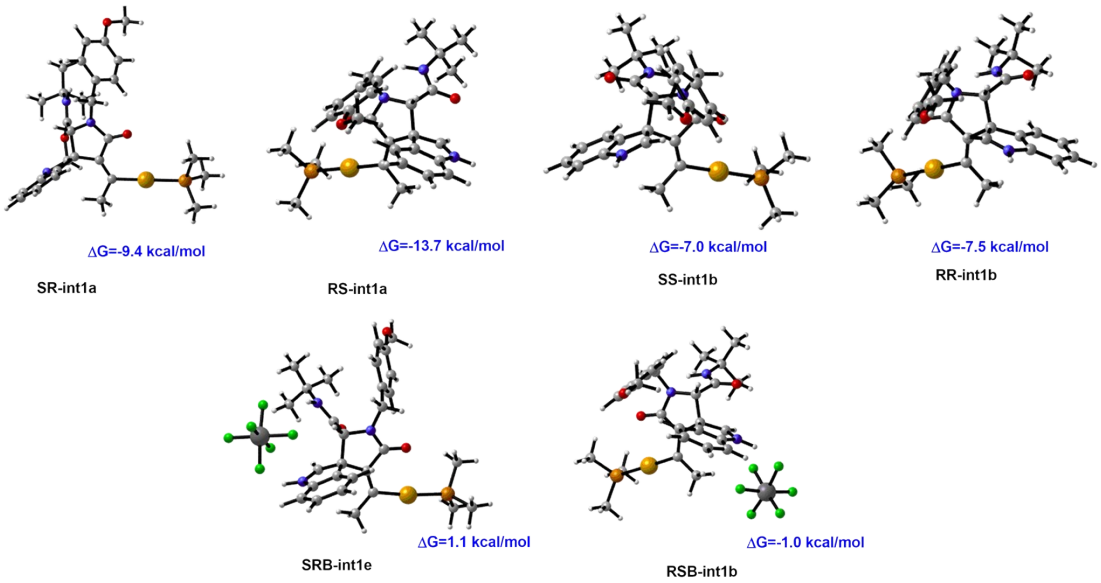


Fig.S7 Optimized structures for spiro-intermediates. The Gibbs relative free energy are in kcal/mol. The distances are in Å.

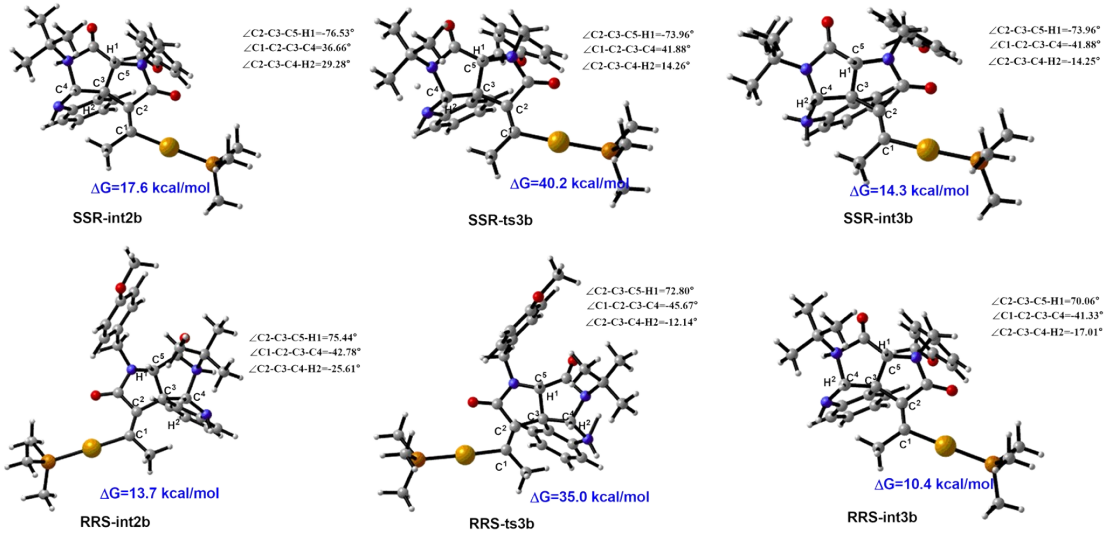


Fig S8. Optimized transition state and intermediates structures for Fig S5.

Table S1. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig. S4

System	ΔErelgas	ΔGrelgas	ΔE≠gas	ΔG≠gas	ΔErelsol	ΔGrelsol	ΔE≠sol	ΔG≠sol
S-A	0	0			0	0		
RS-ts1a	3.8	6.0	3.8	6.0	10.6	10.7	10.6	10.7
RS-int1a	-21.4	-20.3			-13.3	-13.7		
RSS-ts2a	6.5	8.6	27.9	28.9	10.8	11.7	24.1	25.4
RSS-int2a	-8.0	-4.6			-4.5	-0.7		
RSS-ts3a	10.6	13.8	18.5	18.4	18.3	17.0	22.8	17.7
RSS-int3a	-13.1	-8.7			-15.4	-10.9		
RSR-ts2c	35.7	36.8	38.4	36.8	41.8	40.2	43.0	41.8
RSR-int2c	18.0	21.2			21.4	24.1		
SR-ts1a	5.0	5.2	5.0	5.2	10.6	9.3	10.6	9.3
SR-int1a	-15.2	-14.0			-9.6	-9.4		
SRR-ts2a	1.5	3.2	16.7	17.2	4.7	4.4	14.2	13.8
SRR-int2a	-6.0	-4.7			-3.6	-2.2		
SRR-ts3a	11.5	13.0	17.5	17.7	18.9	15.7	22.4	17.9
SRR-int3a	-12.8	-10.5			-15.5	-12.6		
SRS-ts2c	38.7	43.7	44.7	48.9	38.7	47.1	46.6	49.3
SRS-int2c	22.7	26.5			26.1	28.9		

Table S2. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig. S5

System	ΔErelgas	ΔGrelgas	ΔE≠gas	ΔG≠gas	ΔErelsol	ΔGrelsol	ΔE≠sol	ΔG≠sol
S-A	0	0			0	0		
RR-ts1b	6.2	8.0	6.2	8.0	11.5	12.2	11.5	12.2
RR-int1b	-9.5	-9.3			-7.2	-7.0		
RRS-ts2b	14.7	16.3	24.1	25.6	18.4	18.1	25.7	25.1
RRS-int2b	12.9	15.3			15.4	17.6		
RRS-ts3b	32.7	37.7	19.8	22.4	39.7	40.2	24.3	22.6
RRS-int3b	10.8	15.2			9.9	14.3		
SS-ts1b	6.2	8.1	6.2	8.1	11.5	12.3	11.5	12.3
SS-int1b	-9.5	-9.8			-7.2	-7.5		
SSR-ts2b	10.1	13.0	19.6	22.8	14.2	15.8	21.4	23.2
SSR-int2b	8.0	10.1			11.5	13.7		
SSR-ts3b	29.0	31.4	20.9	21.3	36.9	35.0	25.3	21.3
SSR-int3b	9.7	11.6			8.6	10.4		

Table S3. Thermodynamic properties (relative free energies and activation free energies in gas phase and in solution) of the structures in Fig S6

System	ΔErelgas	ΔGrelgas	ΔE≠gas	ΔG≠gas	ΔErelsol	ΔGrelsol	ΔE≠sol	ΔG≠sol
SB-1	0	0			0	0		
RSB-ts1a	26.4	27.5	26.4	27.5	19.1	20.7	19.1	20.7
RSB-int1a	-0.9	1.9			-2.4	1.1		
RSSB-ts2a	14.4	16.6	4.6	7.0	14.4	13.6	16.6	14.7
RSSB-int2a	5.2	8.1			4.8	6.1		
RSSB-ts3a	22.7	26.2	17.5	18.1	26.9	25.0	22.3	18.8
RSSB-int3a	-5.0	-2.6			-8.1	-6.1		
SRB-ts1a	11.5	12.5	11.5	12.5	12.6	12.9	12.6	12.9
SRB-int1a	5.3	3.9			-0.3	-1.0		
SRRB-ts2a	14.3	16.6	9.0	12.7	14.1	13.5	14.4	14.5
SRRB-int2a	5.3	8.6			4.7	6.5		
SRRB-ts3a	22.8	26.2	17.4	17.6	27.0	24.9	22.3	18.4
SRRB-int3a	-5.0	-2.3			-8.2	-6.0		

The Cartesian coordinates of the stationary points discussed in the text

S-A

C	-3.4934376	0.6770843	2.8403626
C	-3.4483016	1.9002033	3.5396206
C	-2.7380556	2.9820463	3.0510076
C	-2.0629286	2.8075503	1.8369616
C	-2.0806476	1.5849333	1.1274186
C	-2.8212826	0.5061793	1.6442506
N	-1.2881386	3.6930233	1.1192506
C	-0.8256646	3.0742243	-0.0165764
C	-1.2611776	1.7736803	-0.0464714
C	-1.0330966	0.7787243	-1.1453604
N	-0.8631006	-0.6257957	-0.7102964
C	-0.0424836	-1.0594267	0.2617116
C	0.5722864	-0.0440987	1.1544996
O	0.2404034	-2.2327187	0.4856686
C	0.1540114	1.0354823	-2.1007734
O	0.0662244	0.6964973	-3.2690084
N	1.2887534	1.5004123	-1.5190094
C	0.9834374	0.6860063	2.0465796
Au	2.8161354	-0.7772777	1.2331966

C	1.2530104	1.6926883	3.0728596
C	2.5923894	1.6078183	-2.1975474
C	3.5678634	2.1790563	-1.1679294
C	3.0472884	0.2127393	-2.6404354
C	2.4932994	2.5512163	-3.4003814
C	-4.3740826	-2.9563087	0.5236066
C	-5.4707556	-2.2912227	-0.0459514
C	-5.2798966	-1.4582867	-1.1495124
C	-3.9939626	-1.2875757	-1.6634844
C	-2.8980036	-1.9312687	-1.0986634
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C	-1.4962526	-1.6532297	-1.5716534
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H	-2.8836346	-0.4359927	1.1093466
H	-1.1822316	4.6731863	1.3261216
H	-0.2263576	3.6175953	-0.7336854
H	-1.9172986	0.7567613	-1.7890854
H	1.2298164	1.7796293	-0.5495104
H	1.9352424	2.4583613	2.6958756
H	0.2953924	2.1608713	3.3256596
H	1.6780494	1.2414393	3.9708546
H	3.2425154	3.1671243	-0.8258404
H	4.5612044	2.2878353	-1.6110574
H	3.6525884	1.5173563	-0.2944754
H	2.3371234	-0.2123307	-3.3520404
H	4.0310474	0.2689383	-3.1175214
H	3.1097464	-0.4539347	-1.7689144
H	1.7797584	2.1665783	-4.1294494
H	3.4721784	2.6481843	-3.8783214
H	2.1688654	3.5443843	-3.0764014
H	-4.5551356	-3.6110687	1.3689016
H	-6.1129036	-0.9464657	-1.6147984
H	-3.8548746	-0.6447737	-2.5296734
H	-2.2568366	-3.2886447	0.4467416
H	-0.8728326	-2.5459617	-1.5183394
H	-1.4708636	-1.2669987	-2.5935894
H	-8.6511936	-2.2200207	0.5931966
H	-7.9632756	-2.2047667	-1.0517844
H	-7.7178026	-0.8062307	0.0354536
P	4.8175054	-1.7997527	0.7600126

C	5.9977704	-0.7002197	-0.0865594
H	6.2318964	0.1526303	0.5540536
H	6.9162514	-1.2456267	-0.3197884
H	5.5462234	-0.3332717	-1.0114944
C	4.5729764	-3.2167317	-0.3575044
H	5.5324404	-3.6962987	-0.5692724
H	3.8959754	-3.9360307	0.1077846
H	4.1243534	-2.8691547	-1.2907604
C	5.6925514	-2.4536907	2.2173716
H	6.6175884	-2.9455987	1.9049476
H	5.9283114	-1.6373877	2.9028636
H	5.0537334	-3.1738697	2.7325206

Zero-point correction= 0.627676 (Hartree/Particle)
Thermal correction to Energy= 0.669078
Thermal correction to Enthalpy= 0.670022
Thermal correction to Gibbs Free Energy= 0.548426
Sum of electronic and zero-point Energies= -1993.115889
Sum of electronic and thermal Energies= -1993.074487
Sum of electronic and thermal Enthalpies= -1993.073543
Sum of electronic and thermal Free Energies= -1993.195139

RS-ts1a

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C	-1.5671059	3.4468553	0.9258280
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C	-0.6079419	2.9571663	-0.0574670
C	0.7033961	2.2998293	0.2961640
C	3.6727891	0.4463853	1.6869880
C	-0.6897699	0.4217813	0.8757010
C	-1.5114389	0.9358033	-0.2582110
C	-2.3957249	0.6656963	-1.1200890
C	-3.0703659	1.2526113	-2.3040760
C	2.4064071	-0.0874787	1.9566190
C	2.2291531	-1.4676357	1.8669680
C	1.4973871	1.9577513	-0.9876880
C	1.2432171	0.8081503	2.3077380
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C	2.6111071	0.1734083	-2.3246650
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C	1.8309581	0.4452113	-3.6135860
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H	3.8327291	1.5201363	1.7536760
H	1.2483851	-1.8883317	2.0727350
H	0.5879631	0.3149153	3.0295900
H	1.5993031	1.7458913	2.7462760
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H	-2.9586279	3.7306213	3.9943690
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H	-3.2398259	0.5017403	-3.0768600
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O	-1.0055689	-0.6112887	1.4543170
O	1.7306161	2.8648343	-1.7764450
O	5.6368781	-2.4812277	0.9229790
Au	-3.1002139	-1.3046887	-0.3970030
P	-4.0057629	-3.3386257	0.2229520
C	-3.0074119	-4.1445207	1.5196960
H	-3.4684639	-5.0858347	1.8305370
H	-2.0043389	-4.3365827	1.1335180

H	-2.9230529	-3.4721017	2.3759030
C	-5.6868409	-3.2181377	0.9207050
H	-6.3639579	-2.8016687	0.1723880
H	-6.0421399	-4.2065597	1.2241990
H	-5.6727089	-2.5539327	1.7871200
C	-4.1361919	-4.5668177	-1.1192300
H	-3.1468539	-4.7487057	-1.5435390
H	-4.5467429	-5.5045927	-0.7354970
H	-4.7869199	-4.1794187	-1.9056480

Zero-point correction= 0.627388 (Hartree/Particle)
Thermal correction to Energy= 0.666864
Thermal correction to Enthalpy= 0.667808
Thermal correction to Gibbs Free Energy= 0.551566
Sum of electronic and zero-point Energies= -1993.109779
Sum of electronic and thermal Energies= -1993.070303
Sum of electronic and thermal Enthalpies= -1993.069359
Sum of electronic and thermal Free Energies= -1993.185601

RS-int1a

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C	-0.7266245	-5.8037508	-0.4409770
C	-0.5572935	-4.4957418	-0.0133690
C	-0.9490885	-3.4147348	-0.8023520
C	-1.5243835	-3.6148728	-2.0451890
C	4.2540075	2.3032992	-1.9137860
C	-0.1213865	-2.6398418	1.2991130
C	-0.6043775	-2.1295658	-0.0887220
C	0.6453565	-1.4354778	-0.7118570
C	3.2626835	1.4302362	-2.3410330
C	-1.1125855	0.1301832	-0.8387510
C	-1.6484445	-1.0223998	-0.0708110
C	-2.8826835	-1.0577728	0.4673170
C	-3.3755785	-2.2923108	1.1734740
C	1.9807625	1.4677662	-1.7794840
C	1.7207335	2.3940422	-0.7676530
C	1.6049305	-1.3402568	0.4687740
C	0.8737205	0.5624402	-2.2723520
C	4.7721675	5.0140672	0.4451050
C	3.6819215	-0.5336738	1.6141440
C	4.1800575	-1.9175908	2.0325300
C	2.9832375	0.1987792	2.7609680
C	4.8349355	0.3062862	1.0708890
C	2.7052335	3.2724932	-0.3233740

C	3.9798945	3.2347642	-0.9054990
H	2.8959155	-0.1009418	-0.3541180
H	3.4823965	0.7237802	-3.1380850
H	0.7218685	2.4371662	-0.3387980
H	0.0965585	1.1597182	-2.7589450
H	1.2662635	-0.1505858	-3.0086190
H	5.7103675	5.5528102	0.5647060
H	3.9875535	5.7117362	0.1328240
H	-2.1645315	-5.1108968	-3.4552460
H	-1.4630825	-7.0137838	-2.0503700
H	-0.4232265	-6.6437608	0.1744640
H	-1.8473535	-2.7686798	-2.6453830
H	-0.1546985	-4.5952198	2.0420080
H	-0.6842745	-2.2717848	2.1577700
H	1.1211425	-2.0475908	-1.4899120
H	-3.6388955	-2.0475928	2.2084120
H	-2.6785515	-3.1389258	1.1754530
H	-4.3035265	-2.6332028	0.7033660
H	4.4921015	4.5540432	1.4002910
H	4.9359235	-1.7933688	2.8117180
H	4.6443085	-2.4325708	1.1874520
H	3.3770975	-2.5378878	2.4322430
H	3.7024105	0.3666352	3.5663490
H	2.6122615	1.1693412	2.4190400
H	2.1515845	-0.3836708	3.1621930
H	5.5897155	0.4286302	1.8501690
H	4.4862965	1.2984282	0.7703950
H	5.3084675	-0.1776728	0.2111100
H	2.4698625	3.9885542	0.4546340
H	5.2482985	2.2908962	-2.3462350
N	0.1934665	-0.1742178	-1.2194760
N	2.7147045	-0.6713878	0.4745770
N	-0.0132405	-4.0422138	1.2089110
O	-1.6478565	1.1778562	-1.1467460
O	1.2233775	-2.0110468	1.5067000
O	5.0078455	4.0317192	-0.5458480
Au	-4.1597015	0.5628642	0.3097840
P	-5.6188415	2.4095382	0.0788180
C	-5.6639255	3.5565612	1.5035770
H	-4.6569635	3.9323042	1.6963430
H	-6.3338925	4.3968702	1.3024730
H	-6.0086545	3.0209212	2.3904400
C	-5.1662685	3.4787562	-1.3339930
H	-5.8297695	4.3452362	-1.3995600

H	-4.1329655	3.8109062	-1.2132810
H	-5.2303495	2.8983592	-2.2567980
C	-7.3789825	2.0069792	-0.2127560
H	-7.7660805	1.4376832	0.6348030
H	-7.9689765	2.9186972	-0.3393730
H	-7.4649195	1.3906412	-1.1099860

Zero-point correction= 0.631457 (Hartree/Particle)
Thermal correction to Energy= 0.670750
Thermal correction to Enthalpy= 0.671694
Thermal correction to Gibbs Free Energy= 0.554004
Sum of electronic and zero-point Energies= -1993.150062
Sum of electronic and thermal Energies= -1993.110769
Sum of electronic and thermal Enthalpies= -1993.109824
Sum of electronic and thermal Free Energies= -1993.227514

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C	-0.8130887	1.3931312	-0.9601802
C	0.0370093	2.4827552	1.2316168
C	0.3781983	2.0697492	-0.1864342
C	0.6621753	3.4241922	-0.8086472
C	0.4039983	4.4265852	0.1212998
C	-2.1587357	1.5310382	-0.2288642
C	1.1944293	5.1274842	-2.3933952
C	-2.2161517	0.3555202	2.0563398
C	-1.0376487	-0.5930858	1.8485458
C	-2.2421167	0.8651952	3.4981728
C	-3.5204397	-0.3741738	1.7257008
C	1.0595093	3.7705642	-2.0890832
C	0.9266133	6.1135622	-1.4419532
C	0.5224423	5.7776922	-0.1490802
C	0.9097043	-0.2225858	-0.8598632
C	1.4790803	0.9918912	-0.2021612
C	2.7414263	1.0705742	0.2565628
H	0.0703463	1.8479152	2.1028678
H	-0.9840597	1.9263662	-1.9047032
H	-1.0452717	-1.0188908	0.8461518
H	-1.1409767	-1.4193198	2.5567898
H	-0.0593597	-0.1363958	2.0282188
H	-3.0799687	1.5505772	3.6625308
H	-2.3621017	0.0228452	4.1831058
H	-1.3150307	1.3825052	3.7673988
H	-4.3855097	0.2773122	1.8867618
H	-3.5265477	-0.7079398	0.6847258
H	-3.6296987	-1.2546438	2.3652368

H	1.2772363	3.0067202	-2.8295022
H	1.5173853	5.4214702	-3.3857632
H	1.0373843	7.1586452	-1.7075772
H	0.3172383	6.5377542	0.5967298
N	-2.1260737	1.5940422	1.1926728
N	0.0805053	3.7860042	1.3520518
N	-0.3874857	0.0488352	-1.2337042
O	-3.1596067	1.7818692	-0.8522222
O	1.4533733	-1.2916038	-1.0719432
H	-2.9376467	2.1630652	1.4405438
H	-0.0051747	4.2745872	2.2357758
Au	4.0150013	-0.5603218	0.0868688
P	5.4335113	-2.4321458	-0.1478642
C	5.6454003	-3.4452518	1.3603908
H	4.6668303	-3.7813458	1.7093028
H	6.2769453	-4.3140028	1.1559388
H	6.1034423	-2.8393228	2.1447768
C	4.7938983	-3.6125468	-1.3887512
H	4.7482023	-3.1193168	-2.3619772
H	5.4328813	-4.4971208	-1.4556302
H	3.7796663	-3.9066208	-1.1103652
C	7.1458463	-2.0918088	-0.6920242
H	7.7063903	-3.0233588	-0.8076042
H	7.1235383	-1.5605398	-1.6457012
H	7.6422923	-1.4575858	0.0452168
C	3.2807463	2.3257932	0.8823188
H	2.5786473	3.1655782	0.9270148
H	3.6361473	2.1103342	1.8954128
H	4.1610773	2.6612692	0.3249688
C	-1.0961867	-0.7710528	-2.2147982
H	-0.3375917	-1.4267378	-2.6514352
H	-1.4760847	-0.1050038	-2.9993582
C	-2.2256467	-1.5912578	-1.6406372
C	-3.5563387	-1.2912868	-1.9100492
C	-1.9362837	-2.7007458	-0.8323482
C	-4.5947467	-2.0646188	-1.3862002
H	-3.7989837	-0.4340368	-2.5324192
C	-2.9516997	-3.4685938	-0.2926582
H	-0.8959057	-2.9533998	-0.6364712
C	-4.2918207	-3.1557468	-0.5694752
H	-5.6204567	-1.8069758	-1.6188502
H	-2.7456137	-4.3310208	0.3317228
O	-5.2109407	-3.9669078	0.0000278
C	-6.5739267	-3.7165778	-0.2798772

H	-7.1377697	-4.4811458	0.2520428
H	-6.8770477	-2.7254008	0.0773188
H	-6.7787847	-3.7929848	-1.3535482

Zero-point correction= 0.629885 (Hartree/Particle)
Thermal correction to Energy= 0.668894
Thermal correction to Enthalpy= 0.669838
Thermal correction to Gibbs Free Energy= 0.553931
Sum of electronic and zero-point Energies= -1993.105463
Sum of electronic and thermal Energies= -1993.066455
Sum of electronic and thermal Enthalpies= -1993.065511
Sum of electronic and thermal Free Energies= -1993.181418

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C	0.9081860	-1.4440421	-1.2524965
C	0.4567650	-2.3194241	1.0525095
C	-0.2010150	-2.0542811	-0.3510305
C	-0.5625920	-3.4549021	-0.7869665
C	-0.0257910	-4.3839941	0.0981275
C	2.1793840	-1.4464141	-0.4231645
C	-1.4706180	-5.2378751	-2.0941105
C	1.9729820	-0.3830711	1.9852245
C	0.8424070	0.6066199	1.7414045
C	1.9475940	-0.9395151	3.4080925
C	3.3241290	0.2571779	1.6779525
C	-1.2881190	-3.8687381	-1.8924375
C	-0.9288080	-6.1607571	-1.1997865
C	-0.1936160	-5.7476481	-0.0872465
C	-0.8063670	0.1766719	-1.1171915
C	-1.2967470	-0.9957831	-0.3435205
C	-2.4927690	-1.0389541	0.2740925
H	-0.1321860	-1.8978661	1.8668295
H	1.1096170	-2.0375161	-2.1535165
H	0.8673690	0.9876519	0.7192815
H	1.0021630	1.4575399	2.4086195
H	-0.1497760	0.1984719	1.9498345
H	2.7674290	-1.6452021	3.5783855
H	2.0768330	-0.1094341	4.1058535
H	0.9997140	-1.4260271	3.6538835
H	4.1436600	-0.4645071	1.7441305
H	3.3407660	0.7229869	0.6896075
H	3.4986690	1.0413409	2.4185735
H	-1.7226250	-3.1389581	-2.5698315
H	-2.0424200	-5.5861631	-2.9466015
H	-1.0813580	-7.2214371	-1.3671255

