Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Regioselectivity of Pd-catalyzed *o*-Carborane Arylation: A Theoretical View

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Part 1: Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Part 2: Comparisons of relative energies calculated by fully optimization in solvent with those by single-point refinement

Table S1 Comparisons of relative energies with in the gas and in hexafluoroisopropanol (HFIP) solvent by the SMD model.

Geometry	Optimization in the solvent[1]			Optimization in the gas[2]		
	G	**Δ*G***	**ΔΔ*G***	***G***	**Δ*G***	**ΔΔ*G***
AgI	-1779.662504			-1779.668161		
AgTFA	-673.299491			-673.297952		
ArI	-757.070592			-757.069943		
HTFA	-526.815271			-526.81539		
4	-1767.813255	0.0		-1767.811893	0.0	
8-ts	-1996.148526	30.5	0.0	-1996.148527	27.8	0.0
23-ts	-1996.12883		10.3	-1996.132156		12.3

[1]the thermal corrections of the Gibbs free energies obtained at *Level C*.(*Level C*: The structures were optimized by using the B3LYP density functional and mixed basis set with the solvent effects simulated by the SMD model in HFIP, i.e. the pseudopotential basis set LanL2DZ was used for Pd, Ag and I, and the split-valence basis set 6-31G(d, p) was used for other atoms) [2]the thermal corrections of the Gibbs free energies obtained at *Level A*.

Part 3: Energies, and frequencies of all the optimized structures

Table S2 Absolute Energies, Enthalpies, and Free Energies

Geometry	*E*(elec-B3LYP)[1]	*G*(corr-B3LYP)[2]	*E*(solv, M06)[3]	IF[4]
1	-1536.82158012	0.282393	-1537.812002	-
2-ts	-1536.79785853	0.278532	-1537.798525	1202.78*i*
3	-1536.82204790	0.281137	-1537.827297	-
4	-1480.94628669	0.367276	-1768.179169	-
5-ts	-1480.91593794	0.369477	-1768.14886	156.19*i*
6	-1480.92653376	0.370223	-1768.156372	-
7	-1995.69336505	0.392236	-1996.56115	-
8-ts	-1995.66842498	0.393732	-1996.542259	248.88*i*
9	-1995.75901647	0.393467	-1996.623899	-
10	-884.468258809	0.273945	-884.2229709	-
11	-1343.41101407	0.385490	-1343.041252	-
12-ts	-1480.926534	0.370746	-1768.123643	117.04*i*
13	-1480.963423	0.373061	-1768.181618	-
14-ts	-1995.73655805	0.389145	-1996.614296	1224.47*i*
15	-1995.75500673	0.392153	-1996.635865	-
16	-1939.87677263	0.481001	-2226.986896	-
17-ts	-1939.85426650	0.480482	-2226.963848	116.89*i*
18	-1939.86631697	0.481412	-2226.967512	-
19	-2454.62802564	0.504782	-2455.374864	-
20-ts	-2454.59995058	0.505803	-2455.352657	255.87*i*
21	-2454.69390354	0.506469	-2455.433551	-
22	-1802.34506172	0.498116	-1801.849607	-
23-ts	-1995.650856	0.393791	-1996.522621	343.15*i*
25-ts	-2110.175876	0.422680	-2111.033432	313.07*i*
26-ts	-2110.193682	0.422401	-2111.050682	250.15*i*
28-ts	-2332.682460	0.394009	-2333.601994	352.38*i*
29-ts	-2332.698575	0.392470	-2333.621382	250.22*i*

31-ts	-1863.830422	0.308624	-1864.813746	323.95*i*
32-ts	-1863.833048	0.309509	-1864.823784	249.34*i*
34-ts	-2224.179331	0.306629	-2225.151787	359.00*i*
35-ts	-2224.190495	0.306730	-2225.17111	252.04*i*
37-ts	-4335.390758	0.305082	-4339.023173	359.52*i*
38-ts	-4335.403167	0.304680	-4339.045318	252.57*i*
40-ts	-1803.927020	0.345828	-1804.878377	275.14*i*
41-ts	-1803.935634	0.344666	-1804.892525	250.48*i*
43-ts	-1882.547046	0.399811	-1883.459884	300.84*i*
44-ts	-1882.562061	0.398616	-1883.482821	247.43*i*
46-ts	-1921.852070	0.426961	-1922.742447	341.46*i*
47-ts	-1921.868877	0.427293	-1922.772656	258.25*i*
49-ts	-1764.628598	0.319279	-1765.595547	282.52*i*
50-ts	-1764.616824	0.318987	-1765.591761	252.33*i*
AgI	-628.979737859	-0.054089	-444.870416	-
AgTFA	-671.960976645	-0.008875	-673.289077	-
ArI	-470.907343974	0.094559	-757.164502	-
HTFA	-526.781571599	0.007745	-526.823016	-

[1]The electronic energy calculated by B3LYP in gas phase. [2]The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. [3]The electronic energy calculated by M06 in HFIP solvent. [4]The B3LYP calculated imaginary frequencies for the transition states.