H	0.2272690	-6.4678681	0.6061615
N	1.8115900	-1.6215961	1.0545375
N	0.6763000	-3.7395081	1.1565055
N	0.4722250	-0.1109481	-1.5658845
O	3.3184310	-1.4314551	-0.7456255
O	-1.3517250	1.2429989	-1.3384445
H	2.4911510	-2.3163451	1.3879615
H	0.5074720	-4.1314771	2.0763045
Au	-3.8152720	0.5480969	0.1156185
P	-5.3101290	2.3639329	-0.1278895
C	-5.3956070	3.5106999	1.2951435
H	-4.3983550	3.9046609	1.5015915
H	-6.0769550	4.3390199	1.0829515
H	-5.7442500	2.9704789	2.1776765
C	-4.8529780	3.4391569	-1.5344075
H	-4.8956210	2.8579469	-2.4579615
H	-5.5277500	4.2960659	-1.6096115
H	-3.8262080	3.7857639	-1.3993815
C	-7.0585070	1.9313579	-0.4453125
H	-7.6611040	2.8332709	-0.5822145
H	-7.1209660	1.3129999	-1.3431055
H	-7.4494480	1.3570329	0.3970775
C	-2.9128490	-2.2423561	1.0761255
H	-2.1523510	-3.0244821	1.1855175
H	-3.2453500	-1.9294881	2.0711225
H	-3.7862240	-2.7040011	0.6023525
C	1.2041000	0.7610699	-2.4798015
H	0.4466900	1.3803499	-2.9686645
H	1.6846940	0.1353029	-3.2404065
C	2.2263320	1.6307369	-1.7846355
C	3.5930600	1.4344979	-1.9491625
C	1.7932220	2.6682659	-0.9445735
C	4.5274920	2.2339929	-1.2868365
H	3.9486660	0.6403449	-2.6003415
C	2.7043170	3.4622269	-0.2710075
H	0.7247290	2.8431139	-0.8329385
C	4.0817090	3.2506139	-0.4392905
H	5.5846470	2.0577419	-1.4419485
H	2.3861790	4.2720829	0.3765235
O	4.8908150	4.0772479	0.2593455
C	6.2868140	3.9475659	0.0721175
H	6.7479040	4.7152869	0.6911235
H	6.6406320	2.9604589	0.3921245
H	6.5623500	4.1091909	-0.9758105

Zero-point correction= 0.632088 (Hartree/Particle)
Thermal correction to Energy= 0.670850
Thermal correction to Enthalpy= 0.671794
Thermal correction to Gibbs Free Energy= 0.558211
Sum of electronic and zero-point Energies= -1993.128567
Sum of electronic and thermal Energies= -1993.089805
Sum of electronic and thermal Enthalpies= -1993.088861
Sum of electronic and thermal Free Energies= -1993.202444

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C	0.8846320	-1.3289729	-1.5091700
C	0.8350650	-1.9844919	0.8551420
C	-0.0270480	-1.9799099	-0.4397860
C	-0.2474530	-3.4523439	-0.6943830
C	0.4321450	-4.2413139	0.2240660
C	2.2908970	-1.2975489	-0.9217490
C	-1.0517030	-5.4497299	-1.7383030
C	2.9789430	-0.6853179	1.4940290
C	2.3064000	0.6839941	1.4960420
C	2.9105780	-1.3556089	2.8685980
C	4.4408880	-0.5700949	1.0604190
C	-1.0016000	-4.0570169	-1.6907510
C	-0.3571360	-6.2238819	-0.8068280
C	0.4038280	-5.6255599	0.1968960
C	-0.8996300	0.1693231	-1.1417350
C	-1.2375250	-1.0574169	-0.3648390
C	-2.3866630	-1.2277119	0.3148470
H	0.4009520	-1.4314609	1.6849770
H	0.9118170	-1.8791959	-2.4587270
H	2.3577020	1.1429971	0.5054910
H	2.8297180	1.3396901	2.1970090
H	1.2568320	0.6322271	1.8056940
H	3.3895100	-2.3407309	2.8571150
H	3.4542360	-0.7351719	3.5838840
H	1.8885870	-1.4522329	3.2486070
H	4.8835770	-1.5532029	0.8797320
H	4.5510150	0.0375121	0.1628100
H	4.9917310	-0.0873309	1.8714310
H	-1.5557880	-3.4507709	-2.4010940
H	-1.6425780	-5.9391369	-2.5044320
H	-0.4103540	-7.3054189	-0.8596900
H	0.9456130	-6.2209229	0.9240930
N	2.2300350	-1.5872589	0.5145800
N	1.1528000	-3.4179609	1.1743720

N	0.3693250	0.0081291	-1.6638740
O	3.3111040	-1.1074099	-1.5092330
O	-1.5609540	1.1791061	-1.3081320
H	2.3152320	-2.8715169	0.8005030
H	1.0298690	-3.6905729	2.1501910
Au	-3.8914990	0.1909951	0.1843810
P	-5.5879270	1.8217931	-0.0258550
C	-5.8784490	2.8545191	1.4561250
H	-4.9477370	3.3507931	1.7385750
H	-6.6464180	3.6070461	1.2578330
H	-6.1974300	2.2194181	2.2850720
C	-5.2050680	3.0323761	-1.3415730
H	-5.1287370	2.5093851	-2.2971940
H	-5.9784600	3.8025001	-1.4051830
H	-4.2378560	3.4935131	-1.1308290
C	-7.2531540	1.2020491	-0.4592580
H	-7.9562760	2.0312171	-0.5751390
H	-7.1976610	0.6394021	-1.3933960
H	-7.6072830	0.5320101	0.3268000
C	-2.6212900	-2.4546909	1.1564830
H	-1.7246040	-3.0521009	1.3643550
H	-3.0796550	-2.1776049	2.1091670
H	-3.3397950	-3.1119759	0.6524180
C	0.9631170	0.9871341	-2.5755610
H	0.1284730	1.4840761	-3.0784490
H	1.5496990	0.4428891	-3.3229910
C	1.8241630	1.9965381	-1.8523990
C	3.2210500	1.9518751	-1.9182800
C	1.2227270	2.9659901	-1.0499640
C	3.9955720	2.8356471	-1.1812050
H	3.7078750	1.2110651	-2.5464900
C	1.9866240	3.8631761	-0.3059840
H	0.1377340	3.0064781	-0.9982920
C	3.3823310	3.7950971	-0.3660080
H	5.0790740	2.8165581	-1.2268040
H	1.4904600	4.6072761	0.3050310
O	4.2197940	4.6062471	0.3204210
C	3.6472840	5.6341581	1.1031380
H	4.4804750	6.1819721	1.5404290
H	3.0467860	6.3138361	0.4882490
H	3.0214650	5.2235821	1.9045770

Zero-point correction= 0.627087 (Hartree/Particle)
Thermal correction to Energy= 0.665599
Thermal correction to Enthalpy= 0.666543

Thermal correction to Gibbs Free Energy= 0.552994
Sum of electronic and zero-point Energies= -1993.099006
Sum of electronic and thermal Energies= -1993.060495
Sum of electronic and thermal Enthalpies= -1993.059551
Sum of electronic and thermal Free Energies= -1993.173100

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C	0.7702135	-1.1826213	-1.5164008
C	0.7175005	-1.8582283	0.8295112
C	-0.1477735	-1.8592223	-0.4669778
C	-0.3890045	-3.3123783	-0.7702768
C	0.2657845	-4.1671403	0.0962302
C	2.1231215	-1.0259803	-0.8252088
C	-1.2200835	-5.2454413	-1.9159798
C	2.9726345	-0.8414573	1.5543022
C	3.4023345	0.6063497	1.2933122
C	2.3665135	-0.9365083	2.9550152
C	4.1688565	-1.7912533	1.4262652
C	-1.1536985	-3.8595853	-1.7954848
C	-0.5396705	-6.0829703	-1.0273688
C	0.2194865	-5.5485453	0.0110222
C	-1.0866855	0.2506097	-1.2076608
C	-1.3719745	-0.9565283	-0.3770828
C	-2.4889375	-1.1229793	0.3536362
H	0.1937745	-1.4793713	1.7059762
H	0.8959875	-1.7642683	-2.4379078
H	3.9306775	0.7006807	0.3450202
H	4.0662465	0.9327157	2.0983262
H	2.5318615	1.2689167	1.2672472
H	2.0373365	-1.9521123	3.2097462
H	3.1340195	-0.6648723	3.6822882
H	1.5282165	-0.2456923	3.0818942
H	3.9028235	-2.8218893	1.6988582
H	4.5599125	-1.7797253	0.4076442
H	4.9634015	-1.4787893	2.1087112
H	-1.6951825	-3.2087013	-2.4749908
H	-1.8133915	-5.6846123	-2.7103908
H	-0.6071845	-7.1589063	-1.1394848
H	0.7416155	-6.1884543	0.7150212
N	1.9374065	-1.2227533	0.5429202
N	0.9623125	-3.4049003	1.1474032
N	0.1577145	0.0988807	-1.7666398
O	3.1652005	-0.7461283	-1.3624088
O	-1.7829015	1.2399327	-1.3695828

H	0.6077155	-3.6446833	2.0790852
H	1.9750075	-3.5721313	1.1456542
Au	-3.9994365	0.2945537	0.2538542
P	-5.6567325	1.9641027	0.0616072
C	-4.9560585	3.5059577	-0.6272728
H	-4.4708915	3.2801747	-1.5792898
H	-5.7328205	4.2613017	-0.7734188
H	-4.1953755	3.8895077	0.0560042
C	-7.0384185	1.5612837	-1.0674418
H	-7.5734775	0.6869987	-0.6912158
H	-7.7295975	2.4045707	-1.1482288
H	-6.6379345	1.3236347	-2.0550998
C	-6.4895315	2.4959097	1.6007052
H	-5.7409865	2.8425937	2.3160362
H	-7.1988105	3.3026147	1.3970432
H	-7.0197375	1.6478667	2.0388272
C	-2.6750965	-2.3237353	1.2430652
H	-1.7838575	-2.9540523	1.3722402
H	-3.0205825	-2.0106463	2.2321802
H	-3.4647035	-2.9649403	0.8350752
C	0.8004515	1.1481737	-2.5511448
H	-0.0086475	1.6875357	-3.0524208
H	1.4262065	0.6713937	-3.3121538
C	1.6267355	2.0987477	-1.7103958
C	2.9893375	2.2624517	-1.9291488
C	1.0128995	2.8564237	-0.7014558
C	3.7469685	3.1553047	-1.1684568
H	3.4828385	1.6749247	-2.6982618
C	1.7513855	3.7386097	0.0683122
H	-0.0570735	2.7567847	-0.5389538
C	3.1263815	3.8938177	-0.1601888
H	4.8060805	3.2602827	-1.3693978
H	1.2913345	4.3382657	0.8463072
O	3.7596865	4.7794707	0.6453662
C	5.1383125	4.9942907	0.4262352
H	5.4490955	5.7424207	1.1539612
H	5.7141785	4.0738827	0.5816662
H	5.3266905	5.3702677	-0.5857828

Zero-point correction= 0.632366 (Hartree/Particle)
Thermal correction to Energy= 0.670395
Thermal correction to Enthalpy= 0.671340
Thermal correction to Gibbs Free Energy= 0.560074
Sum of electronic and zero-point Energies= -1993.136745
Sum of electronic and thermal Energies= -1993.098716

Sum of electronic and thermal Enthalpies= -1993.097772
Sum of electronic and thermal Free Energies= -1993.209037

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C	0.8430446	-1.0783670	-1.9675924
C	0.4606786	-1.2294040	0.3728236
C	-0.0996434	-1.7727350	-1.0208304
C	-0.0425574	-3.2520370	-0.7564834
C	-0.1719624	-3.4369690	0.6221206
C	2.1653266	-1.0591550	-1.1679164
C	0.0075886	-5.6212460	-1.0296204
C	2.9098726	-1.1023850	1.2285486
C	3.3715626	0.3556200	1.1851906
C	2.2987336	-1.4122650	2.5959846
C	4.0745006	-2.0661550	0.9823766
C	0.0536766	-4.3423850	-1.5993494
C	-0.1325294	-5.7872600	0.3456826
C	-0.2248734	-4.6855370	1.2054526
C	-1.0409274	0.3241240	-1.5639354
C	-1.4170544	-1.0639380	-1.0355024
C	-2.6049044	-1.3810570	-0.4139494
H	0.1587516	-0.2037380	0.6252376
H	0.9996296	-1.5481260	-2.9435694
H	3.8710426	0.5747430	0.2411076
H	4.0721576	0.5452910	2.0034666
H	2.5244046	1.0421310	1.2934846
H	1.9609136	-2.4525100	2.6570826
H	3.0688886	-1.2720650	3.3572396
H	1.4778626	-0.7292340	2.8456356
H	3.7199646	-3.1007690	0.9979496
H	4.5523106	-1.8677290	0.0235536
H	4.8162906	-1.9406200	1.7757596
H	0.1518196	-4.2176600	-2.6728444
H	0.0817836	-6.4938850	-1.6684954
H	-0.1652124	-6.7874830	0.7631096
H	-0.3325184	-4.8152850	2.2771756
N	1.8835416	-1.3353570	0.1648266
N	-0.3009814	-2.1398860	1.2233826
N	0.2163436	0.2334760	-2.0872744
O	3.2488016	-0.8397510	-1.6530064
O	-1.7411454	1.3190100	-1.5501584
H	-1.5808454	-1.4954650	0.5563146
H	-0.1937554	-2.0602380	2.2288726
Au	-3.9813324	0.1659100	-0.0629604

P	-5.5205764	1.9157290	0.2585946
C	-4.7647394	3.5434660	-0.0839264
H	-4.3473744	3.5377500	-1.0931284
H	-5.5041174	4.3435140	0.0074086
H	-3.9492104	3.7176040	0.6211246
C	-6.9727644	1.8469090	-0.8485674
H	-7.5350994	0.9307620	-0.6570804
H	-7.6204974	2.7122780	-0.6848234
H	-6.6356744	1.8368280	-1.8870954
C	-6.2374104	2.0829300	1.9311436
H	-5.4355184	2.2168380	2.6598886
H	-6.9131144	2.9413470	1.9730346
H	-6.7883754	1.1747870	2.1838406
C	-3.1189864	-2.8101570	-0.2469474
H	-2.4670654	-3.5945790	-0.6322214
H	-3.3549144	-3.0174970	0.8006486
H	-4.0675064	-2.8588450	-0.7876484
C	0.8986626	1.3853890	-2.6778344
H	0.1168986	2.0023380	-3.1305774
H	1.5509156	1.0112740	-3.4720834
C	1.6956226	2.1845410	-1.6718484
C	3.0710186	2.3367560	-1.8048044
C	1.0465416	2.8274820	-0.6061994
C	3.8054776	3.1123560	-0.9069224
H	3.5908326	1.8338630	-2.6153774
C	1.7628686	3.5894670	0.3001396
H	-0.0334064	2.7459300	-0.5114614
C	3.1506096	3.7376980	0.1553726
H	4.8753506	3.2120180	-1.0421314
H	1.2776586	4.1019690	1.1237276
O	3.7587756	4.5009270	1.0905716
C	5.1558466	4.6881350	0.9790406
H	5.4434386	5.3279240	1.8116936
H	5.6901056	3.7333400	1.0506066
H	5.4164806	5.1793230	0.0349546

Zero-point correction= 0.626755 (Hartree/Particle)
Thermal correction to Energy= 0.664807
Thermal correction to Enthalpy= 0.665751
Thermal correction to Gibbs Free Energy= 0.553758
Sum of electronic and zero-point Energies= -1993.079524
Sum of electronic and thermal Energies= -1993.041472
Sum of electronic and thermal Enthalpies= -1993.040528
Sum of electronic and thermal Free Energies= -1993.152521

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C	-1.3052224	0.8701055	-1.6849827
C	-1.5042924	1.3366395	0.7111743
C	-0.8529234	1.8693875	-0.6186037
C	-1.4602794	3.2427345	-0.7602157
C	-2.1480304	3.5586885	0.4114403
C	-2.4351134	0.0610375	-1.0527377
C	-2.0434574	5.3684015	-1.6900327
C	-3.2740284	-0.4985215	1.2137043
C	-2.5419154	-1.8448385	1.2550883
C	-3.3036904	0.1127155	2.6181023
C	-4.7234724	-0.6698225	0.7447593
C	-1.3934424	4.1386105	-1.8140147
C	-2.7401494	5.6731955	-0.5206337
C	-2.8016724	4.7781815	0.5479663
C	0.9916446	0.5573425	-1.4259037
C	0.6578876	1.7794405	-0.6571447
C	1.5674646	2.6163565	-0.1508577
H	-0.7848944	0.8200475	1.3567053
H	-1.6414154	1.3250595	-2.6222787
H	-2.5021954	-2.2935975	0.2594903
H	-3.0621474	-2.5344135	1.9261063
H	-1.5174994	-1.7209025	1.6231603
H	-3.9436364	1.0000135	2.6556713
H	-3.7401594	-0.6226845	3.2975713
H	-2.3087194	0.3567865	3.0030813
H	-5.1995514	0.3077655	0.6268753
H	-4.7779604	-1.2039675	-0.2015867
H	-5.2749734	-1.2313185	1.5042913
H	-0.8463184	3.8901995	-2.7200787
H	-2.0115024	6.0837855	-2.5035687
H	-3.2467814	6.6288805	-0.4359207
H	-3.3386324	5.0298505	1.4563553
N	-2.5397744	0.3976395	0.2671353
N	-1.9785724	2.5473445	1.3606563
N	-0.1265754	0.0356855	-1.9255737
O	-3.0723144	-0.7682535	-1.6708977
O	2.1175676	0.0300165	-1.6193597
H	-2.6602394	2.4542235	2.0983973
Au	3.9721606	0.1080275	-0.5666577
P	5.9800386	0.0431845	0.4756713
C	6.0959686	-1.2884795	1.7127723
H	5.9331306	-2.2527125	1.2272813
H	7.0836186	-1.2782425	2.1814873

H	5.3287546	-1.1458915	2.4762683
C	7.3672246	-0.2280685	-0.6724837
H	7.3973846	0.5785405	-1.4076157
H	8.3098786	-0.2533305	-0.1193127
H	7.2269496	-1.1752655	-1.1970247
C	6.3733766	1.5801985	1.3705743
H	5.6085236	1.7678675	2.1267893
H	7.3497266	1.4921185	1.8544783
H	6.3895736	2.4173015	0.6698033
C	1.2752446	3.8430605	0.6567423
H	0.3792896	3.7146015	1.2679353
H	2.1182016	4.0841105	1.3069283
H	1.1063906	4.7016085	-0.0036707
C	-0.1749044	-1.2126105	-2.6944697
H	0.7757316	-1.2834005	-3.2303317
H	-0.9860904	-1.1111455	-3.4191677
C	-0.4041074	-2.4291665	-1.8248227
C	-1.4576974	-3.2978585	-2.0874737
C	0.4511666	-2.7179855	-0.7538867
C	-1.6669614	-4.4392625	-1.3141977
H	-2.1486634	-3.0719825	-2.8938027
C	0.2495096	-3.8385045	0.0330503
H	1.2890486	-2.0586985	-0.5411927
C	-0.8124744	-4.7104265	-0.2436557
H	-2.4991434	-5.0921145	-1.5459837
H	0.9009376	-4.0754965	0.8671513
O	-0.9261174	-5.7768425	0.5797773
C	-1.9830574	-6.6842865	0.3369493
H	-1.8960184	-7.4607835	1.0952353
H	-2.9576694	-6.1913095	0.4296593
H	-1.8983484	-7.1354895	-0.6580017
H	2.6164086	2.3969185	-0.3581457

Zero-point correction= 0.632406 (Hartree/Particle)
Thermal correction to Energy= 0.671185
Thermal correction to Enthalpy= 0.672129
Thermal correction to Gibbs Free Energy= 0.556662
Sum of electronic and zero-point Energies= -1993.186548
Sum of electronic and thermal Energies= -1993.147769
Sum of electronic and thermal Enthalpies= -1993.146825
Sum of electronic and thermal Free Energies= -1993.262291

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C	-1.7954584	-2.9207434	2.3655644
C	-1.5060824	-2.8890894	3.7415664

C	-1.1116524	-1.7168094	4.3677454
C	-1.0152414	-0.5783374	3.5683064
C	-1.2812264	-0.5917994	2.1869634
C	-1.6841254	-1.7861934	1.5770184
N	-0.6852734	0.7281146	3.9099134
C	-0.7312834	1.5246746	2.8205274
C	-1.0305924	0.7566786	1.6966294
C	-1.4613254	1.2633606	0.3479074
N	-0.7400414	0.5443946	-0.6957286
C	0.4760516	0.0229126	-0.4411426
C	1.0217416	0.3190926	0.9140454
O	1.1482346	-0.6083744	-1.2494716
C	-1.3276734	2.8012776	0.2507394
O	-1.8876874	3.4924186	1.0890984
N	-0.5965154	3.2713656	-0.7778986
C	2.0503996	0.3548366	1.6450844
Au	3.5115306	-0.7026584	0.3424364
C	2.5192096	0.7770696	2.9889914
C	-0.3641004	4.7068456	-1.0512896
C	0.5036066	4.7656096	-2.3078496
C	-1.7020784	5.4081816	-1.3006496
C	0.3727066	5.3453826	0.1298144
C	-2.3752894	-3.3982664	-1.7936396
C	-3.7315744	-3.3190744	-1.4410986
C	-4.3481984	-2.0706144	-1.3343066
C	-3.5981814	-0.9164394	-1.5615366
C	-2.2469724	-0.9833794	-1.8879596
C	-1.6456524	-2.2442684	-2.0145876
C	-1.4040044	0.2611196	-1.9799726
O	-4.3511454	-4.5003324	-1.2319446
C	-5.7265954	-4.4755134	-0.9012586
H	-2.1169694	-3.8516444	1.9102574
H	-1.6025754	-3.7967494	4.3271294
H	-0.9019454	-1.6852304	5.4316474
H	-1.9166174	-1.8259884	0.5181864
H	-0.4930554	1.0498776	4.8470264
H	-0.5904194	2.5940676	2.8864214
H	-2.5281724	1.0372046	0.2197874
H	-0.1404054	2.6008126	-1.3791806
H	1.8905696	1.5893086	3.3645334
H	2.4540666	-0.0702564	3.6784454
H	3.5558446	1.1139046	2.9651634
H	1.4629586	4.2618416	-2.1473106
H	0.7090856	5.8060006	-2.5685496

H	-0.0051264	4.2984626	-3.1573556
H	-2.3400234	5.3453406	-0.4180066
H	-1.5253604	6.4617956	-1.5331616
H	-2.2196014	4.9509606	-2.1489026
H	-0.2392724	5.2983346	1.0318504
H	0.5871016	6.3940916	-0.0930556
H	1.3217996	4.8308866	0.3102114
H	-1.9285034	-4.3817874	-1.8884426
H	-5.3974804	-1.9842244	-1.0817176
H	-4.0883854	0.0512976	-1.4824916
H	-0.5911684	-2.3065274	-2.2681596
H	-0.6167404	0.1537006	-2.7292786
H	-2.0099644	1.1379596	-2.2294076
H	-6.0281774	-5.5150684	-0.7849976
H	-6.3171164	-4.0118354	-1.6991836
H	-5.8984504	-3.9381564	0.0383924
P	5.1774506	-1.8016434	-0.8187506
C	4.5328046	-2.5582864	-2.3480346
H	4.0888436	-1.7814174	-2.9737736
H	5.3343476	-3.0619774	-2.8949586
H	3.7533986	-3.2784504	-2.0909816
C	5.9637486	-3.1672634	0.0995624
H	6.7153226	-3.6586564	-0.5240936
H	6.4384246	-2.7749624	1.0010514
H	5.2027596	-3.8929534	0.3931904
C	6.5559866	-0.7340704	-1.3543356
H	7.2872836	-1.3170284	-1.9205926
H	6.1690506	0.0719456	-1.9808696
H	7.0391736	-0.2950544	-0.4792786

Zero-point correction= 0.627481 (Hartree/Particle)
Thermal correction to Energy= 0.667965
Thermal correction to Enthalpy= 0.668909
Thermal correction to Gibbs Free Energy= 0.548557
Sum of electronic and zero-point Energies= -1993.107996
Sum of electronic and thermal Energies= -1993.067512
Sum of electronic and thermal Enthalpies= -1993.066568
Sum of electronic and thermal Free Energies= -1993.186919

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C	-2.3761191	-2.9401421	2.0508846
C	-2.9243761	-2.6134531	3.2938556
C	-2.6811131	-1.3737941	3.8868066
C	-1.8765131	-0.5047821	3.1709346
C	-1.3182781	-0.8063861	1.9318986
C	-1.5662371	-2.0405821	1.3541936

N	-1.4343081	0.8033459	3.5217146
C	-0.6981851	1.3347329	2.5898496
C	-0.5530881	0.3991719	1.4238016
C	-1.2512331	0.9830439	0.1337106
N	-0.4250791	0.5754089	-0.9682714
C	0.8194929	0.1080699	-0.5672984
C	0.8804459	0.1399399	0.9241256
O	1.6583949	-0.2956871	-1.3494824
C	-1.4369841	2.5053419	0.2636326
O	-1.8967081	2.9397049	1.3233276
N	-1.1240801	3.2313029	-0.8084534
C	1.9830779	-0.1624261	1.6318686
Au	3.7810879	-0.5398721	0.6689006
C	1.9484009	-0.2553761	3.1306896
C	-1.2817261	4.7006279	-0.9250184
C	-0.8056261	5.0682759	-2.3295494
C	-2.7569511	5.0679629	-0.7503064
C	-0.4163611	5.3964269	0.1293626
C	-1.3929611	-3.6415771	-1.8629934
C	-2.7475041	-3.7593951	-1.5145604
C	-3.5573161	-2.6229901	-1.4841174
C	-2.9962051	-1.3775191	-1.7704064
C	-1.6462411	-1.2423581	-2.0817304
C	-0.8518231	-2.3979201	-2.1413494
C	-1.0109461	0.1162459	-2.2363164
O	-3.1715531	-5.0098181	-1.2187284
C	-4.5462921	-5.1895211	-0.9387674
H	-2.5744571	-3.9138711	1.6133676
H	-3.5462501	-3.3340531	3.8128586
H	-3.1004031	-1.1133401	4.8523756
H	-1.1399061	-2.3072021	0.3925006
H	-1.6494811	1.2612419	4.4006026
H	-0.1873361	2.2754519	2.7365496
H	-2.2594951	0.5586209	0.0491566
H	-0.6422911	2.7402849	-1.5518954
H	0.9424299	-0.2258611	3.5667976
H	2.4172089	-1.1884501	3.4552926
H	2.5476209	0.5498399	3.5703236
H	0.2470599	4.8021639	-2.4709614
H	-0.9035601	6.1450439	-2.4822904
H	-1.4059231	4.5619609	-3.0919084
H	-3.1127761	4.7826119	0.2410996
H	-2.8794941	6.1477369	-0.8682784
H	-3.3679241	4.5679169	-1.5069034

H	-0.7471591	5.1296929	1.1345856
H	-0.4989101	6.4802539	0.0131126
H	0.6344009	5.1170099	0.0091316
H	-0.7941411	-4.5447821	-1.9048684
H	-4.6106601	-2.6915781	-1.2425344
H	-3.6364131	-0.4980591	-1.7532694
H	0.2017959	-2.3065041	-2.3904624
H	-0.1892391	0.0915839	-2.9553834
H	-1.7438761	0.8593709	-2.5677924
H	-4.6824981	-6.2548781	-0.7607284
H	-5.1672451	-4.8782711	-1.7859324
H	-4.8463431	-4.6287401	-0.0450524
P	5.8167109	-0.9856591	-0.4414874
C	5.5591949	-1.5649391	-2.1565054
H	4.9744079	-0.8200851	-2.7003914
H	6.5142109	-1.7286661	-2.6628604
H	4.9902309	-2.4968281	-2.1381654
C	6.8737819	-2.2730551	0.3129326
H	7.7749189	-2.4329301	-0.2851404
H	7.1565849	-1.9649321	1.3215746
H	6.3127359	-3.2072581	0.3819786
C	6.9339869	0.4511499	-0.6216824
H	7.8353299	0.1723259	-1.1741244
H	6.4128109	1.2488799	-1.1548774
H	7.2132729	0.8208029	0.3670476

Zero-point correction= 0.630499 (Hartree/Particle)
Thermal correction to Energy= 0.670228
Thermal correction to Enthalpy= 0.671172
Thermal correction to Gibbs Free Energy= 0.553059
Sum of electronic and zero-point Energies= -1993.140046
Sum of electronic and thermal Energies= -1993.100317
Sum of electronic and thermal Enthalpies= -1993.099373
Sum of electronic and thermal Free Energies= -1993.217485

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C	1.7507038	0.8753786	3.5851529
C	2.1193338	-0.2668914	4.2962279
C	1.9166108	-1.5456084	3.7710429
C	1.3293468	-1.6145884	2.5201159
C	0.9424928	-0.4867894	1.8000109
C	1.1557348	0.7772806	2.3243329
N	0.9884908	-2.7630384	1.7551739
C	0.5730288	-2.4274574	0.5269459
C	0.3306038	-0.9092674	0.4790589
C	1.0660388	-0.2735934	-0.7424821

N	0.0878298	0.4594716	-1.4807001
C	-1.1760412	0.3977326	-0.9317981
C	-1.1426962	-0.5213964	0.2467059
O	-2.1177542	1.0408826	-1.3584441
C	1.6791978	-1.3962264	-1.5695591
C	-2.2422422	-0.8307424	0.9597449
Au	-4.1009322	-0.1141714	0.3702079
C	-2.1949792	-1.6876434	2.1942449
C	1.1365578	4.2963746	0.1737599
C	2.4984908	4.5722146	-0.0301671
C	3.2056528	3.8782556	-1.0115591
C	2.5464908	2.9116076	-1.7757991
C	1.1987148	2.6321976	-1.5862161
C	0.4988818	3.3412046	-0.5964881
C	0.4903778	1.5494016	-2.3661431
O	3.0282788	5.5228606	0.7722259
C	4.3794188	5.8820506	0.5635569
H	1.9257118	1.8537356	4.0182159
H	2.5753568	-0.1646964	5.2746199
H	2.2047648	-2.4345594	4.3216579
H	0.8698388	1.6663416	1.7668729
H	1.0250678	-3.7094124	2.1056159
H	1.8821278	0.3878316	-0.4056211
H	-1.1944152	-1.9545534	2.5431539
H	-2.7068062	-1.1721664	3.0121719
H	-2.7666392	-2.6068174	2.0227769
H	0.6073948	4.8647456	0.9311159
H	4.2544898	4.0783496	-1.1922541
H	3.1019728	2.3763096	-2.5424171
H	-0.5607502	3.1417476	-0.4490361
H	-0.4362582	1.9158816	-2.8141361
H	1.1258898	1.1486516	-3.1604541
H	4.5971788	6.6725106	1.2799029
H	4.5366978	6.2579306	-0.4536581
H	5.0492658	5.0330686	0.7437769
P	-6.1907582	0.7260556	-0.3330631
C	-6.0036642	2.2149936	-1.3775751
H	-5.3547282	1.9759506	-2.2228481
H	-6.9735332	2.5661596	-1.7400321
H	-5.5230782	3.0033306	-0.7943961
C	-7.3528642	1.2424996	0.9814739
H	-8.2710762	1.6484506	0.5485459
H	-7.5957192	0.3827876	1.6093069
H	-6.8782652	2.0024936	1.6054789

C	-7.1778412	-0.4164514	-1.3660891
H	-8.1063682	0.0607176	-1.6909971
H	-6.5926442	-0.7068064	-2.2410611
H	-7.4121582	-1.3154444	-0.7923891
N	2.1072798	-2.4568974	-0.6892821
H	2.7715518	-2.0782334	-0.0060461
C	2.6355868	-3.7477574	-1.2534451
C	2.8751338	-4.6807304	-0.0642681
C	1.6063278	-4.3685974	-2.1986281
C	3.9554768	-3.4670844	-1.9768531
H	3.4964678	-4.2102084	0.7059979
H	1.9323788	-5.0084444	0.3847709
H	3.3971008	-5.5749914	-0.4114241
H	1.4638998	-3.7705154	-3.0974671
H	1.9654858	-5.3574604	-2.4939341
H	0.6394248	-4.5089054	-1.7050991
H	4.3602758	-4.4058464	-2.3634051
H	3.8076828	-2.7851454	-2.8150941
H	4.6957858	-3.0421634	-1.2908611
O	1.7228818	-1.4534444	-2.7635991
H	-0.0385592	-3.1227094	-0.0391731

Zero-point correction= 0.629657 (Hartree/Particle)
Thermal correction to Energy= 0.668660
Thermal correction to Enthalpy= 0.669604
Thermal correction to Gibbs Free Energy= 0.553027
Sum of electronic and zero-point Energies= -1993.113453
Sum of electronic and thermal Energies= -1993.074451
Sum of electronic and thermal Enthalpies= -1993.073506
Sum of electronic and thermal Free Energies= -1993.190084

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C	-1.8750042	-0.1043727	4.1538568
C	-2.2600372	1.1460673	4.6378098
C	-2.0900212	2.3028803	3.8754308
C	-1.5132252	2.1635183	2.6223508
C	-1.1156382	0.9232443	2.1347628
C	-1.2983122	-0.2253057	2.8888368
N	-1.2496782	3.1984423	1.6776228
C	-0.5619492	2.6242203	0.5517288
C	-0.5350562	1.0678713	0.7475338
C	-1.4635862	0.4602023	-0.3286342
N	-0.6102002	-0.2569587	-1.2435942
C	0.6768558	-0.4317687	-0.7397542
C	0.8205138	0.4300843	0.4640378
O	1.4904898	-1.1698747	-1.2613202

C	-2.1166532	1.6123843	-1.0566802
C	1.9808708	0.6004323	1.1274658
Au	3.6863298	-0.4195887	0.5423118
C	2.0658158	1.5098353	2.3243968
C	-2.1612292	-4.1082307	0.0461618
C	-3.5595752	-4.1220587	-0.0795862
C	-4.1909142	-3.1916317	-0.9053912
C	-3.4183292	-2.2569867	-1.5981232
C	-2.0327592	-2.2424777	-1.4896842
C	-1.4109832	-3.1803997	-0.6511422
C	-1.1967022	-1.2030697	-2.1939442
O	-4.2004332	-5.0702897	0.6389288
C	-5.6064182	-5.1520177	0.5165998
H	-2.0212602	-0.9867497	4.7662758
H	-2.7039262	1.2245753	5.6242788
H	-2.3983032	3.2729203	4.2504278
H	-0.9871022	-1.1923327	2.5027528
H	-0.8175912	4.0300843	2.0645658
H	-2.2549122	-0.1816627	0.0815298
H	1.1648708	2.0991213	2.5315928
H	2.2712518	0.9081583	3.2169448
H	2.9170618	2.1895013	2.2200928
H	-1.6987162	-4.8492847	0.6887128
H	-5.2678872	-3.1827777	-1.0176392
H	-3.9142082	-1.5293847	-2.2365302
H	-0.3266442	-3.1799507	-0.5635992
H	-0.3467752	-1.6509387	-2.7146482
H	-1.7992582	-0.6516477	-2.9242782
H	-5.9178162	-5.9813727	1.1494718
H	-5.9028312	-5.3521747	-0.5192322
H	-6.0895382	-4.2301847	0.8606648
P	5.5959368	-1.6331867	-0.1434542
C	5.1564188	-3.0262637	-1.2431232
H	4.6009368	-2.6414797	-2.1010312
H	6.0503958	-3.5543607	-1.5853892
H	4.5071938	-3.7180487	-0.7022992
C	6.5826938	-2.4069397	1.1877448
H	7.4162438	-2.9774337	0.7693348
H	6.9697538	-1.6306027	1.8509128
H	5.9437918	-3.0725517	1.7717268
C	6.8287298	-0.6827437	-1.1049102
H	7.6551618	-1.3270417	-1.4167732
H	6.3475328	-0.2566447	-1.9876332
H	7.2161098	0.1343823	-0.4929022

N	-1.3775202	2.9142043	-0.7101972
H	-2.1157202	3.5675893	-0.4163422
C	-0.6223452	3.5903993	-1.8857602
C	-0.0736132	4.9130783	-1.3470402
C	0.4843518	2.6572633	-2.3606602
C	-1.6275712	3.8729333	-3.0018252
H	-0.8701862	5.5347293	-0.9248902
H	0.7116548	4.7819023	-0.5999342
H	0.3656188	5.4641683	-2.1812832
H	0.0772748	1.7323173	-2.7783762
H	1.0438438	3.1673353	-3.1482972
H	1.1889488	2.3945903	-1.5647062
H	-1.1171582	4.4622423	-3.7668782
H	-2.0016052	2.9626713	-3.4691432
H	-2.4800732	4.4569513	-2.6418702
O	-3.0552252	1.6372513	-1.7798272
H	0.4378428	3.0232363	0.3914638

Zero-point correction= 0.631671 (Hartree/Particle)
Thermal correction to Energy= 0.670802
Thermal correction to Enthalpy= 0.671746
Thermal correction to Gibbs Free Energy= 0.554429
Sum of electronic and zero-point Energies= -1993.125463
Sum of electronic and thermal Energies= -1993.086332
Sum of electronic and thermal Enthalpies= -1993.085388
Sum of electronic and thermal Free Energies= -1993.202705

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C	1.4818865	-0.2615403	4.3037865
C	2.0177515	-1.5089283	4.6304995
C	2.0446215	-2.5447143	3.6971625
C	1.5122825	-2.2775543	2.4469885
C	0.9737565	-1.0455023	2.1019875
C	0.9567965	-0.0179353	3.0351645
N	1.4440765	-3.1984103	1.3290865
C	0.7295905	-2.4922013	0.2128825
C	0.4813685	-1.0301333	0.6745465
C	1.3784175	-0.1739453	-0.2462815
N	0.4751035	0.4104827	-1.2126885
C	-0.8424845	0.4021777	-0.7659685
C	-0.9293345	-0.5284033	0.3941095
O	-1.7260335	1.0518677	-1.2918685
C	2.3037285	-1.1278073	-0.9818105
C	-2.0809915	-0.8650593	1.0051365
Au	-3.8624625	0.0243617	0.4299935
C	-2.1028995	-1.8706213	2.1258595

C	1.3146075	4.4707827	0.1721635
C	2.7035735	4.6721347	0.1725635
C	3.5262235	3.8341007	-0.5805605
C	2.9520255	2.8041527	-1.3288105
C	1.5762485	2.6043857	-1.3460785
C	0.7614075	3.4500467	-0.5782685
C	0.9590595	1.4606117	-2.1122265
O	3.1446395	5.6991557	0.9342485
C	4.5310575	5.9725407	0.9309785
H	1.4701435	0.5260587	5.0488525
H	2.4188935	-1.6785343	5.6233535
H	2.4626045	-3.5149223	3.9437225
H	0.5288035	0.9466507	2.7780885
H	1.0882425	-4.1255123	1.5644885
H	1.9676095	0.5879687	0.2805775
H	-1.1800225	-2.4522513	2.2461085
H	-2.2867605	-1.3536443	3.0751255
H	-2.9355765	-2.5662663	1.9934095
H	0.7007085	5.1432917	0.7611285
H	4.6004725	3.9700947	-0.5952755
H	3.5950875	2.1461137	-1.9083255
H	-0.3160855	3.3023097	-0.5878155
H	0.0817265	1.7811917	-2.6785935
H	1.6845745	1.0262367	-2.8069335
H	4.6710085	6.8384077	1.5761465
H	4.8863545	6.2086407	-0.0784805
H	5.1046465	5.1267747	1.3279085
P	-5.8560735	1.0859147	-0.2636025
C	-5.5162895	2.6319137	-1.1786045
H	-4.8563215	2.4090387	-2.0197795
H	-6.4423515	3.0854997	-1.5418285
H	-5.0003075	3.3326947	-0.5188655
C	-7.0196615	1.5898597	1.0543425
H	-7.8876085	2.1007027	0.6288675
H	-7.3509035	0.7062107	1.6036165
H	-6.5100055	2.2584727	1.7510725
C	-6.8920735	0.1108917	-1.4137005
H	-7.7684535	0.6852637	-1.7258375
H	-6.3008215	-0.1562943	-2.2919775
H	-7.2162315	-0.8083123	-0.9215045
N	1.8730065	-2.5136553	-0.7452695
H	2.3481615	-3.0769283	0.3425945
C	1.7956775	-3.4522303	-1.9454405
C	1.3392815	-4.8250883	-1.4425475

C	0.7990305	-2.8616853	-2.9402245
C	3.1902015	-3.5986303	-2.5584035
H	2.0354745	-5.2289693	-0.6994085
H	0.3264625	-4.8231703	-1.0306505
H	1.3332995	-5.5152703	-2.2886305
H	1.1393885	-1.8879563	-3.3038115
H	0.7033735	-3.5297743	-3.7994805
H	-0.1942585	-2.7381293	-2.4956145
H	3.1448155	-4.3816683	-3.3192235
H	3.5367905	-2.6795413	-3.0251275
H	3.9183255	-3.9029623	-1.8008835
O	3.2238015	-0.8387863	-1.6853155
H	-0.1621745	-3.0040613	-0.1408435

Zero-point correction= 0.626779 (Hartree/Particle)
Thermal correction to Energy= 0.665618
Thermal correction to Enthalpy= 0.666563
Thermal correction to Gibbs Free Energy= 0.549905
Sum of electronic and zero-point Energies= -1993.097582
Sum of electronic and thermal Energies= -1993.058742
Sum of electronic and thermal Enthalpies= -1993.057798
Sum of electronic and thermal Free Energies= -1993.174455

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C	-1.8607161	-0.8135999	3.6866109
C	-2.3851681	0.3161891	4.3221799
C	-2.2689521	1.5774991	3.7422649
C	-1.6127281	1.6358771	2.5243439
C	-1.0751281	0.5403971	1.8771029
C	-1.2018131	-0.7146989	2.4635439
N	-1.3793411	2.8629511	1.7373219
C	-0.5615111	2.4341961	0.4561759
C	-0.4443541	0.8900631	0.5577349
C	-1.2587321	0.3697641	-0.6475091
N	-0.3605081	-0.4657359	-1.4005611
C	0.8982449	-0.5637659	-0.8550421
C	0.9642989	0.3532711	0.3238789
O	1.7683059	-1.3018019	-1.2852301
C	-1.6379021	1.6161861	-1.4450671
C	2.0821779	0.5932651	1.0321769
Au	3.8616399	-0.3112749	0.4706799
C	2.0755389	1.5007171	2.2340339
C	-1.8544471	-4.2455779	0.0129839
C	-3.2372141	-4.3494949	-0.2065811
C	-3.8546471	-3.5173139	-1.1393881
C	-3.0851431	-2.5862979	-1.8425231

C	-1.7151301	-2.4793659	-1.6390441
C	-1.1072621	-3.3235819	-0.6965331
C	-0.8816981	-1.4408939	-2.3529051
O	-3.8781611	-5.2830089	0.5349869
C	-5.2590521	-5.4714639	0.3017819
H	-1.9692771	-1.7847089	4.1567939
H	-2.8893481	0.2135461	5.2761809
H	-2.6734071	2.4607241	4.2260209
H	-0.7989221	-1.5921459	1.9657329
H	-0.8748581	3.5758601	2.2744349
H	-2.1649231	-0.1829839	-0.3647671
H	1.0936649	1.9097961	2.5121339
H	2.4525519	0.9577881	3.1062839
H	2.7704289	2.3331441	2.0781829
H	-1.3990221	-4.9183529	0.7317389
H	-4.9190671	-3.5813249	-1.3283251
H	-3.5706521	-1.9371259	-2.5671781
H	-0.0321121	-3.2569669	-0.5408381
H	-0.0043171	-1.8863329	-2.8280631
H	-1.4665491	-0.9151589	-3.1122341
H	-5.5715861	-6.2777019	0.9635669
H	-5.4498591	-5.7587059	-0.7383961
H	-5.8303191	-4.5657189	0.5370879
P	5.8188439	-1.4054439	-0.2663691
C	5.3981959	-2.8754709	-1.2684941
H	4.7344319	-2.5709849	-2.0806161
H	6.2969429	-3.3463459	-1.6756131
H	4.8599779	-3.5916109	-0.6439131
C	6.9629499	-2.0407449	1.0111599
H	7.8026009	-2.5674169	0.5496949
H	7.3401459	-1.2079709	1.6082009
H	6.4247629	-2.7236469	1.6715989
C	6.8943679	-0.4136009	-1.3644751
H	7.7407369	-1.0091429	-1.7171731
H	6.3114759	-0.0675629	-2.2205371
H	7.2644419	0.4586851	-0.8218821
N	-1.2841671	2.7562691	-0.7157231
C	-1.2432441	4.1133111	-1.3572511
C	-0.8675521	5.1696251	-0.3121851
C	-0.1956071	4.0921291	-2.4732671
C	-2.6345981	4.4514911	-1.9029281
H	-1.6172821	5.2501591	0.4846199
H	0.1225799	5.0116001	0.1258539
H	-0.8401061	6.1427381	-0.8065461

H	-0.4593591	3.3509211	-3.2296131
H	-0.1431521	5.0728661	-2.9528221
H	0.7945239	3.8533241	-2.0711931
H	-2.6198981	5.4666111	-2.3078311
H	-2.9322541	3.7627031	-2.6911431
H	-3.3807261	4.4162751	-1.1021581
O	-2.1230871	1.6142631	-2.5484431
H	0.3998369	2.9398421	0.5495139
H	-2.2588061	3.2809961	1.4137599

Zero-point correction= 0.632578 (Hartree/Particle)
Thermal correction to Energy= 0.670795
Thermal correction to Enthalpy= 0.671739
Thermal correction to Gibbs Free Energy= 0.557095
Sum of electronic and zero-point Energies= -1993.136326
Sum of electronic and thermal Energies= -1993.098109
Sum of electronic and thermal Enthalpies= -1993.097164
Sum of electronic and thermal Free Energies= -1993.211809

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C	-1.3197333	2.9249807	3.8300558
C	-0.5281383	4.0357857	3.5490998
C	0.2529817	4.0971447	2.3886388
C	0.1976327	3.0067517	1.5457768
C	-0.5806383	1.8798807	1.8176188
C	-1.3542893	1.8270157	2.9613478
N	0.9214307	2.7510357	0.3329288
C	0.0762347	1.8640327	-0.4619772
C	-0.3294253	0.8776567	0.7250598
C	-1.4430583	0.1080807	0.0694308
N	-0.7016233	-0.8907223	-0.6912052
C	0.6202287	-1.0033483	-0.3596592
C	0.9041887	0.0318457	0.7376158
O	1.4124527	-1.8023903	-0.8181972
C	-2.0757283	1.1514687	-0.8702162
C	2.1369137	0.2868107	1.2969048
C	-2.7875163	-4.5482843	0.7060498
C	-4.1499963	-4.2154353	0.7443538
C	-4.6166943	-3.1136323	0.0252588
C	-3.7190963	-2.3582253	-0.7305782
C	-2.3681983	-2.6878883	-0.7818872
C	-1.9110893	-3.7904913	-0.0479912
C	-1.3960103	-1.8420973	-1.5634222
O	-4.9259063	-5.0194953	1.5047148
C	-6.3131003	-4.7510403	1.5451068
H	-1.9169333	2.9095787	4.7346578

H	-0.5184493	4.8735267	4.2374658
H	0.8685447	4.9631087	2.1694048
H	-1.9630943	0.9581087	3.1892268
H	1.7810207	1.4726017	0.6239678
H	-2.1943003	-0.3461543	0.7230868
H	-2.4556493	-5.4125103	1.2705018
H	-5.6640533	-2.8389583	0.0401798
H	-4.0791423	-1.4928903	-1.2821482
H	-0.8569683	-4.0562443	-0.0814372
H	-0.6128793	-2.4453363	-2.0279452
H	-1.9162163	-1.2762583	-2.3429252
H	-6.7507063	-5.5148583	2.1858018
H	-6.7583123	-4.8139103	0.5457638
H	-6.5143413	-3.7607343	1.9698828
N	-1.2133093	2.2398887	-0.9873502
C	-1.3694183	3.2003207	-2.1252692
C	-0.2548783	4.2458407	-2.0506542
C	-1.2812733	2.4423287	-3.4538122
C	-2.7163373	3.9137277	-1.9754962
H	-0.2734593	4.7762437	-1.0925002
H	0.7358307	3.8080167	-2.2224232
H	-0.4149453	4.9828377	-2.8403022
H	-2.0981193	1.7249177	-3.5462862
H	-1.3466683	3.1474107	-4.2864832
H	-0.3269243	1.9103657	-3.5389982
H	-2.8132643	4.6603937	-2.7681642
H	-3.5469703	3.2137787	-2.0514122
H	-2.7667173	4.4243107	-1.0099132
O	-3.1268973	1.0005407	-1.4473282
H	0.7127387	1.4145817	-1.2351782
H	1.3761207	3.5287797	-0.1334692
Au	3.8008837	-0.7222163	0.5104408
P	5.6337587	-1.9084273	-0.3672372
C	5.0862207	-3.3828453	-1.2967002
H	5.9405377	-3.9115683	-1.7276162
H	4.5438057	-4.0501383	-0.6236442
H	4.4029627	-3.0728603	-2.0901432
C	6.6738387	-0.9837153	-1.5522972
H	7.1111847	-0.1157223	-1.0548412
H	7.4730277	-1.6219253	-1.9386032
H	6.0556737	-0.6350373	-2.3820512
C	6.8208367	-2.5548483	0.8622468
H	7.6101307	-3.1275473	0.3680718
H	7.2654147	-1.7232513	1.4126878

H	6.2952107	-3.1982223	1.5707678
C	2.3245807	0.9739217	2.6516348
H	3.0261387	1.8087087	2.5710118
H	1.4101077	1.3160167	3.1372158
H	2.7998347	0.2368867	3.3037858

Zero-point correction= 0.626499 (Hartree/Particle)
Thermal correction to Energy= 0.664805
Thermal correction to Enthalpy= 0.665749
Thermal correction to Gibbs Free Energy= 0.551513
Sum of electronic and zero-point Energies= -1993.077090
Sum of electronic and thermal Energies= -1993.038784
Sum of electronic and thermal Enthalpies= -1993.037839
Sum of electronic and thermal Free Energies= -1993.152076