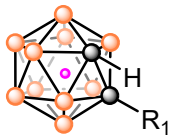
Part 4: Correlation between distortion of *o*-carborane and activation energy

Table S3 Relative geometry deviation, *NICS* of the *o*-carborane moiety, and free energy for the transition states of the reductive elimination for the B(3)-arylation versus the B(4)-arylation when the C(2) vertex is substituted by various groups.

Entry	R_1		Bond Length (Å)			ΔMUD (Å)	*NICS* (ppm)	$\Delta NICS$ (ppm)	$\Delta\Delta G$ (kcal/mol)
			C(1)–B(3)	C(2)–B(3)	C(1)–B(4)				
1	**Ph**	**23-ts**[a]	2.05	2.08	1.74	0.18	-21.82	2.02	12.3
		8-ts[b]	1.70	1.76	1.84		-23.84		
		24[c]	1.72	1.74	1.70		/		
2	**PhOMe**	**25-ts**[a]	1.97	1.99	1.74	0.12	-22.67	1.22	11.0
		26-ts[b]	1.69	1.76	1.83		-23.89		
		27[c]	1.72	1.74	1.70		/		
3	**$PhCF_3$**	**28-ts**[a]	2.08	2.10	1.74	0.19	-22.00	1.80	13.1
		29-ts[b]	1.70	1.76	1.84		-23.80		
		30[c]	1.72	1.74	1.70		/		
4	**F**	**31-ts**[a]	2.01	1.94	1.73	0.12	-24.52	1.35	5.7
		32-ts[b]	1.72	1.76	1.83		-25.87		
		33[c]	1.72	1.73	1.70		/		
5	**Cl**	**34-ts**[a]	2.13	2.13	1.74	0.22	-22.93	2.25	12.1
		35-ts[b]	1.71	1.77	1.84		-25.18		
		36[c]	1.72	1.73	1.70		/		
6	**Br**	**37-ts**[a]	2.14	2.15	1.74	0.23	-22.65	2.32	14.1
		38-ts[b]	1.71	1.76	1.84		-24.97		
		39[c]	1.72	1.73	1.70		/		
7	**Me**	**40-ts**[a]	1.90	1.87	1.73	0.06	-23.84	0.88	9.6
		41-ts[b]	1.71	1.76	1.84		-24.71		
		42[c]	1.71	1.73	1.70		/		
8	***i*-Pr**	**43-ts**[a]	1.97	1.99	1.74	0.13	-23.35	1.00	15.1
		44-ts[b]	1.70	1.76	1.84		-24.35		
		45[c]	1.71	1.74	1.70		/		
9	***t*-Bu**	**46-ts**[a]	2.21	2.34	1.76	0.32	-21.67	2.33	18.7
		47-ts[b]	1.70	1.78	1.87		-24.00		
		48[c]	1.70	1.74	1.69		/		
10	**H**	**49-ts**[a]	1.91	1.83	1.72	0.05	-24.37	0.55	-2.2
		50-ts[b]	1.72	1.75	1.83		-24.92		
		51[c]	1.72	1.72	1.70		/		

[a] Transition state of the reductive elimination for the B(3)-arylation. [b] Transition state of the reductive elimination for the B(4)-arylation. [c] *o*-carborane with C(2) vertex substituted.

Part 5: Position of the ghost atom for NICS calculation



Scheme S1 Position of the ghost atom in the optimized structure

Part 6: Cartesian coordination of all the optimized structures

1

Zero-point correction= 0.341463
Thermal correction to Energy= 0.368465
Thermal correction to Enthalpy= 0.369409
Thermal correction to Gibbs Free Energy= 0.282393
Sum of electronic and zero-point Energies= -1536.480117
Sum of electronic and thermal Energies= -1536.453115
Sum of electronic and thermal Enthalpies= -1536.452171
Sum of electronic and thermal Free Energies= -1536.539187

Cartesian coordinates

B	0.359482	-3.224561	0.360839
B	3.102000	-2.820592	-0.431527
B	1.494769	-3.298284	-1.021800
B	2.085797	-1.664297	-1.321265
B	2.031111	-3.779179	0.615379
B	1.279079	-2.666299	1.793487
B	2.970107	-2.430476	1.298771
B	1.872857	-1.040028	1.457683
H	2.372254	-1.145685	-2.340956
H	2.020259	-0.130688	2.192354
H	-0.662890	-0.938582	1.329782
H	1.005574	-2.970799	2.904712
H	3.919488	-2.471136	2.001848
H	2.303824	-4.899388	0.887588
H	4.140700	-3.128137	-0.904384
H	1.379275	-4.055208	-1.925335
H	-0.577991	-3.941783	0.452387
H	-0.441378	-1.587181	-1.619301
C	4.101132	-0.235399	-0.029377
C	4.779573	-0.101013	-1.252649
C	4.553711	0.505713	1.074972
C	5.865359	0.765450	-1.371058