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C	1.2299239	-0.0932058	4.1649497
C	2.2064409	-1.0464068	4.4553777
C	2.6658499	-1.9384998	3.4868947
C	2.1146889	-1.8577558	2.2119827
C	1.1282819	-0.9147568	1.9202457
C	0.6835619	-0.0231648	2.8827097
N	2.4345449	-2.6271128	1.0849557
C	1.4886479	-2.3423628	0.0061737
C	0.7215459	-1.0541708	0.4745707
C	1.2617029	0.0587012	-0.4439053
N	0.0886899	0.6312402	-1.0972143
C	-1.0527531	0.0436472	-0.7578433
C	-0.7673611	-1.0550558	0.1976227
O	-2.1639471	0.4063572	-1.2249773
C	2.1537449	-0.6355128	-1.4734833
C	-1.6970331	-1.8839888	0.6775807
Au	-4.1766311	0.2871952	-0.5390843
C	-1.4633031	-3.0036048	1.6399957
C	0.6365709	4.8559892	0.1573677
C	2.0079059	5.1144292	0.0142107
C	2.7903429	4.2874512	-0.7944453
C	2.1960519	3.2128022	-1.4558243
C	0.8345489	2.9548042	-1.3253073
C	0.0625189	3.7870392	-0.5054333
C	0.2086269	1.7715162	-2.0162973
O	2.4743199	6.1827752	0.6973947
C	3.8460169	6.5008292	0.5676777
H	0.8961929	0.5917592	4.9358467
H	2.6235329	-1.0952268	5.4557637
H	3.4331789	-2.6692748	3.7190997

H	-0.0817651	0.7109362	2.6433957
H	1.8178139	0.8448712	0.0745327
H	-0.4258841	-3.0577278	1.9729957
H	-2.0943261	-2.8750318	2.5251027
H	-1.7454351	-3.9592058	1.1855637
H	0.0539759	5.5191812	0.7869507
H	3.8507449	4.4681902	-0.9183863
H	2.8029199	2.5559082	-2.0743193
H	-1.0034741	3.5965562	-0.3992293
H	-0.8028571	1.9882612	-2.3637733
H	0.8206179	1.4476912	-2.8617293
H	4.0098679	7.3874362	1.1779947
H	4.1046749	6.7219932	-0.4739233
H	4.4791789	5.6845632	0.9336827
P	-6.3530021	0.2977242	0.0799167
C	-6.8933601	1.9040322	0.7467627
H	-6.7506031	2.6794992	-0.0083903
H	-7.9493521	1.8566912	1.0258407
H	-6.2950501	2.1551112	1.6247637
C	-6.7397121	-0.9243708	1.3742767
H	-7.8002261	-0.8710128	1.6343627
H	-6.5048611	-1.9271888	1.0120117
H	-6.1371261	-0.7192528	2.2612937
C	-7.4858771	-0.0700878	-1.2978053
H	-8.5208411	-0.0475388	-0.9462753
H	-7.3531691	0.6719182	-2.0876273
H	-7.2600441	-1.0580038	-1.7039433
N	2.1158519	-1.9775168	-1.2543793
C	2.9235969	-2.9315308	-2.0671293
C	2.5661579	-4.3674478	-1.6759393
C	2.5864759	-2.7440888	-3.5514633
C	4.4090939	-2.6664418	-1.8026433
H	2.8219869	-4.5984358	-0.6380613
H	1.5057429	-4.5801608	-1.8416723
H	3.1435269	-5.0476548	-2.3057293
H	2.8603209	-1.7489488	-3.8980883
H	3.1379399	-3.4845068	-4.1370273
H	1.5168599	-2.9004268	-3.7211153
H	5.0204959	-3.3661738	-2.3792743
H	4.6703819	-1.6492818	-2.1014573
H	4.6328549	-2.7931708	-0.7398943
O	2.7432899	-0.0371088	-2.3561043
H	0.8087119	-3.1844518	-0.1559793
H	-2.7239851	-1.7495378	0.3333167

H	2.6514669	-3.6006938	1.2519877

Zero-point correction= 0.632152 (Hartree/Particle)
Thermal correction to Energy= 0.670423
Thermal correction to Enthalpy= 0.671367
Thermal correction to Gibbs Free Energy= 0.557118
Sum of electronic and zero-point Energies= -1993.188929
Sum of electronic and thermal Energies= -1993.150658
Sum of electronic and thermal Enthalpies= -1993.149714
Sum of electronic and thermal Free Energies= -1993.263964

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C	0.6130115	-0.2800769	4.5377629
C	0.2799635	0.9536601	5.0960799
C	0.1217035	2.0912401	4.2996409
C	0.3308905	1.9321041	2.9428859
C	0.6638205	0.7012601	2.3626209
C	0.7849705	-0.4245719	3.1584989
N	0.3380805	2.9515591	1.9298159
C	0.7206825	2.3989561	0.7695369
C	0.5458925	0.8946501	0.8670829
N	0.0232325	2.2938031	-1.1278851
C	1.1120675	1.3666721	-1.4418141
C	1.4059125	0.3667961	-0.2819521
O	1.7590615	1.4307491	-2.4481631
N	0.8836085	-0.9361769	-0.5913731
C	-0.4438195	-1.0416689	-0.2487491
C	-0.8300725	0.2096061	0.4996949
O	-1.1480775	-1.9878209	-0.5459321
C	-2.1132965	0.5294551	0.7561699
C	-2.5188035	1.7929661	1.4749449
Au	-3.6268155	-0.7885829	0.1881999
C	5.3318485	-1.5213419	-1.4486251
C	5.6639995	-2.4140669	-0.4223181
C	4.6535215	-3.1221469	0.2360189
C	3.3270115	-2.9311019	-0.1425571
C	2.9854235	-2.0530289	-1.1682611
C	4.0069635	-1.3464489	-1.8136891
C	1.5430885	-1.8294549	-1.5411671
O	6.9816175	-2.5217719	-0.1411491
C	7.3712295	-3.4415459	0.8588329
C	-0.2284435	3.4937051	-1.9860251
C	-1.3764335	4.2413511	-1.3063691
C	-0.6475805	3.0481711	-3.3912371
C	1.0203985	4.3737911	-2.0321011
H	0.7340335	-1.1421059	5.1839239

H	0.1409845	1.0368561	6.1681129
H	-0.1388795	3.0515941	4.7311059
H	1.0175965	-1.3894399	2.7193869
H	0.5869185	3.9039561	2.1641589
H	1.5897625	2.8511721	0.2982199
H	-0.8428835	1.7686301	-0.9534371
H	2.4870265	0.3373851	-0.1120371
H	-3.5785895	2.0060101	1.3380719
H	-1.9548975	2.6778621	1.1623399
H	-2.3505255	1.6660031	2.5526239
H	6.1348975	-0.9883619	-1.9452211
H	4.8884585	-3.8229489	1.0275339
H	2.5441395	-3.4884199	0.3664409
H	3.7548235	-0.6522449	-2.6119371
H	1.4737695	-1.4096069	-2.5533251
H	0.9624465	-2.7546679	-1.5206001
H	8.4572695	-3.3872929	0.9131909
H	7.0700515	-4.4624069	0.5979789
H	6.9447245	-3.1749129	1.8328509
H	-1.1018595	4.5473891	-0.2912201
H	-2.2769125	3.6201291	-1.2494101
H	-1.6213815	5.1391381	-1.8782731
H	0.1648045	2.5326271	-3.9033751
H	-1.5182255	2.3864111	-3.3430841
H	-0.9274755	3.9285461	-3.9759201
H	1.8695545	3.8556841	-2.4800911
H	1.2946685	4.7288911	-1.0328511
H	0.8050305	5.2560221	-2.6394681
P	-5.3156325	-2.3082319	-0.4339081
C	-4.6789415	-3.5946509	-1.5658411
H	-5.4546455	-4.3272979	-1.8040541
H	-4.3272975	-3.1215359	-2.4850901
H	-3.8288155	-4.0928179	-1.0949141
C	-6.0426635	-3.2539609	0.9521739
H	-6.5240995	-2.5657309	1.6499199
H	-6.7789635	-3.9732989	0.5837099
H	-5.2489865	-3.7849879	1.4817189
C	-6.7679015	-1.6183759	-1.3050351
H	-6.4378785	-1.1037409	-2.2097041
H	-7.4689565	-2.4129029	-1.5743861
H	-7.2692035	-0.8950559	-0.6586971

Zero-point correction= 0.624815 (Hartree/Particle)
Thermal correction to Energy= 0.664091
Thermal correction to Enthalpy= 0.665036

Thermal correction to Gibbs Free Energy= 0.549443
Sum of electronic and zero-point Energies= -1657.683536
Sum of electronic and thermal Energies= -1657.644259
Sum of electronic and thermal Enthalpies= -1657.643314
Sum of electronic and thermal Free Energies= -1657.758907

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C	0.6797539	1.0621488	4.5104060
C	0.5171859	2.4454498	4.5982940
C	0.3560379	3.2326828	3.4574070
C	0.3732909	2.5919438	2.2278660
C	0.5476819	1.2047028	2.1287530
C	0.6811999	0.4272098	3.2683720
N	0.1977289	3.2009638	0.9384090
C	0.7397739	2.2062998	0.0606550
C	0.3624339	0.8435398	0.6803620
N	0.3322449	2.0213738	-1.3609100
C	1.0758259	0.6111448	-1.5759720
C	1.2418289	-0.0682612	-0.1811150
O	1.3249359	0.2243408	-2.6601500
N	0.6022379	-1.3433802	-0.2229270
C	-0.7683281	-1.1908602	-0.0685100
C	-1.0333861	0.2161108	0.3957330
O	-1.5534731	-2.0912702	-0.2893010
C	-2.2992551	0.6438628	0.6261530
C	-2.6230481	1.9918088	1.2183880
Au	-3.9128461	-0.6165322	0.2444220
C	4.9595379	-2.3720542	-1.2808550
C	5.3800759	-2.7845612	-0.0107540
C	4.4295769	-3.1128122	0.9617400
C	3.0750289	-3.0284672	0.6502490
C	2.6447869	-2.6264422	-0.6128780
C	3.6071659	-2.2933152	-1.5722720
C	1.1759959	-2.4963492	-0.9173690
O	6.7168379	-2.8320362	0.1791720
C	7.1917349	-3.2872032	1.4307930
C	0.5825819	3.0988208	-2.4188080
C	0.0071189	4.4102718	-1.8815090
C	-0.1798611	2.6724648	-3.6742360
C	2.0800319	3.2358008	-2.6796130
H	0.8001099	0.4773678	5.4151960
H	0.5120599	2.9218968	5.5726640
H	0.2182539	4.3062718	3.5331170
H	0.7879139	-0.6503032	3.1892530
H	0.6395889	4.1110718	0.8705710

H	1.8411099	2.2629358	0.0256390
H	-0.6780871	1.7942158	-1.3486670
H	2.3019689	-0.1257152	0.0862580
H	-3.6855241	2.2189138	1.1415000
H	-2.0521911	2.8152388	0.7818520
H	-2.3687191	1.9721908	2.2875010
H	5.7165719	-2.1292812	-2.0181340
H	4.7318709	-3.4406272	1.9486240
H	2.3385659	-3.2891772	1.4065550
H	3.2884799	-1.9774572	-2.5625820
H	1.0156019	-2.4019602	-1.9995420
H	0.6032949	-3.3619782	-0.5761700
H	8.2783749	-3.2700132	1.3662120
H	6.8548209	-4.3097832	1.6344780
H	6.8652889	-2.6282222	2.2436590
H	0.6475619	4.8501438	-1.1134650
H	-1.0000251	4.2811208	-1.4745760
H	-0.0466331	5.1251078	-2.7056080
H	0.1789149	1.7231978	-4.0708020
H	-1.2539481	2.5982978	-3.4728080
H	-0.0410321	3.4385598	-4.4402640
H	2.5048039	2.3432698	-3.1408650
H	2.6333609	3.4727808	-1.7657960
H	2.2268949	4.0702488	-3.3693590
P	-5.7405611	-2.0553622	-0.1439940
C	-5.1964121	-3.7663442	-0.4882810
H	-6.0515801	-4.4211032	-0.6761190
H	-4.5348891	-3.7626742	-1.3571230
H	-4.6281971	-4.1387642	0.3666700
C	-6.9180961	-2.2303222	1.2441870
H	-7.3663631	-1.2593672	1.4645620
H	-7.7051461	-2.9472702	0.9954070
H	-6.3818261	-2.5723162	2.1317210
C	-6.8045561	-1.6303362	-1.5699870
H	-6.1972621	-1.5956752	-2.4767660
H	-7.5991781	-2.3711782	-1.6929570
H	-7.2476231	-0.6449922	-1.4117580

Zero-point correction= 0.631171 (Hartree/Particle)
Thermal correction to Energy= 0.669483
Thermal correction to Enthalpy= 0.670427
Thermal correction to Gibbs Free Energy= 0.557077
Sum of electronic and zero-point Energies= -1993.087253
Sum of electronic and thermal Energies= -1993.048942
Sum of electronic and thermal Enthalpies= -1993.047997

Sum of electronic and thermal Free Energies= -1993.161347

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C	-4.4864581	-3.0449870	-2.5318384
C	-5.2914851	-3.3749840	-1.4424924
C	-5.2702371	-2.6165240	-0.2685374
C	-4.4326291	-1.5176450	-0.2535954
C	-3.6168581	-1.1685900	-1.3391714
C	-3.6196071	-1.9500070	-2.4818844
C	-0.4894311	2.9188630	2.3632616
C	-3.5018161	0.4503140	0.3327816
C	-2.6825641	-0.0955920	-0.8244704
C	6.0886589	1.4151120	-0.5897074
C	-1.8499811	2.1099890	-0.2741994
C	-2.1101721	1.1719890	-1.4871474
C	-1.8109891	2.1444570	2.2916606
C	-0.4225261	-0.4315450	-1.6331464
C	-1.3433041	-0.8667240	-0.5272174
C	-0.9366811	-1.7024010	0.4493926
C	-1.8364171	-2.1961770	1.5563076
C	-1.8530631	1.0754070	3.3835456
C	-3.0147961	3.0768320	2.4220106
C	3.6910379	1.2527090	-2.0326594
C	3.7839639	1.9186350	-0.8094144
C	2.6619009	2.5751530	-0.2897064
C	1.4592219	2.5393590	-0.9772334
C	1.3364249	1.8352400	-2.1817444
C	2.4650769	1.2063590	-2.6947814
C	-0.0041931	1.6777130	-2.8683754
H	4.5528439	0.7651930	-2.4726694
H	-3.9541331	2.5132640	2.4200436
H	-2.9523411	3.5958080	3.3814686
H	-3.0387021	3.8290000	1.6323716
H	-0.4704071	3.7417770	1.6477456
H	0.3593739	2.2543990	2.1684616
H	-4.5271981	-3.6523470	-3.4288134
H	-5.9473141	-4.2362560	-1.5020434
H	-5.8924711	-2.8737340	0.5818036
H	-2.9691421	-1.7141430	-3.3179064
H	-5.0902911	-0.3212420	1.3835406
H	-3.9509521	1.4415120	0.2975556
H	-2.7860041	1.6969160	-2.1699014
H	-2.3486741	-1.3878170	2.0885376
H	-1.2806151	-2.7767860	2.2913006
H	-2.6159551	-2.8459530	1.1393296

H	-0.3729141	3.3312520	3.3689516
H	2.7700619	3.1232290	0.6402946
H	0.6114929	3.0901420	-0.5802384
H	2.3860009	0.6442740	-3.6204444
H	-0.5281571	2.6358370	-2.9404664
H	0.1382589	1.2932740	-3.8825444
H	6.8715749	1.5881820	0.1471986
H	5.9759409	0.3352880	-0.7546514
H	6.3621419	1.8960130	-1.5352114
H	-2.7840381	0.5009900	3.3364986
H	-1.7980621	1.5524590	4.3645276
H	-1.0098571	0.3813280	3.2953976
N	-1.8766501	1.3951160	0.9954556
N	-0.8920171	0.7609020	-2.1388744
N	-4.3020131	-0.5307820	0.7846726
O	-1.7806201	3.3039130	-0.3533184
O	0.5824869	-0.9821640	-2.0346704
O	4.9087209	1.9772410	-0.0518144
H	-1.2029351	0.6167420	0.9758876
Au	1.0982219	-2.1686620	0.5031266
P	3.4300869	-2.4806510	0.5127136
C	4.3707509	-1.1788280	1.3883126
H	4.0872529	-1.1708680	2.4429456
H	5.4460589	-1.3643450	1.3067826
H	4.1359799	-0.2006680	0.9589406
C	4.0815529	-4.0417760	1.2064466
H	3.6356859	-4.8870950	0.6783066
H	5.1695389	-4.0841080	1.1070806
H	3.8105069	-4.1117260	2.2618956
C	4.0825909	-2.4247800	-1.1931664
H	5.1750749	-2.4824350	-1.2003824
H	3.6682769	-3.2571920	-1.7661884
H	3.7479099	-1.4926480	-1.6559284

Zero-point correction= 0.629617 (Hartree/Particle)
Thermal correction to Energy= 0.667926
Thermal correction to Enthalpy= 0.668870
Thermal correction to Gibbs Free Energy= 0.558263
Sum of electronic and zero-point Energies= -1993.054213
Sum of electronic and thermal Energies= -1993.015904
Sum of electronic and thermal Enthalpies= -1993.014960
Sum of electronic and thermal Free Energies= -1993.125566

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C	4.1812937	-2.4301417	3.4082510
C	5.1795547	-2.8692487	2.5384750

C	5.2505277	-2.4114057	1.2218740
C	4.2962947	-1.4949357	0.8094300
C	3.2960647	-1.0396517	1.6791760
C	3.2176667	-1.5176507	2.9778250
C	1.7993117	1.8562813	-3.3924200
C	3.3654647	0.2484723	-0.2363640
C	2.3765787	-0.1762877	0.8604230
C	-6.5321383	1.5741573	0.6392580
C	1.6575877	1.8168813	-0.1955110
C	1.7909367	1.1919933	1.2364680
C	3.0016937	1.5771743	-2.4895820
C	0.0532777	-0.3084527	1.4659690
C	1.0444287	-0.8886197	0.4899530
C	0.6289087	-1.7277887	-0.4840680
C	1.5234187	-2.3472527	-1.5270740
C	3.9425607	0.5808093	-3.1689520
C	3.7475407	2.8549753	-2.1164790
C	-4.0619753	1.4883963	1.9587000
C	-4.2318823	2.1299243	0.7302390
C	-3.1430603	2.7651213	0.1213300
C	-1.8961873	2.7310783	0.7238340
C	-1.6998723	2.0561543	1.9336480
C	-2.7954343	1.4513153	2.5396750
C	-0.3201643	1.9207073	2.5410120
H	-4.8941023	1.0126703	2.4637160
H	4.5556377	2.6627213	-1.4039560
H	4.2085617	3.2523023	-3.0238080
H	3.0838327	3.6222463	-1.7162400
H	1.0847827	2.5349273	-2.9273450
H	1.2903807	0.9242303	-3.6624730
H	4.1508577	-2.8060677	4.4244670
H	5.9170277	-3.5833597	2.8884470
H	6.0256157	-2.7621997	0.5485220
H	2.4259967	-1.1868307	3.6429560
H	5.0737137	-0.7073947	-0.9244120
H	3.9730787	1.0798113	0.1600250
H	2.4387577	1.8316413	1.8465250
H	2.5920597	-2.1560907	-1.4099200
H	1.1976687	-2.0369177	-2.5296940
H	1.3670497	-3.4307317	-1.5108760
H	2.1579477	2.3156163	-4.3161820
H	-3.3087373	3.2840343	-0.8163650
H	-1.0641323	3.2394153	0.2470180
H	-2.6581983	0.9121453	3.4721600

H	0.2144147	2.8753243	2.5155400
H	-0.4047003	1.6116913	3.5880060
H	-7.3575943	1.7224933	-0.0554610
H	-6.3712073	0.4984783	0.7915460
H	-6.7757613	2.0397553	1.6005970
H	4.9030707	0.5146913	-2.6518190
H	4.1449687	0.9340663	-4.1824230
H	3.5017267	-0.4185007	-3.2347470
N	2.4572477	0.8952563	-1.2304400
N	0.5156857	0.9449133	1.8303620
N	4.1763867	-0.9062177	-0.4965810
O	1.0838517	2.7732943	-0.5732630
O	-0.9769373	-0.7899727	1.8864940
O	-5.4024493	2.1795983	0.0458580
H	1.7735197	0.1760113	-1.5217110
Au	-1.4227683	-2.0816487	-0.6307660
P	-3.7733663	-2.2770627	-0.6356900
C	-4.6700933	-0.9197487	-1.4726920
H	-4.4008413	-0.8969677	-2.5306850
H	-5.7509843	-1.0621527	-1.3792520
H	-4.3899343	0.0360163	-1.0212360
C	-4.5159803	-3.7975307	-1.3290970
H	-4.1013653	-4.6684447	-0.8173420
H	-5.6024863	-3.7874347	-1.2074490
H	-4.2703003	-3.8712517	-2.3904690
C	-4.3883713	-2.2031247	1.0839380
H	-5.4818783	-2.2239837	1.1131740
H	-3.9905063	-3.0492897	1.6483240
H	-4.0135383	-1.2824357	1.5396290

Zero-point correction= 0.631213 (Hartree/Particle)
Thermal correction to Energy= 0.670084
Thermal correction to Enthalpy= 0.671028
Thermal correction to Gibbs Free Energy= 0.558058
Sum of electronic and zero-point Energies= -1993.079781
Sum of electronic and thermal Energies= -1993.040911
Sum of electronic and thermal Enthalpies= -1993.039966
Sum of electronic and thermal Free Energies= -1993.152937

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C	0.1696635	4.2498790	2.7138226
C	0.1128885	3.8420760	4.0600376
C	0.4136805	2.5409740	4.4259536
C	0.7688245	1.6634110	3.4011716
C	0.8166895	2.0405930	2.0423056
C	0.5141485	3.3693950	1.7017906

C	4.8735915	-2.7029790	-0.4514114
C	1.3158515	-0.1724830	2.2437606
C	1.1193445	0.8321390	1.2939716
C	1.5380595	0.6242510	-0.1415024
C	3.9116765	-1.9650400	-1.1444004
C	-0.3977835	-0.8714910	-0.2105674
C	-0.9107745	-0.0050630	0.8853896
C	-1.9164985	0.3922130	1.5390546
C	2.5538485	-2.2013730	-0.9672574
C	1.4396665	1.9079760	-0.9894844
C	2.1553065	-3.2036110	-0.0688364
C	1.5046895	-1.3704650	-1.6629844
C	0.2486155	3.0477780	-2.8708834
C	-0.0408165	4.3452230	-2.1108344
C	1.4879045	3.2063160	-3.7567124
C	-0.9620385	2.6559470	-3.7172154
C	-2.3706485	1.2835290	2.6418296
C	6.6913945	-4.2805630	0.9912336
C	3.0940555	-3.9383570	0.6309866
C	4.4642595	-3.6921280	0.4429906
H	1.6815035	2.2833210	-4.3115634
H	4.2383745	-1.1949170	-1.8390624
H	1.0948895	-3.4096660	0.0632726
H	1.9527565	-0.7243170	-2.4252794
H	0.7429755	-1.9927250	-2.1362144
H	7.1776845	-5.0008420	1.6468196
H	6.9847455	-4.4749620	-0.0463394
H	-0.0580525	5.2806130	2.4654426
H	-0.1620915	4.5609970	4.8239596
H	0.3771095	2.2187790	5.4612736
H	0.5639995	3.7064030	0.6743666
H	1.1243855	-0.2250370	4.3307436
H	1.6106635	-1.2023710	2.0773336
H	2.6032905	0.3654890	-0.1638634
H	-0.0992455	1.1069490	-2.0361884
H	-0.2768175	5.1419150	-2.8216054
H	-0.8989455	4.2132300	-1.4441114
H	0.8288565	4.6488880	-1.5256054
H	1.3275005	4.0129340	-4.4772624
H	6.9977275	-3.2666100	1.2724056
H	2.3620925	3.4479880	-3.1497364
H	-1.1671515	3.4341580	-4.4554284
H	-0.7771395	1.7209160	-4.2569134
H	-1.8534055	2.5357060	-3.0924054

H	-1.7770775	2.2008400	2.6637426
H	-2.2349775	0.7648530	3.5959616
H	-3.4260835	1.5374250	2.5448416
H	2.8064835	-4.7259840	1.3188266
H	5.9236965	-2.4971010	-0.6162784
N	0.8104945	-0.5130380	-0.6939574
N	0.4586895	1.9396850	-1.9144414
N	1.0799045	0.3129150	3.4782976
O	-1.0667795	-1.8118110	-0.6269304
O	2.2353345	2.8062750	-0.7698904
O	5.2998115	-4.4631890	1.1707816
Au	-3.4840375	-0.8898540	0.6018846
P	-5.2485935	-2.1406860	-0.2054154
C	-4.6569915	-3.5520220	-1.1974784
H	-5.5003735	-4.1278570	-1.5878484
H	-4.0478005	-3.1801130	-2.0237854
H	-4.0310535	-4.1926140	-0.5729564
C	-6.3119745	-2.8698750	1.0845476
H	-6.7611315	-2.0733650	1.6809906
H	-7.1014055	-3.4723910	0.6273266
H	-5.7075175	-3.4993860	1.7405296
C	-6.3874405	-1.2266100	-1.2983414
H	-5.8312905	-0.8230560	-2.1467064
H	-7.1758435	-1.8908860	-1.6622754
H	-6.8353515	-0.3971420	-0.7476754

Zero-point correction= 0.627607 (Hartree/Particle)
Thermal correction to Energy= 0.667132
Thermal correction to Enthalpy= 0.668076
Thermal correction to Gibbs Free Energy= 0.551301
Sum of electronic and zero-point Energies= -1993.106066
Sum of electronic and thermal Energies= -1993.066541
Sum of electronic and thermal Enthalpies= -1993.065597
Sum of electronic and thermal Free Energies= -1993.182372

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C	-1.0681433	3.5110492	-3.0907564
C	-1.8208593	2.9973972	-4.1526874
C	-2.2017903	1.6579742	-4.1838664
C	-1.7985413	0.8907192	-3.1039344
C	-1.0524933	1.3758342	-2.0332194
C	-0.6709423	2.7078542	-2.0228724
C	-3.9672363	-3.3808438	0.8114016
C	-1.4356593	-0.8946388	-1.7739794
C	-0.7743753	0.2460972	-1.0808264
C	-1.4443413	0.3520862	0.3485506

C	-3.2686923	-2.4135098	1.5389896
C	0.6786067	-0.6549668	0.6481636
C	0.6945607	-0.1153438	-0.7436944
C	1.7851077	-0.0904558	-1.5290404
C	-1.8786073	-2.3870978	1.5656566
C	-1.6930653	1.8217002	0.7458416
C	-1.1756403	-3.3655048	0.8424296
C	-1.1138393	-1.2689288	2.2365926
C	-0.8992143	3.6988052	2.1914626
C	-0.8031393	4.7527862	1.0848446
C	-2.2234383	3.8322492	2.9497766
C	0.2785557	3.8385342	3.1546706
C	1.7351547	0.3052572	-2.9784914
C	-5.2306803	-5.4399238	-0.6220324
C	-1.8513723	-4.3261088	0.1089386
C	-3.2566413	-4.3402448	0.0892796
H	-2.2909603	3.0725242	3.7341266
H	-3.8306433	-1.6684118	2.0973346
H	-0.0880183	-3.3667968	0.8664026
H	-1.7581073	-0.6884478	2.9038766
H	-0.2635873	-1.6441508	2.8100816
H	-5.4725893	-6.3052078	-1.2366544
H	-5.5883713	-5.6054028	0.3999606
H	-0.7867673	4.5582892	-3.1013424
H	-2.1105083	3.6501272	-4.9681084
H	-2.7773893	1.2479902	-5.0063274
H	-0.0841063	3.1076142	-1.2023014
H	-2.5017303	-1.1151768	-3.5109204
H	-1.4926343	-1.9205578	-1.4126864
H	-2.4417583	-0.1023398	0.3364086
H	-0.1118013	1.7083982	1.9865586
H	-0.8979453	5.7517812	1.5189776
H	0.1692327	4.6924792	0.5848546
H	-1.6006093	4.6125412	0.3521036
H	-2.2804523	4.8171322	3.4210306
H	-5.7183993	-4.5504058	-1.0375804
H	-3.0693423	3.7188512	2.2699186
H	0.2666827	4.8296082	3.6135176
H	0.2199097	3.0951892	3.9564676
H	1.2310577	3.7177372	2.6287526
H	0.7329797	0.3282542	-3.4180624
H	2.3553977	-0.3718988	-3.5709914
H	2.1756567	1.3023472	-3.0977834
H	-1.3239963	-5.1007838	-0.4375464

H	-5.0501603	-3.3767978	0.8216026
N	-0.5560653	-0.3782988	1.2145696
N	-0.7948313	2.3469172	1.5996666
N	-1.9914703	-0.5040018	-2.8800934
O	1.5503327	-1.2801358	1.2220076
O	-2.6451963	2.4015382	0.2491266
O	-3.8211313	-5.3161378	-0.6548834
Au	3.6341097	-0.6063988	-0.7319214
P	5.7274587	-1.2030268	0.1810666
C	5.5626417	-2.2910808	1.6408286
H	6.5416867	-2.5259628	2.0669076
H	4.9428817	-1.7930448	2.3894096
H	5.0609107	-3.2147288	1.3448636
C	6.8562567	-2.1130658	-0.9329244
H	7.0851877	-1.4937768	-1.8026004
H	7.7840297	-2.3711328	-0.4152814
H	6.3666717	-3.0260728	-1.2778334
C	6.7372767	0.1986722	0.7816046
H	6.1737787	0.7534922	1.5345516
H	7.6733207	-0.1595688	1.2184396
H	6.9578367	0.8705512	-0.0503734

Zero-point correction= 0.629994 (Hartree/Particle)
Thermal correction to Energy= 0.669972
Thermal correction to Enthalpy= 0.670916
Thermal correction to Gibbs Free Energy= 0.551014
Sum of electronic and zero-point Energies= -1993.130992
Sum of electronic and thermal Energies= -1993.091014
Sum of electronic and thermal Enthalpies= -1993.090069
Sum of electronic and thermal Free Energies= -1993.209972

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C	1.6380006	1.4196624	2.7792861
C	2.0812886	0.5403954	3.7670481
C	1.9598746	-0.8420806	3.6115591
C	1.3820856	-1.2864576	2.4349821
C	0.9230356	-0.4238346	1.4361171
C	1.0408286	0.9492654	1.6070331
N	1.1713276	-2.6233106	2.0006901
C	0.8007536	-2.6259176	0.7102701
C	0.2701496	-1.2579876	0.3362741
C	0.7563586	-0.9639166	-1.0917219
N	0.0773236	0.2420354	-1.4305659
C	-1.1783794	0.2339954	-0.8414779
C	-1.2195694	-0.8900116	0.1630941
O	-2.0507034	1.0344494	-1.1183209

C	2.2433116	-1.1117556	-1.0485869
C	-2.3369564	-1.3253646	0.7636981
Au	-4.1624314	-0.4572976	0.2942461
C	-2.3168064	-2.4135666	1.7989871
C	0.5616306	4.4364854	-0.2734849
C	1.9348506	4.6117334	-0.0517579
C	2.8477906	3.7347214	-0.6396959
C	2.3787466	2.6818704	-1.4267079
C	1.0179326	2.4905574	-1.6418379
C	0.1118966	3.3926134	-1.0640079
C	0.4983086	1.2768294	-2.3784859
O	2.2738506	5.6549774	0.7420141
C	3.6489456	5.9052634	0.9460471
H	1.7504426	2.4891234	2.9201651
H	2.5303746	0.9321194	4.6730311
H	2.3022496	-1.5294246	4.3776931
H	0.6878156	1.6461954	0.8526171
H	1.4552526	-3.4449686	2.5146171
H	-1.3254934	-2.8265186	2.0140841
H	-2.7278104	-2.0264476	2.7371661
H	-2.9782504	-3.2316126	1.4973421
H	-0.1251454	5.1425794	0.1802321
H	3.9141716	3.8591994	-0.4970919
H	3.0937306	1.9956394	-1.8697989
H	-0.9527104	3.2520854	-1.2255009
H	-0.3777554	1.5315174	-2.9817129
H	1.2657096	0.8533424	-3.0310179
H	3.7061336	6.7875904	1.5816191
H	4.1616306	6.1049214	-0.0017169
H	4.1373326	5.0620664	1.4494071
P	-6.2069264	0.5910694	-0.2472989
C	-5.9573744	2.3188504	-0.7913359
H	-5.2598764	2.3288024	-1.6316989
H	-6.9038144	2.7790124	-1.0876309
H	-5.5125274	2.8904704	0.0259341
C	-7.4397924	0.7176724	1.0976111
H	-8.3310114	1.2512854	0.7565641
H	-7.7201794	-0.2844396	1.4283761
H	-6.9988654	1.2494584	1.9432101
C	-7.1361824	-0.1756856	-1.6238239
H	-8.0436664	0.3938054	-1.8418899
H	-6.5029604	-0.2054646	-2.5129099
H	-7.4047804	-1.1995646	-1.3559259
N	2.4824856	-2.3656906	-0.2867469

H	3.1363066	-2.1220146	0.4648981
C	3.0832386	-3.5258126	-1.0505289
C	3.1245166	-4.7088216	-0.0822009
C	2.2044356	-3.8377266	-2.2584619
C	4.5043836	-3.1669586	-1.4938049
H	3.6931406	-4.4607806	0.8205951
H	2.1233876	-5.0416416	0.2068741
H	3.6234516	-5.5532116	-0.5629749
H	2.1817506	-3.0027896	-2.9660839
H	2.6170056	-4.7007576	-2.7855959
H	1.1787916	-4.0871276	-1.9680059
H	4.9492176	-4.0300266	-1.9956999
H	4.5135426	-2.3213576	-2.1825819
H	5.1325486	-2.9176946	-0.6328049
O	3.1222226	-0.4354456	-1.4885809
H	0.4484666	-3.5439576	0.2519931
H	0.4279396	-1.8142216	-1.7253009

Zero-point correction= 0.629103 (Hartree/Particle)
Thermal correction to Energy= 0.668146
Thermal correction to Enthalpy= 0.669091
Thermal correction to Gibbs Free Energy= 0.552503
Sum of electronic and zero-point Energies= -1993.092508
Sum of electronic and thermal Energies= -1993.053464
Sum of electronic and thermal Enthalpies= -1993.052520
Sum of electronic and thermal Free Energies= -1993.169108

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C	1.6245725	1.6058100	2.6257839
C	2.1099495	0.7660230	3.6301619
C	2.0569335	-0.6204650	3.4962539
C	1.4897575	-1.1325380	2.3375269
C	0.9854855	-0.3044900	1.3309329
C	1.0466545	1.0793890	1.4718389
N	1.4146055	-2.5129060	1.9664179
C	0.9886025	-2.5154980	0.5992009
C	0.3186235	-1.1670160	0.2605879
C	0.7718655	-0.9112030	-1.1848801
N	0.0990795	0.2836270	-1.5504541
C	-1.1464435	0.2927750	-0.9249611
C	-1.1619865	-0.8122640	0.1039149
O	-2.0157395	1.0960520	-1.1977241
C	2.2361825	-1.1337440	-1.1104261
C	-2.2616375	-1.2289070	0.7500569
Au	-4.1054845	-0.3933460	0.3128599
C	-2.1767215	-2.2803740	1.8200779

C	0.7043825	4.4446520	-0.3891031
C	2.0754865	4.5232590	-0.1064631
C	2.9549445	3.6019980	-0.6784451
C	2.4513185	2.5964090	-1.5040991
C	1.0904365	2.4962370	-1.7727591
C	0.2208075	3.4446390	-1.2155531
C	0.5230595	1.3055240	-2.5086061
O	2.4463765	5.5207050	0.7301029
C	3.8234335	5.6650380	1.0110639
H	1.6871725	2.6827480	2.7416639
H	2.5449865	1.1956640	4.5261219
H	2.4493775	-1.2778230	4.2647089
H	0.6509015	1.7427560	0.7091689
H	0.9072025	-3.1295740	2.5906869
H	-1.1603005	-2.6448740	2.0141239
H	-2.5715245	-1.8790520	2.7588999
H	-2.8099275	-3.1362780	1.5663189
H	0.0464525	5.1843720	0.0535449
H	4.0200895	3.6544200	-0.4899761
H	3.1392755	1.8732450	-1.9331581
H	-0.8444845	3.3696560	-1.4135451
H	-0.3592395	1.5842910	-3.0911741
H	1.2627995	0.8612620	-3.1806871
H	3.9089965	6.5209910	1.6786129
H	4.3977185	5.8566640	0.0976309
H	4.2234185	4.7732940	1.5087699
P	-6.1709525	0.6310080	-0.2031741
C	-5.9396615	2.3089750	-0.8918421
H	-5.2918585	2.2470340	-1.7688851
H	-6.8980545	2.7567520	-1.1679911
H	-5.4434185	2.9353470	-0.1475571
C	-7.3265865	0.8753940	1.1931329
H	-8.2313405	1.3914840	0.8608319
H	-7.5957285	-0.0947480	1.6157819
H	-6.8354915	1.4658160	1.9693379
C	-7.1813725	-0.2286610	-1.4627921
H	-8.0952345	0.3331110	-1.6741051
H	-6.5994635	-0.3348710	-2.3806331
H	-7.4424985	-1.2254120	-1.1014971
N	2.3287035	-2.4024570	-0.2194201
H	3.0316945	-2.1782970	0.4978019
C	2.8432675	-3.6802730	-0.9141371
C	2.8210695	-4.8001370	0.1272529
C	1.9484785	-3.9978060	-2.1059501

C	4.2824085	-3.4202280	-1.3612841
H	3.3777525	-4.5213650	1.0261409
H	1.8084515	-5.0872130	0.4189259
H	3.2976815	-5.6803130	-0.3098621
H	2.0022935	-3.2187940	-2.8727021
H	2.2987725	-4.9270820	-2.5608021
H	0.9036435	-4.1493310	-1.8182741
H	4.6807955	-4.3476050	-1.7788471
H	4.3501105	-2.6444410	-2.1238391
H	4.9168575	-3.1367710	-0.5156701
O	3.2148225	-0.6181040	-1.5320611
H	0.4621065	-3.4150580	0.2865499
H	0.4252925	-1.7771020	-1.7894491

Zero-point correction= 0.630996 (Hartree/Particle)
Thermal correction to Energy= 0.670061
Thermal correction to Enthalpy= 0.671005
Thermal correction to Gibbs Free Energy= 0.555574
Sum of electronic and zero-point Energies= -1993.095318
Sum of electronic and thermal Energies= -1993.056253
Sum of electronic and thermal Enthalpies= -1993.055309
Sum of electronic and thermal Free Energies= -1993.170739

RRS-ts3b

C	1.5256190	1.9085130	2.4018888
C	2.2113100	1.1942260	3.3879018
C	2.3042690	-0.1938250	3.3268308
C	1.6787480	-0.8174660	2.2586668
C	0.9867570	-0.1346670	1.2685348
C	0.8985770	1.2548680	1.3442008
N	1.7628270	-2.2319850	1.9461118
C	1.0251970	-2.4238780	0.6541348
C	0.3302950	-1.1031100	0.2912248
C	0.7763000	-0.9545330	-1.1702682
N	0.0985110	0.2168000	-1.6074812
C	-1.1463090	0.2558730	-0.9859142
C	-1.1491350	-0.7740100	0.1233388
O	-2.0233340	1.0377030	-1.2966872
C	2.2424180	-1.2595730	-1.1128822
C	-2.2185420	-1.1385890	0.8454498
Au	-4.0859430	-0.3834200	0.3753178
C	-2.0540850	-2.0736850	2.0120538
C	0.6862510	4.4229070	-0.6030492
C	2.0332750	4.4567650	-0.2167932
C	2.9168640	3.4857400	-0.6919932
C	2.4365200	2.4692130	-1.5176022

C	1.0958400	2.4109730	-1.8844462
C	0.2262850	3.4119900	-1.4311202
C	0.5395920	1.2007160	-2.5958312
O	2.3776020	5.4601570	0.6265468
C	3.7346380	5.5608700	1.0060608
H	1.4697230	2.9910580	2.4579838
H	2.6805610	1.7227250	4.2102768
H	2.8450800	-0.7590440	4.0785078
H	0.3523430	1.8264330	0.6013098
H	1.5665370	-2.8800730	2.7086778
H	-1.0065770	-2.3067760	2.2558638
H	-2.5093770	-1.6368350	2.9056108
H	-2.5855470	-3.0136140	1.8287848
H	0.0275030	5.2025680	-0.2364922
H	3.9656570	3.5038390	-0.4225052
H	3.1215080	1.6997000	-1.8640532
H	-0.8237850	3.3691520	-1.7058302
H	-0.3303060	1.4623030	-3.2041462
H	1.2913530	0.7297470	-3.2348342
H	3.8040760	6.4297480	1.6587078
H	4.3819800	5.7074280	0.1341768
H	4.0621890	4.6673380	1.5519568
P	-6.1691540	0.5601660	-0.2194622
C	-5.9528570	2.1476490	-1.1004422
H	-5.3132230	1.9863800	-1.9708312
H	-6.9159320	2.5572660	-1.4165642
H	-5.4514990	2.8574790	-0.4391152
C	-7.3107670	0.9596560	1.1523228
H	-8.2213740	1.4305020	0.7722788
H	-7.5709540	0.0438910	1.6870788
H	-6.8147800	1.6378560	1.8496718
C	-7.1870710	-0.4451100	-1.3594252
H	-8.1061520	0.0838910	-1.6256042
H	-6.6132140	-0.6549820	-2.2643802
H	-7.4390840	-1.3940820	-0.8817322
N	2.2950810	-2.4339370	-0.1880712
H	2.7171530	-2.3313950	1.0652338
C	2.7711340	-3.7524960	-0.7866602
C	2.7649790	-4.8045810	0.3262098
C	1.8474920	-4.1630200	-1.9308232
C	4.2064800	-3.5598860	-1.2800562
H	3.4209270	-4.5153970	1.1536968
H	1.7645030	-5.0148220	0.7151568
H	3.1494310	-5.7415410	-0.0821032

H	1.8786400	-3.4357440	-2.7479892
H	2.1775260	-5.1234730	-2.3338102
H	0.8103660	-4.2830580	-1.5993542
H	4.5948910	-4.5322980	-1.5923952
H	4.2650500	-2.8772420	-2.1268592
H	4.8454450	-3.1746410	-0.4809472
O	3.1998290	-0.8141730	-1.6639472
H	0.4436590	-3.3416680	0.5996628
H	0.3902120	-1.8454580	-1.7089272

Zero-point correction= 0.626446 (Hartree/Particle)
Thermal correction to Energy= 0.664108
Thermal correction to Enthalpy= 0.665052
Thermal correction to Gibbs Free Energy= 0.555197
Sum of electronic and zero-point Energies= -1993.063817
Sum of electronic and thermal Energies= -1993.026155
Sum of electronic and thermal Enthalpies= -1993.025211
Sum of electronic and thermal Free Energies= -1993.135066

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C	1.5272388	1.6363667	2.3988257
C	2.1539628	0.8338717	3.3538397
C	2.1354228	-0.5547663	3.2316187
C	1.4799908	-1.0610613	2.1253837
C	0.8541918	-0.3005833	1.1527017
C	0.8638428	1.0848667	1.3026747
N	1.3498038	-2.4945903	1.7971957
C	0.9729978	-2.5081433	0.3035077
C	0.1962808	-1.1898313	0.0980927
C	0.6143178	-0.8845793	-1.3343873
N	-0.0740352	0.3299997	-1.6251543
C	-1.2969752	0.3087837	-0.9744873
C	-1.2928442	-0.8585873	0.0007347
O	-2.1781662	1.1252137	-1.1655623
C	2.0863418	-1.2039783	-1.3335523
C	-2.3747822	-1.3245843	0.6381597
Au	-4.2300652	-0.4756433	0.2743157
C	-2.2610882	-2.4427023	1.6349547
C	0.7031418	4.4249017	-0.3471133
C	2.0701208	4.3853487	-0.0394433
C	2.8898888	3.4261097	-0.6374993
C	2.3287578	2.4939337	-1.5107563
C	0.9684448	2.5097747	-1.8032483
C	0.1618648	3.4978737	-1.2233633
C	0.3314428	1.3729637	-2.5659043
O	2.4972898	5.3079787	0.8577957

C	3.8795328	5.3507067	1.1459817
H	1.5523278	2.7167407	2.5025957
H	2.6577668	1.2879417	4.1994427
H	2.6117688	-1.1955303	3.9666787
H	0.3787828	1.7349247	0.5835857
H	0.6105848	-2.9389123	2.3561287
H	-1.2485862	-2.8701503	1.7177637
H	-2.5638002	-2.0909093	2.6266637
H	-2.9366602	-3.2638573	1.3795657
H	0.0947048	5.1940237	0.1160407
H	3.9519688	3.3891637	-0.4283443
H	2.9613768	1.7274357	-1.9509333
H	-0.9030702	3.5094577	-1.4383803
H	-0.5667172	1.7023067	-3.0950993
H	1.0293808	0.9302127	-3.2813583
H	4.0180288	6.1686977	1.8513257
H	4.4686098	5.5444867	0.2426427
H	4.2205698	4.4135757	1.6034487
P	-6.2939032	0.5695477	-0.1948663
C	-6.0521572	2.2706497	-0.8195713
H	-5.3991722	2.2378297	-1.6943553
H	-7.0072062	2.7321807	-1.0843843
H	-5.5572872	2.8670267	-0.0501743
C	-7.4546942	0.7644827	1.2047827
H	-8.3565682	1.2948057	0.8874397
H	-7.7284932	-0.2199583	1.5896767
H	-6.9661102	1.3248117	2.0044917
C	-7.2991112	-0.2408843	-1.4903243
H	-8.2102712	0.3307927	-1.6861103
H	-6.7119152	-0.3147673	-2.4079663
H	-7.5648022	-1.2495713	-1.1675523
N	2.1898098	-2.3078883	-0.4512053
C	3.1590438	-3.4125373	-0.7644803
C	3.0598458	-4.5345583	0.2768667
C	2.8172648	-3.9762223	-2.1476413
C	4.5880628	-2.8598183	-0.7265433
H	3.4888878	-4.2444173	1.2451287
H	2.0456508	-4.9228363	0.4143157
H	3.6681348	-5.3718993	-0.0711783
H	2.8817648	-3.1938563	-2.9073563
H	3.5220678	-4.7664713	-2.4177863
H	1.8082368	-4.4027093	-2.1582983
H	5.2930378	-3.6881883	-0.8385983
H	4.7593588	-2.1386313	-1.5229293

H	4.7790858	-2.3700053	0.2331057
O	2.9692998	-0.7717253	-2.0290893
H	0.4362868	-3.4374213	0.0952487
H	0.2200248	-1.7058413	-1.9682723
H	2.2218698	-3.0111733	1.9405497

Zero-point correction= 0.632440 (Hartree/Particle)
Thermal correction to Energy= 0.670271
Thermal correction to Enthalpy= 0.671216
Thermal correction to Gibbs Free Energy= 0.560322
Sum of electronic and zero-point Energies= -1993.098754
Sum of electronic and thermal Energies= -1993.060923
Sum of electronic and thermal Enthalpies= -1993.059979
Sum of electronic and thermal Free Energies= -1993.170873

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C	0.1715131	4.2463891	-2.7179215
C	0.1142451	3.8368841	-4.0635975
C	0.4143071	2.5351611	-4.4279065
C	0.7692471	1.6587441	-3.4020745
C	0.8176331	2.0376611	-2.0437145
C	0.5158001	3.3670361	-1.7048375
C	4.8711441	-2.7061759	0.4519735
C	1.3155811	-0.1759419	-2.2424095
C	1.1198291	0.8300201	-1.2938755
C	1.5390691	0.6238511	0.1416885
C	3.9107741	-1.9665479	1.1453175
C	-0.3981359	-0.8699469	0.2141285
C	-0.9105729	-0.0052829	-0.8834795
C	-1.9161429	0.3913551	-1.5377795
C	2.5525051	-2.2017719	0.9700925
C	1.4421171	1.9088851	0.9878715
C	2.1519351	-3.2046579	0.0732975
C	1.5049321	-1.3688279	1.6658045
C	0.2530901	3.0521231	2.8684795
C	-0.9572789	2.6622911	3.7161375
C	1.4930561	3.2110441	3.7532865
C	-0.0359579	4.3487021	2.1068095
C	-2.3699569	1.2813341	-2.6417795
C	6.6856901	-4.2869169	-0.9913595
C	3.0891221	-3.9410839	-0.6268535
C	4.4597891	-3.6959169	-0.4408385
H	2.3670111	3.4512881	3.1454135
H	4.2390531	-1.1959339	1.8386865
H	1.0911631	-3.4098089	-0.0573605
H	1.9544311	-0.7221379	2.4267905

H	0.7429671	-1.9895819	2.1406075
H	7.1704811	-5.0083319	-1.6468085
H	6.9802551	-4.4804449	0.0460315
H	-0.0556699	5.2775451	-2.4708095
H	-0.1605599	4.5549561	-4.8283815
H	0.3773161	2.2116471	-5.4628005
H	0.5659981	3.7053271	-0.6778515
H	1.1235861	-0.2311029	-4.3292705
H	1.6099011	-1.2057669	-2.0747105
H	2.6041041	0.3642791	0.1638835
H	-0.0965729	1.1103471	2.0367785
H	-1.1614079	3.4416711	4.4533895
H	-1.8491189	2.5417451	3.0920685
H	-0.7726479	1.7278991	4.2570325
H	1.3336711	4.0187551	4.4728385
H	6.9925301	-3.2735369	-1.2740435
H	1.6863921	2.2886791	4.3092765
H	-0.8946299	4.2163611	1.4408535
H	-0.2709449	5.1465491	2.8166225
H	0.8335261	4.6509511	1.5205695
H	-1.7759569	2.1983311	-2.6650625
H	-3.4252569	1.5358991	-2.5450215
H	-2.2346939	0.7612421	-3.5951965
H	2.7999561	-4.7292029	-1.3134615
H	5.9216431	-2.5010909	0.6153105
N	0.8108451	-0.5120089	0.6961575
N	0.4617861	1.9425631	1.9134415
N	1.0795791	0.3079731	-3.4775105
O	-1.0681109	-1.8084719	0.6329455
O	2.2382361	2.8063301	0.7664385
O	5.2937101	-4.4685239	-1.1688635
Au	-3.4845399	-0.8889599	-0.5996335
P	-5.2510399	-2.1375479	0.2071775
C	-5.9579329	-3.2928099	-1.0146955
H	-5.1765009	-3.9672399	-1.3703265
H	-6.7639309	-3.8757569	-0.5609785
H	-6.3490829	-2.7311099	-1.8652385
C	-4.7373139	-3.1811859	1.6117985
H	-5.5716109	-3.7969629	1.9582435
H	-3.9090449	-3.8201889	1.2988015
H	-4.3888199	-2.5430599	2.4263295
C	-6.6686919	-1.1657949	0.8171225
H	-7.0774059	-0.5659319	0.0016095
H	-7.4445509	-1.8316499	1.2043215

H	-6.3354409	-0.4946039	1.6110235

Zero-point correction= 0.627599 (Hartree/Particle)
Thermal correction to Energy= 0.667126
Thermal correction to Enthalpy= 0.668070
Thermal correction to Gibbs Free Energy= 0.551368
Sum of electronic and zero-point Energies= -1993.106071
Sum of electronic and thermal Energies= -1993.066544
Sum of electronic and thermal Enthalpies= -1993.065600
Sum of electronic and thermal Free Energies= -1993.182302

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C	1.0716616	3.5135851	-3.0890289
C	1.8233736	2.9995551	-4.1514869
C	2.2024606	1.6596271	-4.1835869
C	1.7984626	0.8922691	-3.1040119
C	1.0533686	1.3777431	-2.0327899
C	0.6736606	2.7102831	-2.0215239
C	3.9633706	-3.3845669	0.8103751
C	1.4336236	-0.8933809	-1.7749879
C	0.7740206	0.2478201	-1.0809879
C	1.4446336	0.3521911	0.3482121
C	3.2660706	-2.4164229	1.5380841
C	-0.6794184	-0.6525029	0.6479811
C	-0.6952274	-0.1121329	-0.7436139
C	-1.7860484	-0.0854099	-1.5285529
C	1.8760266	-2.3880299	1.5644911
C	1.6951556	1.8212841	0.7463131
C	1.1718116	-3.3652089	0.8408071
C	1.1127056	-1.2690799	2.2357831
C	0.9035846	3.6984731	2.1931061
C	-0.2740294	3.8390261	3.1563871
C	2.2279706	3.8298211	2.9515101
C	0.8088206	4.7532551	1.0871421
C	-1.7361864	0.3114321	-2.9777029
C	5.2241356	-5.4451229	-0.6234119
C	1.8463036	-4.3265719	0.1071881
C	3.2515556	-4.3427469	0.0878421
H	3.0737356	3.7159121	2.2715641
H	3.8289686	-1.6722959	2.0967671
H	0.0841826	-3.3649449	0.8645441
H	1.7578086	-0.6894819	2.9030271
H	0.2621266	-1.6433519	2.8094131
H	5.4648856	-6.3105899	-1.2382369
H	5.5814176	-5.6114179	0.3985931
H	0.7917156	4.5612161	-3.0988829

H	2.1136986	3.6523881	-4.9665849
H	2.7772966	1.2493551	-5.0064399
H	0.0876106	3.1103491	-1.2005399
H	2.4989256	-1.1143069	-3.5123599
H	1.4893626	-1.9195649	-1.4142729
H	2.4415146	-0.1034119	0.3354591
H	0.1137736	1.7091541	1.9870001
H	-0.2609734	4.8298041	3.6158431
H	-1.2266744	3.7196861	2.6303911
H	-0.2162794	3.0951181	3.9577281
H	2.2861576	4.8142971	3.4234721
H	5.7132216	-4.5562039	-1.0386299
H	2.2946056	3.0694551	3.7353161
H	-0.1636524	4.6945251	0.5871571
H	0.9049336	5.7518561	1.5218921
H	1.6060886	4.6124391	0.3542871
H	-0.7341264	0.3342431	-3.4175309
H	-2.1761834	1.3088581	-3.0960889
H	-2.3569904	-0.3648939	-3.5705549
H	1.3179336	-5.1003269	-0.4396419
H	5.0462966	-3.3820649	0.8207771
N	0.5557756	-0.3776249	1.2140541
N	0.7975716	2.3470761	1.6004751
N	1.9896246	-0.5028419	-2.8810359
O	-1.5517204	-1.2767259	1.2219651
O	2.6479636	2.4002651	0.2498971
O	3.8147746	-5.3192739	-0.6564589
Au	-3.6353014	-0.6000489	-0.7310809
P	-5.7281814	-1.1992479	0.1816551
C	-6.4447804	-2.7419409	-0.4903899
H	-5.7429874	-3.5638609	-0.3347969
H	-7.3923204	-2.9740169	0.0032011
H	-6.6120634	-2.6279189	-1.5633689
C	-5.6411234	-1.4978059	1.9832401
H	-6.6106354	-1.8175959	2.3744421
H	-4.8901454	-2.2654029	2.1817481
H	-5.3294764	-0.5792319	2.4848111
C	-7.0704784	0.0281491	-0.0067849
H	-7.2556024	0.2031201	-1.0685559
H	-7.9881544	-0.3276689	0.4692011
H	-6.7659884	0.9716081	0.4507761

Zero-point correction= 0.629932 (Hartree/Particle)
Thermal correction to Energy= 0.669944
Thermal correction to Enthalpy= 0.670888

Thermal correction to Gibbs Free Energy= 0.550220
Sum of electronic and zero-point Energies= -1993.131040
Sum of electronic and thermal Energies= -1993.091028
Sum of electronic and thermal Enthalpies= -1993.090084
Sum of electronic and thermal Free Energies= -1993.210753

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C	0.7637226	0.3934784	0.5388896
C	0.6782506	1.9910754	-1.2875944
C	-0.0858714	1.5220254	-0.0571104
C	-0.1356454	2.8294044	0.7234066
C	0.2163046	3.8784954	-0.1284754
C	2.0977216	1.0026034	0.7920026
C	-0.5554424	4.4387174	2.4409976
C	3.5150086	0.9684704	-1.3261294
C	3.0819356	-0.4592076	-1.6518394
C	3.6724416	1.8029164	-2.5970044
C	4.8267956	0.9524304	-0.5360764
C	-0.5359174	3.1067094	2.0223626
C	-0.2040114	5.4711374	1.5708526
C	0.1905766	5.2074424	0.2583086
C	-1.3619464	-0.1704856	1.0903896
C	-1.4518014	0.8016504	-0.0578424
C	-2.5535834	0.9778224	-0.8054074
H	0.7690226	1.3926524	-2.1879704
H	2.9744126	-1.0707516	-0.7491854
H	3.8527866	-0.9260076	-2.2700874
H	2.1452306	-0.4919516	-2.2177464
H	3.9383286	2.8389574	-2.3609244
H	4.4767316	1.3870944	-3.2079574
H	2.7633166	1.7992004	-3.2057944
H	5.1282126	1.9628504	-0.2432454
H	4.7433716	0.3415164	0.3651226
H	5.6154786	0.5333474	-1.1662214
H	-0.8207124	2.3041144	2.6944856
H	-0.8532504	4.6749364	3.4562276
H	-0.2361414	6.4982834	1.9168336
H	0.4609706	6.0078984	-0.4219244
N	2.4474866	1.6545894	-0.4952984
N	0.5896696	3.3283554	-1.3833744
N	-0.0451014	-0.1583886	1.5745966
O	2.7720886	1.0705204	1.7733606
O	-2.2353774	-0.8716776	1.5563406
H	2.7954856	2.5908314	-0.2645934
H	0.9184166	3.8678424	-2.1710694

Au	-4.2608374	-0.1393286	-0.4290644
P	-6.1901574	-1.4095846	0.0596486
C	-6.4740634	-2.8548556	-1.0252484
H	-5.6016654	-3.5104646	-0.9879604
H	-7.3602724	-3.4098366	-0.7058624
H	-6.6084454	-2.5161116	-2.0545364
C	-6.1232794	-2.1235106	1.7415066
H	-6.0666214	-1.3135296	2.4717386
H	-7.0041924	-2.7388336	1.9431426
H	-5.2185904	-2.7278246	1.8361766
C	-7.7818294	-0.5100576	0.0173966
H	-8.6071114	-1.1710736	0.2954606
H	-7.7398694	0.3312004	0.7122286
H	-7.9514524	-0.1193006	-0.9879884
C	-2.6010954	1.9926484	-1.9113464
H	-1.6758924	2.5608914	-2.0532834
H	-2.8625544	1.5061924	-2.8564134
H	-3.4066754	2.7064514	-1.7101834
C	0.4715706	-1.2499696	2.4060966
H	-0.4095464	-1.7670326	2.7952176
H	1.0265336	-0.8232916	3.2457036
C	1.3614786	-2.1753686	1.6088396
C	2.7281876	-2.2513186	1.8548156
C	0.8293666	-2.9245776	0.5479546
C	3.5634436	-3.0675176	1.0857376
H	3.1577776	-1.6671566	2.6646476
C	1.6428776	-3.7240636	-0.2348714
H	-0.2394974	-2.8781646	0.3469796
C	3.0188486	-3.8060446	0.0339056
H	4.6201056	-3.1192806	1.3183246
H	1.2452466	-4.3154736	-1.0523364
O	3.7273046	-4.6165526	-0.7838464
C	5.1060286	-4.7790966	-0.5166944
H	5.4776136	-5.4845046	-1.2580004
H	5.6447306	-3.8288866	-0.6160394
H	5.2704016	-5.1843146	0.4878396
H	0.9331656	-0.3393576	-0.2709904

Zero-point correction= 0.629697 (Hartree/Particle)
Thermal correction to Energy= 0.668541
Thermal correction to Enthalpy= 0.669485
Thermal correction to Gibbs Free Energy= 0.555115
Sum of electronic and zero-point Energies= -1993.099773
Sum of electronic and thermal Energies= -1993.060929
Sum of electronic and thermal Enthalpies= -1993.059985

Sum of electronic and thermal Free Energies= -1993.174355

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C	-0.8333257	0.3692879	-0.6931081
C	-0.9288187	1.9108819	1.1321259
C	-0.0157967	1.4920439	-0.0500341
C	0.0446863	2.8241009	-0.7853201
C	-0.3503857	3.8495799	0.0767009
C	-2.1709057	0.9764129	-0.8522481
C	0.5906843	4.4655099	-2.4408021
C	-3.3986707	0.9580849	1.4537779
C	-2.9880277	-0.4900121	1.6993599
C	-3.4480487	1.7686849	2.7491179
C	-4.7524317	1.0198479	0.7449249
C	0.5228013	3.1283409	-2.0558091
C	0.2038673	5.4809769	-1.5631981
C	-0.2812537	5.1865609	-0.2908481
C	1.2964113	-0.1620281	-1.1986561
C	1.3421163	0.7857059	-0.0291051
C	2.4217993	0.9615969	0.7518989
H	-0.8225617	1.3370539	2.0505569
H	-2.9888007	-1.0810681	0.7765379
H	-3.7202287	-0.9404821	2.3741399
H	-2.0087857	-0.5771671	2.1802979
H	-3.6590807	2.8240049	2.5528699
H	-4.2527227	1.3723589	3.3722499
H	-2.5232467	1.6984899	3.3262639
H	-5.0231767	2.0466609	0.4803389
H	-4.7726397	0.4085669	-0.1583151
H	-5.5123687	0.6408889	1.4319639
H	0.8412073	2.3374779	-2.7271601
H	0.9538163	4.7212889	-3.4297791
H	0.2726933	6.5165219	-1.8783121
H	-0.5981787	5.9709459	0.3880449
N	-2.3636267	1.6438239	0.5367599
N	-0.8716587	3.3304749	1.3019639
N	-0.0128807	-0.1436861	-1.7358241
O	-2.9932967	1.0723469	-1.6969641
O	2.1799583	-0.8581751	-1.6494291
H	-2.7343727	2.5848189	0.3507749
H	-0.4489077	3.6628569	2.1607539
Au	4.1567803	-0.1205221	0.4230259
P	6.1265733	-1.3487821	-0.0198161
C	6.4129533	-2.7951721	1.0630109
H	5.5576413	-3.4706681	0.9965549

H	7.3205953	-3.3270921	0.7652849
H	6.5103313	-2.4610251	2.0979629
C	6.1269603	-2.0512141	-1.7078561
H	6.0709023	-1.2374601	-2.4339201
H	7.0291253	-2.6420531	-1.8874951
H	5.2417683	-2.6782901	-1.8335351
C	7.6944603	-0.4122781	0.0756169
H	8.5430483	-1.0515441	-0.1824321
H	7.6529583	0.4329729	-0.6143901
H	7.8252123	-0.0252341	1.0882209
C	2.4003493	1.9679179	1.8670139
H	1.4615713	2.5285899	1.9495609
H	2.6018543	1.4780299	2.8250909
H	3.2094183	2.6907799	1.7216069
C	-0.4960507	-1.2644121	-2.5526771
H	0.3997203	-1.7533101	-2.9438601
H	-1.0714387	-0.8667421	-3.3930141
C	-1.3440717	-2.2083791	-1.7325261
C	-2.7207767	-2.2852091	-1.9136281
C	-0.7622747	-2.9535391	-0.6945121
C	-3.5193397	-3.0980781	-1.1024101
H	-3.1890127	-1.7076291	-2.7067731
C	-1.5383067	-3.7494591	0.1287719
H	0.3144563	-2.9047411	-0.5432161
C	-2.9256987	-3.8323481	-0.0743231
H	-4.5853307	-3.1532961	-1.2867881
H	-1.1024887	-4.3387001	0.9281559
O	-3.5945587	-4.6397341	0.7786189
C	-4.9823647	-4.8131111	0.5705839
H	-5.3171407	-5.5180321	1.3296199
H	-5.5233377	-3.8663541	0.6890119
H	-5.1857607	-5.2235521	-0.4245791
H	-0.9945707	-0.3939061	0.0935269

Zero-point correction= 0.631306 (Hartree/Particle)
Thermal correction to Energy= 0.670319
Thermal correction to Enthalpy= 0.671263
Thermal correction to Gibbs Free Energy= 0.555374
Sum of electronic and zero-point Energies= -1993.103103
Sum of electronic and thermal Energies= -1993.064090
Sum of electronic and thermal Enthalpies= -1993.063146
Sum of electronic and thermal Free Energies= -1993.179035

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C	0.8734599	0.4034760	0.7159692
C	1.0036509	1.8472520	-1.1191078

C	0.0614909	1.5158970	0.0523682
C	0.0105559	2.8445550	0.7896592
C	0.5496619	3.8670540	0.0223582
C	2.2578619	0.9634860	0.7724442
C	-0.5932661	4.4859580	2.4275442
C	3.4099759	0.8919710	-1.5109588
C	3.0063769	-0.5640610	-1.7411958
C	3.4384979	1.6741510	-2.8266438
C	4.7866219	0.9746250	-0.8484778
C	-0.5758631	3.1570330	2.0143332
C	-0.0469661	5.4970360	1.6318212
C	0.5456349	5.1983940	0.4084272
C	-1.2624661	-0.0857580	1.2378482
C	-1.2998601	0.8323180	0.0424622
C	-2.3661801	1.0247140	-0.7511998
H	0.7900839	1.3962030	-2.0859288
H	3.0104699	-1.1377590	-0.8070788
H	3.7260359	-1.0324900	-2.4176008
H	2.0173609	-0.6510820	-2.2046258
H	3.7239489	2.7186020	-2.6628628
H	4.1897769	1.2284060	-3.4819358
H	2.4874799	1.6408250	-3.3664548
H	5.0293069	2.0043490	-0.5732778
H	4.8485229	0.3545620	0.0457302
H	5.5332449	0.6234620	-1.5649478
H	-1.0143081	2.3768600	2.6268222
H	-1.0454501	4.7428010	3.3789362
H	-0.0800291	6.5263980	1.9706052
H	0.9851259	5.9725440	-0.2115878
N	2.4037109	1.5700720	-0.5906178
N	1.2009299	3.3351790	-1.1605698
N	0.0433869	-0.0547380	1.7828092
O	3.1248749	0.9561150	1.5870932
O	-2.1588291	-0.7581450	1.7009642
H	2.3567509	2.8968810	-0.7854628
H	1.0071309	3.8163720	-2.0387298
Au	-4.1134431	-0.0383090	-0.4377768
P	-6.0835081	-1.2679560	0.0018572
C	-6.3629041	-2.7159940	-1.0803378
H	-5.5048331	-3.3878570	-1.0126478
H	-7.2685161	-3.2514680	-0.7828378
H	-6.4609221	-2.3831130	-2.1156338
C	-6.0801731	-1.9685890	1.6905022
H	-6.0289001	-1.1538530	2.4158142

H	-6.9788561	-2.5645830	1.8704972
H	-5.1911661	-2.5900800	1.8170062
C	-7.6547941	-0.3374060	-0.0949638
H	-8.5008271	-0.9800270	0.1631042
H	-7.6171711	0.5082910	0.5947062
H	-7.7868691	0.0483770	-1.1078758
C	-2.2944941	2.0307740	-1.8665158
H	-1.3644211	2.6178470	-1.8846248
H	-2.4128131	1.5344570	-2.8356568
H	-3.1271701	2.7355940	-1.7840188
C	0.5092839	-1.1614350	2.6291472
H	-0.3884581	-1.5838160	3.0869802
H	1.1468639	-0.7530590	3.4173642
C	1.2638099	-2.1865130	1.8152012
C	2.6442189	-2.3165830	1.9199582
C	0.5880169	-2.9556180	0.8546822
C	3.3562579	-3.2035990	1.1067322
H	3.1840749	-1.7177480	2.6488542
C	1.2783029	-3.8258980	0.0305172
H	-0.4925421	-2.8643460	0.7642622
C	2.6704809	-3.9598640	0.1548692
H	4.4286399	-3.2955160	1.2288282
H	0.7704419	-4.4334290	-0.7104708
O	3.2517709	-4.8389180	-0.6924228
C	4.6439729	-5.0491300	-0.5688828
H	4.9043479	-5.8024050	-1.3105778
H	5.2045329	-4.1286200	-0.7725368
H	4.9029679	-5.4158810	0.4305242
H	0.9860819	-0.3972440	-0.0425588

Zero-point correction= 0.626672 (Hartree/Particle)
Thermal correction to Energy= 0.665267
Thermal correction to Enthalpy= 0.666211
Thermal correction to Gibbs Free Energy= 0.551279
Sum of electronic and zero-point Energies= -1993.069720
Sum of electronic and thermal Energies= -1993.031125
Sum of electronic and thermal Enthalpies= -1993.030180
Sum of electronic and thermal Free Energies= -1993.145112

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C	-2.9674745	2.5504809	1.3676207
C	-3.8643105	2.1467679	2.3612167
C	-3.6859995	0.9482129	3.0500597
C	-2.5856555	0.1968059	2.6752077
C	-1.6883875	0.5626889	1.6754677
C	-1.8656305	1.7680319	1.0139347

C	-0.2255235	-2.6829541	0.2024587
C	-1.0340015	-1.4510551	2.6412597
C	-0.6550175	-0.5370321	1.5113817
C	-0.8917225	-1.2896481	0.1551097
C	0.3639895	-5.4062961	-1.0743543
C	0.5525225	0.4363959	-0.8397473
C	1.3641135	0.4017489	0.4144277
C	0.8018305	-0.0489181	1.5464397
C	1.4488625	-0.0272101	2.9022967
C	2.1775025	-4.1048821	-2.2232133
C	1.3509715	-4.2435751	-0.9456223
C	-4.7813585	1.0010119	-1.2001483
C	-4.5882735	2.3578519	-1.4625263
C	-3.3716295	2.7984379	-2.0031023
C	-2.3504865	1.8968149	-2.2441043
C	-2.5190895	0.5331469	-1.9608013
C	-3.7436635	0.1041059	-1.4573733
C	-1.3665405	-0.4217201	-2.1356003
C	2.2704435	-4.4360361	0.2635937
C	-6.7649895	2.9238279	-0.7216073
H	2.7532635	-5.0174061	-2.3915203
H	2.8811815	-3.2692861	-2.1467943
H	1.5316995	-3.9467651	-3.0926703
H	1.6851755	-4.5278461	1.1801247
H	2.8606205	-5.3472191	0.1347007
H	2.9563995	-3.5889191	0.3593037
H	0.8117735	0.4973459	3.6269827
H	-3.1335715	3.4928429	0.8570447
H	-4.7050705	2.7836649	2.6127387
H	-4.3633645	0.6345129	3.8367367
H	-1.1721575	2.1002049	0.2481257
H	-2.5510555	-1.5050611	4.0095497
H	-0.5155455	-2.3387681	2.9703827
H	-1.9682275	-1.4839661	0.0703247
H	2.4108465	0.4851459	2.8582787
H	1.6221085	-1.0409711	3.2838167
H	-5.7221245	0.6338009	-0.8090803
H	-3.2606835	3.8553449	-2.2212363
H	-1.3993385	2.2392259	-2.6419233
H	-3.9108145	-0.9553351	-1.2731313
H	-0.7375915	-0.1213231	-2.9748363
H	-1.7247295	-1.4413021	-2.3152853
H	-7.3522425	3.8340849	-0.6113603
H	-6.6690785	2.4301809	0.2535667

H	-7.2700135	2.2465219	-1.4193293
H	0.7844425	-2.2316311	-1.4641673
H	0.9161695	-6.3394891	-1.2135543
H	-0.2497875	-5.4932021	-0.1764013
H	-0.2880415	-5.2601371	-1.9400613
N	-2.1127145	-1.0286661	3.2270987
N	-0.4920315	-0.4670681	-0.9498433
N	0.6050945	-2.9728631	-0.7986883
O	0.7840615	1.2231079	-1.7467473
O	-0.5321395	-3.4369781	1.1271867
O	-5.5043065	3.3246039	-1.2176953
Au	3.2321545	1.2729509	0.2094837
P	5.3290205	2.3135159	-0.1077253
C	5.4619835	3.9814459	0.6300777
H	6.4441525	4.4162659	0.4261767
H	4.6852275	4.6243979	0.2109887
H	5.3108025	3.9151559	1.7094727
C	6.7703415	1.4146979	0.5700987
H	6.8278785	0.4244919	0.1135547
H	7.6950735	1.9621479	0.3690137
H	6.6482095	1.2919179	1.6482197
C	5.7539385	2.5738369	-1.8667363
H	6.7184925	3.0798659	-1.9608133
H	5.7976055	1.6088229	-2.3757793
H	4.9764335	3.1770949	-2.3399433

Zero-point correction= 0.631241 (Hartree/Particle)
Thermal correction to Energy= 0.670725
Thermal correction to Enthalpy= 0.671669
Thermal correction to Gibbs Free Energy= 0.555013
Sum of electronic and zero-point Energies= -1993.142636
Sum of electronic and thermal Energies= -1993.103152
Sum of electronic and thermal Enthalpies= -1993.102208
Sum of electronic and thermal Free Energies= -1993.218864

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C	1.6280465	5.2731540	0.4945043
C	0.5738095	5.9697930	-0.1291597
C	-0.4451795	5.2998700	-0.7852327
C	-0.3884375	3.9019910	-0.8031657
C	0.6662945	3.1848360	-0.1883227
C	1.6825205	3.8905110	0.4732633
C	-0.7912645	1.7176140	-1.0888947
C	0.3786285	1.7901890	-0.3804077
C	1.1339435	0.6462070	0.2193203
C	0.5347665	-0.7061370	-0.2255747

C	0.2468625	1.0323250	2.5442803
C	-0.9716335	1.6984010	2.0263753
C	0.3823395	-2.2217880	-2.2336987
C	0.8035065	-3.4862870	-1.4792747
C	1.0789875	-2.1799330	-3.5935557
C	-1.1359005	-2.1641900	-2.4078617
C	-1.9737925	2.3612310	1.7940923
H	2.4052205	5.8347870	1.0020673
H	0.5602545	7.0541380	-0.0936617
H	-1.2561475	5.8359770	-1.2680497
H	2.4897255	3.3543570	0.9646563
H	-2.1452225	3.1465530	-1.7861287
H	-1.3749245	0.8537910	-1.3771077
H	2.1663525	0.6817120	-0.1443207
H	1.3544775	-0.3346630	-2.0240267
H	0.4947355	-4.3713540	-2.0428757
H	0.3438495	-3.5173850	-0.4899127
H	1.8919565	-3.5114890	-1.3650677
H	0.7752425	-3.0418880	-4.1921947
H	0.8039015	-1.2745160	-4.1446317
H	2.1672585	-2.2075290	-3.4753377
H	-1.4923405	-3.0724900	-2.9036207
H	-1.6248265	-2.0676520	-1.4389127
H	-1.4332565	-1.3034980	-3.0143347
N	-1.2516105	2.9785050	-1.3449217
N	1.2448115	0.6898620	1.6794283
N	0.8450335	-1.0306820	-1.4961757
O	-0.1365145	-1.3933140	0.5397553
O	0.3078615	0.8117060	3.7425743
Au	-2.5595615	-0.0168790	1.8762803
P	-3.6825865	-2.0115640	1.9559183
C	-5.4954965	-1.8516230	2.0219513
H	-5.9570415	-2.8422940	2.0585663
H	-5.7756225	-1.2780340	2.9076443
H	-5.8223845	-1.3227550	1.1259563
C	-3.2298115	-3.0094580	3.4183373
H	-3.4676385	-2.4540340	4.3276613
H	-3.7718415	-3.9592000	3.4152703
H	-2.1546615	-3.1996000	3.3981433
C	-3.3229525	-3.0825570	0.5308913
H	-3.7763875	-4.0671900	0.6751543
H	-3.7324515	-2.6071340	-0.3617597
H	-2.2379055	-3.1691310	0.4332383
Sb	-4.6132005	0.3873940	-1.4257167

F	-4.2470855	-0.1067070	-3.0732277
F	-5.3742755	-1.1736540	-1.0490227
F	-6.1442005	1.1039710	-1.8872977
F	-4.8624955	0.8778450	0.2776183
F	-3.7511155	1.9352890	-1.6741327
F	-3.0447085	-0.3335320	-0.9142737
C	-3.0723685	3.2441300	1.4008333
H	-3.8032135	3.3408310	2.2059563
H	-2.6498085	4.2266340	1.1683313
H	-3.5698625	2.8442670	0.5136323
C	2.2572545	-0.1869740	2.3168813
H	2.5868925	0.3190150	3.2260563
H	1.7542175	-1.1110720	2.6254923
C	3.4258035	-0.5001890	1.4238133
C	4.4871205	0.3916960	1.2917733
C	3.4554385	-1.6842700	0.6766653
C	5.5541565	0.1322840	0.4328723
H	4.4831135	1.3128010	1.8695013
C	4.5067515	-1.9602570	-0.1817227
H	2.6333275	-2.3905160	0.7698083
C	5.5627315	-1.0502220	-0.3105557
H	6.3641675	0.8470560	0.3564873
H	4.5437015	-2.8759970	-0.7622767
O	6.5452755	-1.4055230	-1.1753047
C	7.6358565	-0.5224630	-1.3239037
H	8.1672855	-0.3816730	-0.3753237
H	8.3054975	-0.9853290	-2.0476607
H	7.3107515	0.4539040	-1.7024437

Zero-point correction= 0.648373 (Hartree/Particle)
Thermal correction to Energy= 0.697995
Thermal correction to Enthalpy= 0.698940
Thermal correction to Gibbs Free Energy= 0.559879
Sum of electronic and zero-point Energies= -2597.436046
Sum of electronic and thermal Energies= -2597.386423
Sum of electronic and thermal Enthalpies= -2597.385479
Sum of electronic and thermal Free Energies= -2597.524540

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C	0.3582400	-2.4948822	4.9080704
C	-0.3771190	-3.6856762	4.7689844
C	-1.1947600	-3.9035102	3.6709574
C	-1.2596530	-2.8918382	2.7123644
C	-0.5269980	-1.6897282	2.8323344
C	0.2948100	-1.4954252	3.9493714

C	-0.8166040	4.9137778	1.3417924
C	-1.7545150	-1.6491812	0.9243514
C	-0.8295350	-0.9094562	1.6484134
C	-0.4955660	0.5355468	1.4284654
C	-0.1717060	3.8888218	2.0164024
C	1.7419970	-0.1709702	0.9507524
C	1.0555880	-1.3772522	0.3985774
C	1.0507740	-2.3853662	-0.3538546
C	0.1987120	-3.4663052	-0.9140326
C	0.8596620	3.1648178	1.4119324
C	1.2468970	3.5103628	0.1195714
C	-0.9224980	0.9875418	0.0002844
C	1.4708110	1.9688808	2.0992034
C	-0.8870250	6.4716458	-1.9289136
C	-2.8813270	1.5420138	-1.4533996
C	-2.5889740	0.4600908	-2.4973216
C	-2.3558060	2.9052758	-1.9151316
C	-4.3850590	1.6065328	-1.1884836
C	0.6142090	4.5368368	-0.5731916
C	-0.4369290	5.2298558	0.0342174
H	-2.8617770	0.9469668	0.5990954
H	-0.4816860	3.6390108	3.0287974
H	2.0271820	2.9358468	-0.3714596
H	2.5518490	1.9256988	1.9576174
H	1.2636600	2.0101138	3.1756544
H	-1.5986490	7.2367358	-2.2370226
H	0.1330090	6.8475758	-2.0724226
H	0.9846360	-2.3588052	5.7834104
H	-0.3051210	-4.4477082	5.5377634
H	-1.7683770	-4.8176522	3.5613344
H	0.8692800	-0.5804042	4.0601144
H	-2.7002010	-3.4781272	1.2058204
H	-2.2571750	-1.4021562	0.0030184
H	-0.9821300	1.1678098	2.1812754
H	0.5736940	-3.8138492	-1.8769346
H	-0.8296950	-3.1122572	-1.0420116
H	0.1956130	-4.3141612	-0.2224716
H	-1.0306820	5.5714208	-2.5387006
H	-3.0813690	0.7257138	-3.4376216
H	-2.9905500	-0.5046622	-2.1805846
H	-1.5154160	0.3728148	-2.6727176
H	-2.8404460	3.1824608	-2.8566806
H	-2.5750690	3.6759128	-1.1681956
H	-1.2747660	2.8625638	-2.0690286

H	-4.9034700	1.8938328	-2.1063436
H	-4.6133480	2.3521528	-0.4189036
H	-4.7602290	0.6280558	-0.8776686
H	0.9229460	4.7659918	-1.5856086
H	-1.6279210	5.4733388	1.7935884
N	0.9394800	0.7033728	1.5855284
N	-2.2417090	1.1999508	-0.1602306
N	-1.9876110	-2.8254552	1.5373224
O	2.9580120	-0.0548932	0.8190404
O	-0.0791870	1.0886558	-0.8790566
O	-1.1542070	6.2113148	-0.5675706
Au	3.1874640	-2.3029822	-0.8894836
P	5.3925850	-2.2976892	-1.5231886
C	5.6945770	-1.8152572	-3.2580306
H	5.2544360	-0.8323332	-3.4376196
H	6.7676190	-1.7803532	-3.4651146
H	5.2162070	-2.5355572	-3.9245986
C	6.3288410	-1.0865722	-0.5293706
H	7.3734580	-1.0403852	-0.8488166
H	5.8586090	-0.1066112	-0.6342976
H	6.2735800	-1.3729322	0.5229234
C	6.2910870	-3.8740012	-1.3193466
H	5.8292670	-4.6387902	-1.9469086
H	7.3412470	-3.7554732	-1.5996056
H	6.2244040	-4.1938222	-0.2775776
Sb	-4.7639050	-2.8206982	-0.9942406
F	-4.4302080	-1.4158122	0.0705744
F	-5.1270930	-1.6981202	-2.3056876
F	-6.4257930	-2.8688352	-0.4310146
F	-4.9832570	-4.2267142	-2.0242986
F	-4.2496400	-3.8703692	0.3716624
F	-3.0196790	-2.7762782	-1.4358266

Zero-point correction= 0.647449 (Hartree/Particle)
Thermal correction to Energy= 0.695529
Thermal correction to Enthalpy= 0.696473
Thermal correction to Gibbs Free Energy= 0.560676
Sum of electronic and zero-point Energies= -2597.393943
Sum of electronic and thermal Energies= -2597.345863
Sum of electronic and thermal Enthalpies= -2597.344919
Sum of electronic and thermal Free Energies= -2597.480716

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C	-1.2999398	-4.5140217	2.9717737
C	-2.3266178	-5.2090877	2.3245447
C	-2.7360378	-4.8615117	1.0389917

C	-2.0639568	-3.8011187	0.4574287
C	-1.0545328	-3.0792767	1.0861457
C	-0.6529778	-3.4373847	2.3632217
C	-0.4171758	4.6728673	1.7838487
C	-1.4554338	-2.2320377	-1.0325763
C	-0.6175278	-1.9630317	0.1691877
C	-1.0194858	-0.5481697	0.7521417
C	-0.5072288	3.3747673	2.2635317
C	1.3281282	-0.7061797	0.8763027
C	0.9062282	-1.8385507	-0.0010143
C	1.7459812	-2.6267877	-0.6864073
C	1.2461772	-3.8016967	-1.4801793
C	0.2683072	2.3479413	1.7176637
C	1.1235062	2.6493233	0.6595777
C	-1.3308588	0.4458643	-0.3911933
C	0.2539712	0.9670673	2.3419707
C	1.2486392	6.5698383	-0.8157463
C	-2.9238408	2.1774903	-1.2262793
C	-3.3364528	1.5249223	-2.5477073
C	-1.8015868	3.1951673	-1.4397703
C	-4.1093448	2.8865683	-0.5685493
C	1.2199092	3.9466483	0.1607467
C	0.4516662	4.9655463	0.7281847
H	-3.1854378	0.7503593	0.3435987
H	-1.1880018	3.1567123	3.0828567
H	1.7276372	1.8612993	0.2205977
H	1.1726542	0.8207423	2.9194887
H	-0.5954308	0.8781313	3.0285537
H	1.0945262	7.6303733	-1.0126123
H	2.3143742	6.3877553	-0.6312603
H	-1.0065968	-4.8148447	3.9718427
H	-2.8185248	-6.0303617	2.8335957
H	-3.5520128	-5.3609057	0.5312517
H	0.1391822	-2.8942147	2.8686207
H	-3.0399208	-3.4568237	-1.4308873
H	-1.5021198	-1.6298347	-1.9326603
H	-1.8484618	-0.6483597	1.4550477
H	1.3193192	-3.5855267	-2.5522703
H	0.2116472	-4.0857727	-1.2527083
H	1.8742022	-4.6782917	-1.3006523
H	0.9314582	5.9865163	-1.6888843
H	-3.6761278	2.2924753	-3.2499543
H	-4.1421398	0.8082873	-2.3841353
H	-2.4802048	1.0069473	-2.9888383

H	-2.1835058	4.0127633	-2.0593923
H	-1.4876798	3.6067233	-0.4774363
H	-0.9369608	2.7470923	-1.9289863
H	-4.4722388	3.6748263	-1.2334183
H	-3.7937758	3.3514493	0.3714637
H	-4.9283028	2.1917683	-0.3758813
H	1.8868782	4.1462743	-0.6689583
H	-1.0161288	5.4764603	2.1979087
N	0.1995132	-0.1483607	1.4159707
N	-2.4784258	1.1323463	-0.2751093
N	-2.2453758	-3.2337207	-0.8308843
O	2.4635712	-0.3408967	1.1507697
O	-0.5046188	0.5621593	-1.2914043
O	0.4677272	6.2605743	0.3161167
Au	3.7546512	-2.1718837	-0.6534203
P	5.9831162	-1.4581227	-0.4748403
C	7.0761152	-1.5310197	-1.9422453
H	6.6125232	-0.9788457	-2.7623073
H	8.0568902	-1.1009097	-1.7210583
H	7.1960202	-2.5709727	-2.2529873
C	6.0138982	0.3046203	0.0150997
H	7.0313922	0.6460203	0.2246747
H	5.5839502	0.9032773	-0.7910903
H	5.3811942	0.4291653	0.8969957
C	6.9675242	-2.2830307	0.8307177
H	7.0741612	-3.3431267	0.5915307
H	7.9573842	-1.8271637	0.9218257
H	6.4363582	-2.1960287	1.7809287
Sb	-5.2016708	-1.6704997	-0.4678053
F	-3.7490478	-1.4295627	0.5697947
F	-5.3906128	0.0892833	-0.4568643
F	-6.1841838	-1.8948307	0.9672787
F	-6.5596108	-1.8760667	-1.5558133
F	-4.8246808	-3.4237597	-0.5043853
F	-4.0755848	-1.5558257	-1.8632183

Zero-point correction= 0.650906 (Hartree/Particle)
Thermal correction to Energy= 0.698267
Thermal correction to Enthalpy= 0.699211
Thermal correction to Gibbs Free Energy= 0.566803
Sum of electronic and zero-point Energies= -2597.437423
Sum of electronic and thermal Energies= -2597.390062
Sum of electronic and thermal Enthalpies= -2597.389118
Sum of electronic and thermal Free Energies= -2597.521526

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C	2.9538962	1.2741175	3.6223789
C	2.1564652	2.2554145	4.2088859
C	0.9342462	2.6316175	3.6438769
C	0.5570902	1.9822595	2.4823749
C	1.3387652	0.9875495	1.8858529
C	2.5492272	0.6265085	2.4503859
N	-0.6194588	2.1406835	1.7118229
C	-0.5537158	1.4358735	0.5867599
C	0.6202812	0.4732505	0.6585539
N	0.2468742	2.6151005	-0.8670031
C	0.9921782	1.6191575	-1.5676861
C	1.4719322	0.4946605	-0.6373761
O	1.1425032	1.6037055	-2.7597201
N	1.2717792	-0.7809335	-1.2680751
C	0.4472702	-1.6343935	-0.5530241
C	-0.0226138	-0.9294355	0.6701529
O	0.2300432	-2.7835425	-0.8902631
C	-1.0098328	-1.3955705	1.4630439
C	5.9047972	-0.7429425	-1.3684771
C	6.0830592	-1.6680465	-0.3360961
C	5.0158072	-2.4791305	0.0626419
C	3.7853442	-2.3562935	-0.5790711
C	3.5966872	-1.4406565	-1.6146961
C	4.6714592	-0.6330785	-1.9952491
C	2.2278782	-1.2920845	-2.2403561
O	7.3225492	-1.7047825	0.2185549
C	7.5525112	-2.6517265	1.2379489
C	-0.6485808	3.5625645	-1.6098601
C	-1.4900958	4.2816435	-0.5520191
C	-1.5760368	2.7756365	-2.5380811
C	0.2096032	4.5614725	-2.3891091
H	3.8970892	1.0052135	4.0849089
H	2.4881592	2.7403005	5.1206129
H	0.3110782	3.3939485	4.0983129
H	3.1608042	-0.1495305	1.9966699
H	-1.4957248	2.5606405	2.0067489
H	-1.4594838	1.2017755	0.0412629
H	2.5382082	0.6579935	-0.4118621
H	6.7482082	-0.1254605	-1.6572441
H	5.1328272	-3.2083095	0.8551639
H	2.9544522	-2.9903565	-0.2766611
H	4.5381822	0.0901775	-2.7962931
H	2.2589472	-0.6244655	-3.1044971
H	1.8280232	-2.2590725	-2.5556491

H	8.5946952	-2.5348295	1.5329669
H	7.3891652	-3.6744425	0.8781729
H	6.9075892	-2.4708725	2.1064959
H	-0.8609308	4.7296075	0.2270049
H	-2.2194108	3.6069945	-0.0949811
H	-2.0498898	5.0865325	-1.0342081
H	-1.0337218	2.3389105	-3.3763741
H	-2.1161418	1.9929755	-1.9986831
H	-2.3304658	3.4643835	-2.9262971
H	0.8390462	4.0470525	-3.1171161
H	0.8442802	5.1443025	-1.7121311
H	-0.4414298	5.2599515	-2.9217071
H	0.8449882	3.1095795	-0.2001061
Sb	-4.4534338	1.0721745	0.2240009
F	-3.2559108	1.9428885	1.2605939
F	-4.4386768	-0.2465135	1.4100419
F	-5.7798378	1.8655845	1.0537089
F	-5.5391848	0.1439255	-0.8171391
F	-3.0507988	0.3152805	-0.6072981
F	-4.3290108	2.4018415	-0.9374781
Au	-2.4271588	-2.6615455	0.6614699
P	-4.3480508	-3.4761475	-0.3903431
C	-4.5398098	-2.7132235	-2.0407291
H	-3.6755788	-2.9634275	-2.6594361
H	-5.4578008	-3.0584965	-2.5250351
H	-4.5845308	-1.6299835	-1.9062751
C	-4.5315008	-5.2729325	-0.7013911
H	-4.5253548	-5.8080085	0.2505769
H	-5.4654068	-5.4823985	-1.2306371
H	-3.6868038	-5.6220415	-1.2989771
C	-5.8897998	-3.0047665	0.4691759
H	-6.7656758	-3.3315905	-0.0983001
H	-5.9049338	-3.4497965	1.4661269
H	-5.8942078	-1.9180275	0.5703769
C	-1.4177858	-0.7047595	2.7383919
H	-0.6287108	-0.1034175	3.2001259
H	-2.2915868	-0.0708085	2.5372139
H	-1.7489098	-1.4454125	3.4696559

Zero-point correction= 0.650099 (Hartree/Particle)
Thermal correction to Energy= 0.697294
Thermal correction to Enthalpy= 0.698238
Thermal correction to Gibbs Free Energy= 0.565210
Sum of electronic and zero-point Energies= -2597.413165
Sum of electronic and thermal Energies= -2597.365970

Sum of electronic and thermal Enthalpies= -2597.365026
Sum of electronic and thermal Free Energies= -2597.498054

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C	-2.1316608	-1.7734170	4.3937523
C	-1.3082878	-2.8576010	4.6959433
C	-0.3412858	-3.3060240	3.7945763
C	-0.2145738	-2.6279890	2.5908583
C	-1.0256518	-1.5313680	2.2849873
C	-1.9903088	-1.0975740	3.1801133
N	0.6948122	-2.9153500	1.5406663
C	0.3891782	-2.0384190	0.4500313
C	-0.5932278	-0.9380540	0.9674523
N	-0.3867068	-2.8546000	-0.6024307
C	-1.7135528	-2.1535950	-0.8250707
C	-1.6971468	-0.8343760	-0.0936457
O	-2.5740678	-2.6570140	-1.4743277
N	-1.2140688	0.1775530	-1.0010267
C	-0.3229068	1.0538540	-0.3575307
C	0.0876352	0.4310140	0.9261633
O	-0.0136108	2.1211890	-0.8500617
C	1.0745622	0.9333710	1.6977443
C	-5.7507088	0.9584160	-1.1533957
C	-5.7783648	2.2145410	-0.5393967
C	-4.6039308	2.9652640	-0.4375367
C	-3.4158088	2.4548600	-0.9555927
C	-3.3787708	1.2079560	-1.5786437
C	-4.5600238	0.4641820	-1.6639777
C	-2.0677068	0.6543480	-2.0835257
O	-6.9882798	2.6161800	-0.0720797
C	-7.0606708	3.8810520	0.5479413
C	0.4211932	-3.2606390	-1.8648697
C	1.6496692	-4.0131360	-1.3558057
C	0.7900512	-2.0032140	-2.6406047
C	-0.4445308	-4.1978860	-2.7069227
H	-2.8777218	-1.4471660	5.1098503
H	-1.4226298	-3.3675730	5.6468513
H	0.2967052	-4.1519280	4.0268913
H	-2.6012318	-0.2286710	2.9520363
H	1.6873212	-2.9309910	1.7643793
H	1.2693692	-1.6209350	-0.0275017
H	-2.7012858	-0.6211300	0.2982653
H	-6.6752958	0.3952300	-1.2154817
H	-4.6024588	3.9397500	0.0352003
H	-2.4975718	3.0311730	-0.8738247

H	-4.5421688	-0.5166750	-2.1337327
H	-2.2491428	-0.1697690	-2.7840907
H	-1.4831438	1.4216010	-2.5961137
H	-8.1003058	4.0156160	0.8443803
H	-6.7733998	4.6822000	-0.1433097
H	-6.4205848	3.9282820	1.4370163
H	1.3546482	-4.9082580	-0.7976207
H	2.3040612	-3.3985830	-0.7389847
H	2.2365372	-4.3237280	-2.2230177
H	-0.1043928	-1.4593930	-2.9614517
H	1.4439592	-1.3312740	-2.0814517
H	1.3367252	-2.3166980	-3.5334817
H	-1.2853558	-3.6874920	-3.1749397
H	-0.8291028	-5.0345900	-2.1143917
H	0.1911552	-4.6116350	-3.4932707
H	-0.6108878	-3.7400480	-0.1275657
Sb	4.2263662	-0.9274440	-0.2890997
F	3.2908022	-2.0560880	0.7612583
F	4.4147422	0.1346390	1.1148953
F	5.7128322	-1.7838610	0.0803513
F	5.0613192	0.2625910	-1.2998907
F	2.6590862	-0.1605770	-0.7091917
F	3.9338782	-2.0090540	-1.6671227
Au	2.3229272	2.3981870	0.9413013
P	4.0039552	3.5946440	-0.1498407
C	3.9476662	3.2461350	-1.9440057
H	2.9660682	3.5246660	-2.3333677
H	4.7327552	3.7899130	-2.4774047
H	4.0910812	2.1707070	-2.0735737
C	4.0427072	5.4248140	-0.0504167
H	4.1654492	5.7288070	0.9912763
H	4.8647632	5.8301780	-0.6472537
H	3.0947262	5.8240630	-0.4172507
C	5.6914612	3.0824600	0.3292633
H	6.4425882	3.5998850	-0.2743147
H	5.8516362	3.2974010	1.3876793
H	5.7655272	2.0045770	0.1747943
C	1.5795902	0.2287560	2.9292003
H	0.8835362	-0.4777480	3.3875103
H	2.4960202	-0.3041530	2.6407503
H	1.8834692	0.9556620	3.6860303

Zero-point correction= 0.652051 (Hartree/Particle)
Thermal correction to Energy= 0.699432
Thermal correction to Enthalpy= 0.700376

Thermal correction to Gibbs Free Energy= 0.568239
Sum of electronic and zero-point Energies= -2597.427785
Sum of electronic and thermal Energies= -2597.380404
Sum of electronic and thermal Enthalpies= -2597.379460
Sum of electronic and thermal Free Energies= -2597.511597

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C	-0.4750192	-0.1436298	1.8761915
C	-1.4650012	-1.0986438	-0.1598735
C	-0.4344772	-1.3962788	0.9701865
C	-1.0340282	-2.6056028	1.6487725
C	-2.2946472	-2.8907308	1.1349425
C	-1.6334252	0.7197612	1.3822185
C	-1.2644872	-4.4412998	3.1617815
C	-2.3416752	1.2041132	-1.0197275
C	-0.9831482	1.8448202	-1.2958135
C	-2.8657002	0.4672422	-2.2522075
C	-3.3780922	2.2457902	-0.5953705
C	-0.5046712	-3.3799298	2.6704875
C	-2.5316372	-4.7073968	2.6401275
C	-3.0748092	-3.9319838	1.6158695
C	1.7025508	-0.2422588	0.9682915
C	1.0096748	-1.4743488	0.4954475
C	1.5942578	-2.4275778	-0.2538085
H	-1.0491172	-1.1607678	-1.1624875
H	-0.6340482	-0.3741068	2.9369865
H	-0.6352412	2.4227712	-0.4357805
H	-1.0711432	2.5285362	-2.1443905
H	-0.2228732	1.0945362	-1.5463285
H	-3.8522602	0.0412962	-2.0833185
H	-2.9514052	1.2031952	-3.0554595
H	-2.1921202	-0.3146498	-2.6128155
H	-4.2940122	1.7498972	-0.2683375
H	-3.0042142	2.8977252	0.1931775
H	-3.6085752	2.8568432	-1.4724595
H	0.4881708	-3.1701658	3.0585065
H	-0.8664592	-5.0668258	3.9534935
H	-3.1107262	-5.5340588	3.0376795
H	-4.0641762	-4.1085438	1.2115335
N	-2.1450162	0.2014292	0.1236395
N	-2.6374312	-1.9700468	0.0900065
N	0.7897978	0.5211882	1.6581475
O	-2.0758992	1.6769632	1.9461825
O	2.8647978	0.1022932	0.8019915
H	-3.1027422	-0.6747988	0.3253575

H	-3.1294042	-2.3515238	-0.7277655
Au	3.5947178	-2.2594838	-0.7117425
P	5.8815908	-1.9053258	-1.1295315
C	6.5732268	-2.3940188	-2.7527765
H	6.0111368	-1.8986048	-3.5470905
H	7.6287628	-2.1179468	-2.8262455
H	6.4692788	-3.4735208	-2.8802935
C	6.2752428	-0.1228578	-0.9999285
H	5.9112318	0.2444322	-0.0377125
H	7.3497418	0.0578472	-1.0919815
H	5.7431618	0.4163062	-1.7868185
C	7.0225968	-2.6851818	0.0719515
H	8.0592958	-2.4050598	-0.1344575
H	6.7512248	-2.3632738	1.0795655
H	6.9203188	-3.7710178	0.0184055
C	0.8147698	-3.6186078	-0.7473595
H	-0.2710762	-3.5420798	-0.6231815
H	1.0318218	-3.8003188	-1.8036105
H	1.1418518	-4.5156528	-0.2084255
C	1.1725218	1.7507732	2.3467545
H	2.2233038	1.6313012	2.6282965
H	0.5690248	1.8288802	3.2568155
C	0.9940798	2.9829602	1.4893125
C	-0.0262522	3.8953412	1.7312095
C	1.8316658	3.1870382	0.3828585
C	-0.2428782	4.9842982	0.8838215
H	-0.6904932	3.7456912	2.5771315
C	1.6306098	4.2616412	-0.4655225
H	2.6286558	2.4741642	0.1887985
C	0.5850478	5.1636692	-0.2242995
H	-1.0536932	5.6701772	1.0962255
H	2.2636238	4.4312182	-1.3297615
O	0.4596928	6.1737392	-1.1217715
C	-0.5965292	7.0888242	-0.9278585
H	-0.5365122	7.8021462	-1.7489605
H	-1.5702442	6.5850332	-0.9537345
H	-0.4938412	7.6220202	0.0246715
Sb	-6.0074342	-1.6402978	-0.9425235
F	-4.5274322	-2.1427708	-1.8556575
F	-4.9596922	-0.4207128	-0.1167485
F	-5.4632032	-2.8001998	0.2952905
F	-7.3652382	-1.1311208	0.0444715
F	-6.9467722	-2.8684798	-1.7701125
F	-6.3084692	-0.4342038	-2.1925505

Zero-point correction= 0.646907 (Hartree/Particle)
Thermal correction to Energy= 0.693275
Thermal correction to Enthalpy= 0.694219
Thermal correction to Gibbs Free Energy= 0.563456
Sum of electronic and zero-point Energies= -2597.393489
Sum of electronic and thermal Energies= -2597.347121
Sum of electronic and thermal Enthalpies= -2597.346176
Sum of electronic and thermal Free Energies= -2597.476939

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C	-2.1759597	-1.8401669	4.1774843
C	-1.3992307	-2.9708479	4.4379533
C	-0.3909327	-3.3584129	3.5559303
C	-0.2200557	-2.5775659	2.4283663
C	-0.9746827	-1.4526319	2.1421873
C	-1.9707287	-1.0711059	3.0330793
N	0.8169193	-2.7572569	1.4087543
C	0.4261943	-1.8491119	0.2259843
C	-0.5470347	-0.8056379	0.8543253
N	-0.2950377	-2.5918539	-0.7626117
C	-1.5031077	-1.9676859	-1.0651247
C	-1.6680007	-0.7299049	-0.1895857
O	-2.2711067	-2.2790339	-1.9479917
N	-1.3204627	0.4304411	-0.9792647
C	-0.4301357	1.2810831	-0.3406887
C	0.0865543	0.5837601	0.8727893
O	-0.1672357	2.3963111	-0.7544567
C	1.0910263	1.0609481	1.6315203
C	-5.8708697	0.7811151	-1.0216937
C	-6.0249297	2.0164421	-0.3844687
C	-4.9409167	2.8928701	-0.2923527
C	-3.7154407	2.5261361	-0.8454317
C	-3.5542357	1.3038741	-1.4947227
C	-4.6452567	0.4315021	-1.5687487
C	-2.2020387	0.9061891	-2.0365697
O	-7.2632137	2.2725091	0.1163643
C	-7.4642387	3.5161031	0.7483633
C	0.4804853	-3.3270169	-1.8208247
C	1.6575163	-4.0641229	-1.1714537
C	1.0065583	-2.2982859	-2.8264997
C	-0.4126517	-4.3705769	-2.4989057
H	-2.9509627	-1.5546519	4.8805083
H	-1.5758777	-3.5525789	5.3355173
H	0.2303113	-4.2260249	3.7526463
H	-2.5657487	-0.1842229	2.8391163

H	1.7612643	-2.4498439	1.7095633
H	1.3525763	-1.4076449	-0.1381537
H	-2.6844007	-0.6672439	0.2213043
H	-6.7282697	0.1190131	-1.0737937
H	-5.0379927	3.8534851	0.1987023
H	-2.8643957	3.1988031	-0.7699407
H	-4.5189687	-0.5337679	-2.0538707
H	-2.3063897	0.1196161	-2.7893127
H	-1.6886347	1.7611761	-2.4817017
H	-8.5067307	3.5328021	1.0648423
H	-7.2806187	4.3497511	0.0599623
H	-6.8170357	3.6297641	1.6265913
H	1.3040233	-4.8724239	-0.5155317
H	2.3511203	-3.4040639	-0.6445427
H	2.2443803	-4.5368109	-1.9619447
H	0.1738773	-1.7353299	-3.2584697
H	1.7108123	-1.6054519	-2.3559777
H	1.5346813	-2.8099999	-3.6357287
H	-1.1800887	-3.9127199	-3.1180477
H	-0.9031857	-4.9996269	-1.7499297
H	0.2198573	-5.0081069	-3.1230537
Sb	4.3482053	-0.8833559	-0.1396387
F	3.2939713	-1.8817019	0.9632473
F	4.4598103	0.3054341	1.1704833
F	5.7602493	-1.7325509	0.4640283
F	5.2944763	0.1639981	-1.1983717
F	2.8395913	-0.1308509	-0.7328047
F	4.1216173	-2.1224679	-1.3855177
Au	2.3192163	2.5380761	0.8713903
P	4.0255523	3.6652601	-0.2533957
C	4.0500333	3.1337651	-2.0033007
H	3.0858603	3.3610181	-2.4629487
H	4.8550453	3.6285501	-2.5543327
H	4.2055073	2.0522911	-2.0205227
C	4.0449933	5.4959481	-0.3398737
H	4.1260913	5.9058691	0.6690683
H	4.8852553	5.8485461	-0.9447307
H	3.1077483	5.8434821	-0.7795247
C	5.6979573	3.2232011	0.3373703
H	6.4675533	3.6896691	-0.2840967
H	5.8161123	3.5395901	1.3756843
H	5.7885803	2.1364001	0.2911383
C	1.6405433	0.3153401	2.8202413
H	1.0173823	-0.5017799	3.1995783

H	2.6320083	-0.0717249	2.5560073
H	1.8079073	1.0094081	3.6485403
H	0.8973753	-3.7233789	1.0818223

Zero-point correction= 0.653477 (Hartree/Particle)
Thermal correction to Energy= 0.700757
Thermal correction to Enthalpy= 0.701701
Thermal correction to Gibbs Free Energy= 0.568785
Sum of electronic and zero-point Energies= -2597.444015
Sum of electronic and thermal Energies= -2597.396736
Sum of electronic and thermal Enthalpies= -2597.395792
Sum of electronic and thermal Free Energies= -2597.528708

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C	-2.7410770	1.0237373	3.9147397
C	-1.9877370	2.0828773	4.4182327
C	-0.8383650	2.5330093	3.7618217
C	-0.4862150	1.8754763	2.5970877
C	-1.2228630	0.8032343	2.0830507
C	-2.3623630	0.3700523	2.7374287
N	0.6227480	2.0979513	1.7466317
C	0.5418800	1.3514043	0.6492807
C	-0.5430140	0.3019353	0.8284787
C	-1.4703900	0.2076063	-0.4096953
N	-1.1944620	-1.0664857	-1.0159523
C	-0.2514970	-1.8198487	-0.3355813
C	0.2157600	-1.0423797	0.8442977
O	0.0601690	-2.9485007	-0.6657583
C	-1.1537090	1.3397033	-1.3978213
C	1.2815120	-1.3986017	1.5908837
Au	2.7510270	-2.5784137	0.7504727
C	1.7028220	-0.6333057	2.8184957
C	-4.9519640	-2.6278787	0.3731087
C	-6.0315790	-1.9153597	-0.1698043
C	-5.8439980	-1.1326477	-1.3072363
C	-4.5758870	-1.0685417	-1.8921023
C	-3.5014070	-1.7780887	-1.3718913
C	-3.7057760	-2.5574827	-0.2231403
C	-2.1160610	-1.6710317	-1.9659983
O	-7.2134060	-2.0512067	0.4852627
C	-8.3324090	-1.3784937	-0.0470333
H	-3.6279300	0.6976953	4.4467347
H	-2.2970640	2.5709473	5.3361197
H	-0.2493520	3.3559993	4.1514407
H	-2.9399880	-0.4645597	2.3482097
H	1.4805070	2.5928213	1.9714837

H	-2.5315750	0.2848533	-0.1236943
H	2.5048270	0.0649173	2.5438867
H	0.8939410	-0.0849437	3.3108437
H	2.1399690	-1.3175547	3.5489137
H	-5.1294190	-3.2354617	1.2539577
H	-6.6615740	-0.5710437	-1.7423203
H	-4.4275550	-0.4486647	-2.7729743
H	-2.8709090	-3.1183117	0.1923517
H	-1.6951930	-2.6572407	-2.1803933
H	-2.1338950	-1.0876787	-2.8894783
H	-9.1734670	-1.6258617	0.5996397
H	-8.5491760	-1.7112897	-1.0691053
H	-8.1831840	-0.2918807	-0.0485213
P	4.6733790	-3.2866567	-0.3723553
C	4.9865660	-5.0765127	-0.6112133
H	4.1439490	-5.5201667	-1.1457003
H	5.9064790	-5.2374627	-1.1804733
H	5.0719660	-5.5628687	0.3628137
C	6.2133020	-2.6538767	0.3806477
H	7.0827950	-2.9323617	-0.2213953
H	6.1318170	-1.5670857	0.4406547
H	6.3174780	-3.0533737	1.3914877
C	4.7200940	-2.5954497	-2.0643943
H	5.6351560	-2.8967737	-2.5824953
H	3.8463900	-2.9396157	-2.6215993
H	4.6896910	-1.5064007	-1.9836093
N	-0.4396520	2.4114073	-0.7788123
H	-1.0295620	2.8840113	-0.0890063
C	0.3294210	3.3958353	-1.6102593
C	1.1819730	4.2131613	-0.6358783
C	1.2497650	2.6456893	-2.5751003
C	-0.6519530	4.3007383	-2.3585633
H	0.5730950	4.6422093	0.1694537
H	1.9889300	3.6116603	-0.2082783
H	1.6460690	5.0386403	-1.1808083
H	0.6867970	2.1357413	-3.3566643
H	1.9188130	3.3737383	-3.0404543
H	1.8858730	1.9289043	-2.0488983
H	-0.0924800	5.0276253	-2.9535763
H	-1.2865190	3.7167403	-3.0270793
H	-1.2837130	4.8571443	-1.6570213
O	-1.3943070	1.2811903	-2.5738563
H	1.4276040	1.1684173	0.0537557
Sb	4.4276510	1.2799433	0.0517807

F	5.5154280	0.3926663	-1.0225583
F	4.5983590	0.0190343	1.2879087
F	3.2338210	2.0960343	1.1361477
F	3.0406990	0.3805063	-0.6529323
F	5.7370720	2.2128233	0.7526847
F	4.1170540	2.5432773	-1.1487083

Zero-point correction= 0.650104 (Hartree/Particle)
Thermal correction to Energy= 0.697295
Thermal correction to Enthalpy= 0.698239
Thermal correction to Gibbs Free Energy= 0.565293
Sum of electronic and zero-point Energies= -2597.413313
Sum of electronic and thermal Energies= -2597.366122
Sum of electronic and thermal Enthalpies= -2597.365178
Sum of electronic and thermal Free Energies= -2597.498124

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C	2.0842189	1.6355261	-4.4302085
C	1.3112249	2.7631001	-4.7053015
C	0.3804109	3.2456311	-3.7836305
C	0.2374709	2.5575531	-2.5874595
C	0.9981789	1.4185431	-2.3085325
C	1.9272559	0.9503771	-3.2237045
N	-0.6430511	2.8731481	-1.5206925
C	-0.3672801	1.9653271	-0.4474675
C	0.5564909	0.8280931	-0.9928635
C	1.6699749	0.6600001	0.0497275
N	1.1570589	-0.3430869	0.9501525
C	0.2125309	-1.1660669	0.3115945
C	-0.1855431	-0.5087789	-0.9586485
O	-0.1417191	-2.2222659	0.7974825
C	1.7551799	1.9658811	0.8000265
C	-1.2023441	-0.9575229	-1.7244305
Au	-2.5049641	-2.3766449	-0.9714725
C	-1.6882141	-0.2192219	-2.9435075
C	4.3915369	-3.2499499	0.2517855
C	5.6136709	-2.5730169	0.3689075
C	5.6680569	-1.3458199	1.0281895
C	4.4970599	-0.8096619	1.5694735
C	3.2820629	-1.4775989	1.4697025
C	3.2413479	-2.7068589	0.7945075
C	2.0075409	-0.8744479	2.0093605
O	6.6836579	-3.1910639	-0.1935685
C	7.9347519	-2.5495899	-0.0901625
H	2.8021349	1.2825011	-5.1622035
H	1.4365429	3.2799861	-5.6510865

H	-0.2188981	4.1245841	-3.9953865
H	2.4968819	0.0486991	-3.0167995
H	-1.6365571	2.9389411	-1.7311035
H	2.6579349	0.4088611	-0.3603215
H	-2.5881671	0.3355511	-2.6454305
H	-0.9725961	0.4727131	-3.3936875
H	-2.0149601	-0.9261239	-3.7098965
H	4.3805949	-4.2019689	-0.2674315
H	6.5997559	-0.8024819	1.1268985
H	4.5380229	0.1525201	2.0751205
H	2.2918079	-3.2281229	0.7023585
H	1.3985899	-1.6234199	2.5209475
H	2.2391299	-0.0710069	2.7190725
H	8.6527569	-3.1988829	-0.5898275
H	8.2311899	-2.4180899	0.9574285
H	7.9248839	-1.5708749	-0.5850325
P	-4.2253851	-3.5172909	0.1171875
C	-4.3427541	-5.3422419	-0.0100335
H	-3.4095431	-5.7872579	0.3416025
H	-5.1762131	-5.7216409	0.5880595
H	-4.4873711	-5.6241279	-1.0551205
C	-5.8927201	-2.9261369	-0.3410575
H	-6.6614471	-3.4211799	0.2591315
H	-5.9194291	-1.8489789	-0.1673875
H	-6.0687961	-3.1158709	-1.4017515
C	-4.1419561	-3.1991429	1.9159855
H	-4.9464961	-3.7162359	2.4469235
H	-3.1709841	-3.5261689	2.2941115
H	-4.2373531	-2.1205229	2.0621925
N	0.4569679	2.7274561	0.6092715
H	0.7128069	3.6113331	0.1477055
C	-0.3159851	3.1441501	1.8900165
C	-1.5178411	3.9574891	1.4118815
C	-0.7298881	1.8901321	2.6482855
C	0.6006629	4.0272411	2.7366585
H	-1.1927341	4.8491361	0.8649665
H	-2.2064371	3.3826051	0.7938695
H	-2.0789261	4.2774621	2.2926805
H	0.1430169	1.2995471	2.9446825
H	-1.2476751	2.2111771	3.5556115
H	-1.4222851	1.2598441	2.0868525
H	-0.0056991	4.4524681	3.5398635
H	1.4251379	3.4723571	3.1827555
H	1.0125929	4.8580201	2.1542705

O	2.6468899	2.4215661	1.4425945
H	-1.2611591	1.5822571	0.0334255
Sb	-4.2459871	1.0159521	0.3028815
F	-5.1188651	-0.1615019	1.2964755
F	-4.4717931	-0.0167089	-1.1180515
F	-3.2714791	2.1289661	-0.7290275
F	-2.7050371	0.1900731	0.7067375
F	-5.7030311	1.9256901	-0.0548915
F	-3.9184171	2.0651121	1.6977605

Zero-point correction= 0.652155 (Hartree/Particle)
Thermal correction to Energy= 0.699428
Thermal correction to Enthalpy= 0.700372
Thermal correction to Gibbs Free Energy= 0.568803
Sum of electronic and zero-point Energies= -2597.427556
Sum of electronic and thermal Energies= -2597.380283
Sum of electronic and thermal Enthalpies= -2597.379339
Sum of electronic and thermal Free Energies= -2597.510908

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C	-1.8996631	1.5863816	4.4098570
C	-1.2377421	2.8051356	4.5716550
C	-0.4135481	3.3112556	3.5676480
C	-0.2697411	2.5499216	2.4191030
C	-0.9100691	1.3282676	2.2452090
C	-1.7418851	0.8391076	3.2437100
N	0.5020419	2.9033896	1.2531140
C	0.3840689	1.7713156	0.2870630
C	-0.5319641	0.6945656	0.9317650
C	-1.6982041	0.5683566	-0.0614200
N	-1.2896511	-0.5167344	-0.9241180
C	-0.3488721	-1.3564484	-0.3103830
C	0.1561089	-0.6637034	0.9008450
O	-0.0577471	-2.4463184	-0.7629440
C	-1.7040261	1.8498106	-0.8809500
C	1.2244439	-1.0651514	1.6189890
Au	2.5486319	-2.4470404	0.8562960
C	1.7272109	-0.2160124	2.7667100
C	-4.7256641	-3.1227084	-0.0328840
C	-5.8893371	-2.3498214	-0.1502010
C	-5.8579851	-1.1489174	-0.8574390
C	-4.6613011	-0.7347864	-1.4473670
C	-3.5048381	-1.4997674	-1.3488110
C	-3.5489021	-2.6997354	-0.6241030
C	-2.1995351	-1.0268404	-1.9419750
O	-6.9930381	-2.8525534	0.4618250

C	-8.1883751	-2.1130674	0.3563440
H	-2.5350251	1.2128116	5.2054240
H	-1.3655491	3.3686896	5.4893970
H	0.0999869	4.2597746	3.6829070
H	-2.2299571	-0.1235314	3.1233600
H	1.4773999	3.1711256	1.4197590
H	-2.6829941	0.4033456	0.3952530
H	2.1799269	0.7029406	2.3666670
H	0.9353849	0.0708836	3.4657460
H	2.5157469	-0.7210474	3.3237310
H	-4.7811231	-4.0514934	0.5242810
H	-6.7430721	-0.5325004	-0.9560650
H	-4.6316971	0.2089096	-1.9869590
H	-2.6438261	-3.2955004	-0.5329240
H	-1.6629721	-1.8465554	-2.4256570
H	-2.3823831	-0.2415124	-2.6840890
H	-8.9464971	-2.6794814	0.8961390
H	-8.4967291	-1.9983544	-0.6898020
H	-8.0863561	-1.1196334	0.8098990
P	4.3646689	-3.4820634	-0.1827780
C	4.5078069	-5.3092434	-0.1916300
H	3.6248119	-5.7365034	-0.6715280
H	5.4056369	-5.6265604	-0.7296270
H	4.5521399	-5.6740264	0.8367270
C	5.9616629	-2.9048824	0.4927850
H	6.8001339	-3.3236244	-0.0709440
H	5.9733869	-1.8153714	0.4236540
H	6.0388729	-3.1929174	1.5431940
C	4.4605759	-3.0171624	-1.9485220
H	5.3344549	-3.4699884	-2.4258300
H	3.5493639	-3.3374444	-2.4578700
H	4.5377399	-1.9285364	-1.9986790
N	-0.4078231	2.5125776	-0.7436740
H	-0.2338201	3.3733956	0.2207280
C	0.3324089	2.9591756	-2.0049420
C	1.5203179	3.8106816	-1.5537670
C	0.7978559	1.7185976	-2.7637610
C	-0.5999371	3.8190416	-2.8597110
H	1.1770419	4.7249976	-1.0563410
H	2.2162709	3.2740096	-0.9078730
H	2.0920399	4.1006636	-2.4379140
H	-0.0474131	1.0630856	-2.9985350
H	1.2550769	2.0374726	-3.7041870
H	1.5486279	1.1527616	-2.2057810

H	0.0078489	4.2920316	-3.6353020
H	-1.3838271	3.2353306	-3.3395480
H	-1.0700131	4.6063546	-2.2638280
O	-2.5949361	2.2628586	-1.5656320
H	1.3407559	1.3976676	-0.0641430
Sb	4.3380639	1.1003336	-0.1012970
F	5.3458759	-0.0384374	-1.0071190
F	4.4467499	0.0669466	1.3295560
F	3.2164279	2.1875706	0.8166260
F	2.8689329	0.2233416	-0.6457510
F	5.7087829	2.0632946	0.4204760
F	4.1227569	2.1378016	-1.5218370

Zero-point correction= 0.647786 (Hartree/Particle)
Thermal correction to Energy= 0.694614
Thermal correction to Enthalpy= 0.695558
Thermal correction to Gibbs Free Energy= 0.564692
Sum of electronic and zero-point Energies= -2597.399748
Sum of electronic and thermal Energies= -2597.352920
Sum of electronic and thermal Enthalpies= -2597.351976
Sum of electronic and thermal Free Energies= -2597.482843

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C	-2.1723606	1.5715315	4.2343820
C	-1.4781566	2.7593715	4.4729630
C	-0.5144846	3.2121225	3.5722990
C	-0.3027226	2.4350945	2.4488960
C	-0.9759296	1.2547675	2.1843470
C	-1.9275586	0.8087055	3.0936380
N	0.7042004	2.6801955	1.4128010
C	0.3705864	1.7289385	0.2460670
C	-0.5206996	0.6270415	0.8964930
C	-1.6486926	0.4625905	-0.1297920
N	-1.2492926	-0.6948305	-0.8979890
C	-0.2879076	-1.4700075	-0.2665640
C	0.2063854	-0.7154915	0.9214550
O	0.0416804	-2.5728705	-0.6647670
C	-1.5698986	1.6889525	-1.0334150
C	1.2584664	-1.1073295	1.6644870
Au	2.5797884	-2.4985055	0.8989510
C	1.7766784	-0.3051565	2.8300880
C	-4.7860416	-3.1591745	-0.0321730
C	-5.9152966	-2.3527955	-0.2296600
C	-5.8137506	-1.1865935	-0.9867360
C	-4.5818516	-0.8404345	-1.5478590
C	-3.4593866	-1.6413675	-1.3717130

C	-3.5736536	-2.8033495	-0.5958630
C	-2.1166136	-1.2392695	-1.9327770
O	-7.0599266	-2.7892285	0.3607460
C	-8.2241346	-2.0197085	0.1661280
H	-2.9129556	1.2358235	4.9521800
H	-1.6839676	3.3348905	5.3683300
H	0.0438384	4.1249615	3.7522270
H	-2.4569376	-0.1223195	2.9165300
H	1.6729764	2.4500855	1.7048570
H	-2.6542896	0.3522135	0.2971440
H	2.7323974	0.1477395	2.5405560
H	1.1036624	0.4708885	3.2105320
H	2.0091894	-0.9723445	3.6647420
H	-4.8962066	-4.0593645	0.5626740
H	-6.6716066	-0.5447015	-1.1459850
H	-4.4908926	0.0784195	-2.1221600
H	-2.6939316	-3.4242825	-0.4427630
H	-1.5811396	-2.1017245	-2.3363610
H	-2.2410166	-0.4935675	-2.7232280
H	-9.0239676	-2.5357405	0.6964010
H	-8.4819236	-1.9456055	-0.8972630
H	-8.1104766	-1.0088035	0.5765790
P	4.3531174	-3.5051195	-0.2366930
C	4.5001694	-5.3301385	-0.3182620
H	3.5872624	-5.7435945	-0.7520480
H	5.3600104	-5.6251115	-0.9264140
H	4.6145324	-5.7303085	0.6913680
C	5.9934494	-2.9446505	0.3437200
H	6.7905824	-3.3555485	-0.2822490
H	6.0066944	-1.8540065	0.2979940
H	6.1398314	-3.2517785	1.3812500
C	4.3304924	-2.9789815	-1.9881850
H	5.1686554	-3.4135495	-2.5405530
H	3.3849204	-3.2810615	-2.4433600
H	4.4031204	-1.8889205	-2.0103250
N	-0.4086956	2.4026495	-0.7478900
C	0.3041024	3.1803745	-1.8198610
C	1.4223934	4.0154715	-1.1854250
C	0.9032384	2.1810715	-2.8142140
C	-0.6685176	4.1432105	-2.5080460
H	1.0085464	4.8037445	-0.5404550
H	2.1657124	3.4185425	-0.6513610
H	1.9698384	4.5196515	-1.9846590
H	0.1133444	1.5527765	-3.2363530

H	1.3899534	2.7205945	-3.6313020
H	1.6588684	1.5490605	-2.3381560
H	-0.0880356	4.8191055	-3.1422780
H	-1.3998776	3.6197725	-3.1187990
H	-1.2039616	4.7426635	-1.7655410
O	-2.3592866	1.9273925	-1.9202810
H	1.3238754	1.3501075	-0.1195870
Sb	4.3480544	1.0591265	-0.1671180
F	5.3620234	0.0849195	-1.2323050
F	4.5920344	-0.0947335	1.1543080
F	3.2355144	1.9785095	0.9466790
F	2.8984424	0.1676355	-0.7168000
F	5.6902424	2.0452435	0.3869110
F	3.9814054	2.2508535	-1.4263290
H	0.7057714	3.6452605	1.0731970

Zero-point correction= 0.653629 (Hartree/Particle)
Thermal correction to Energy= 0.700817
Thermal correction to Enthalpy= 0.701761
Thermal correction to Gibbs Free Energy= 0.569384
Sum of electronic and zero-point Energies= -2597.443958
Sum of electronic and thermal Energies= -2597.396770
Sum of electronic and thermal Enthalpies= -2597.395825
Sum of electronic and thermal Free Energies= -2597.528203