H	4.470915	-0.684247	-2.111621
C	5.639461	1.371566	0.951843
H	4.068268	0.399504	2.037241
C	6.296109	1.508787	-0.271621
H	6.376773	0.852480	-2.324711
H	5.972990	1.934650	1.817900
H	7.141787	2.183176	-0.365329
C	1.216004	0.756293	-0.479191
H	2.169747	1.237579	-0.709569
N	0.156527	1.469046	-0.520107
C	0.287055	2.908823	-0.798534
H	-0.146164	3.109008	-1.785198
H	1.330404	3.236894	-0.792377
C	-0.535644	3.696513	0.245784
O	-0.260849	4.845928	0.514968
O	-1.539444	3.017408	0.759020
Pd	-1.809908	1.193742	0.015727
O	-2.667254	-0.658134	-0.667547
C	-3.757734	-0.289631	-0.140666
O	-3.841471	0.834324	0.438914
C	-4.970540	-1.232183	-0.167531
C	2.957444	-1.211820	0.108881
C	1.316489	-0.686159	-0.133261
B	0.255053	-1.534902	0.887439
B	0.383091	-1.922711	-0.846527
F	-4.847476	-2.141193	0.815839
F	-6.106971	-0.552937	0.015263
F	-5.030979	-1.877769	-1.339825

2-ts

Zero-point correction= 0.336866
Thermal correction to Energy= 0.363537
Thermal correction to Enthalpy= 0.364481
Thermal correction to Gibbs Free Energy= 0.278532
Sum of electronic and zero-point Energies= -1536.460992
Sum of electronic and thermal Energies= -1536.434322
Sum of electronic and thermal Enthalpies= -1536.433378
Sum of electronic and thermal Free Energies= -1536.519326

Cartesian coordinates

B	0.134511	-2.705966	-0.967508
B	-1.866350	-2.410139	1.085291
B	-0.116150	-2.310107	0.755999
B	-1.073462	-0.842880	0.849058

B	-1.114985	-3.566007	-0.037894
B	-1.464190	-3.024381	-1.706512
B	-2.693763	-2.851976	-0.430963
B	-2.419247	-1.549175	-1.605512
H	-1.057746	0.027878	1.639718
H	-3.221684	-1.108692	-2.348860
H	-0.342061	-0.967073	-2.964370
H	-1.623159	-3.764308	-2.617407
H	-3.754728	-3.371899	-0.402682
H	-1.027642	-4.712512	0.245957
H	-2.378673	-2.623155	2.128718
H	0.674386	-2.546496	1.605473
H	1.115569	-3.232779	-1.362443
H	1.653788	-0.763036	-0.684907
C	-3.843879	-0.466389	0.526594
C	-3.854463	0.295912	1.705267
C	-5.026175	-0.557849	-0.226189
C	-5.008898	0.969740	2.103198
H	-2.968630	0.358786	2.324491
C	-6.178493	0.115387	0.176556
H	-5.054182	-1.166954	-1.121624
C	-6.172954	0.886842	1.339128
H	-4.994776	1.554793	3.017485
H	-7.082002	0.029505	-0.419191
H	-7.070699	1.411259	1.651818
C	-1.567285	1.015871	-1.080407
H	-2.525719	1.430158	-1.394564
N	-0.516277	1.729903	-0.966776
C	-0.453563	3.167863	-1.215909
H	-1.426909	3.646902	-1.076222
H	-0.131895	3.317593	-2.253594
C	0.631875	3.818510	-0.311092
O	0.600456	5.021600	-0.141600
O	1.531861	2.993674	0.153760
Pd	1.204903	1.003264	-0.195387
O	2.931680	-1.296959	-0.692518
C	3.503136	-0.564907	0.155123
O	3.027961	0.488691	0.660519
C	4.884697	-1.008081	0.683103
C	-2.611261	-1.227663	0.092308
C	-1.419704	-0.432532	-0.792963
B	-0.664871	-1.454689	-1.936573
B	0.174001	-0.994060	-0.420441
F	5.682217	0.047761	0.877358

F	5.481946	-1.847093	-0.169381
F	4.712929	-1.641202	1.857926

3

Zero-point correction= 0.341970
Thermal correction to Energy= 0.369448
Thermal correction to Enthalpy= 0.370392
Thermal correction to Gibbs Free Energy= 0.281137
Sum of electronic and zero-point Energies= -1536.480078
Sum of electronic and thermal Energies= -1536.452600
Sum of electronic and thermal Enthalpies= -1536.451656
Sum of electronic and thermal Free Energies= -1536.540911

Cartesian coordinates

B	0.150616	-2.481878	-0.840156
B	-2.035592	-2.382509	1.036724
B	-0.265577	-2.196603	0.872035
B	-1.292993	-0.774537	0.947557
B	-1.137082	-3.444787	-0.071143
B	-1.367471	-2.827948	-1.733561
B	-2.709235	-2.771704	-0.565831
B	-2.394168	-1.396277	-1.642393
H	-1.379016	0.054281	1.779074
H	-3.145784	-0.950671	-2.434171
H	-0.248194	-0.671922	-2.787449
H	-1.416700	-3.524055	-2.690989
H	-3.743169	-3.337660	-0.656316
H	-1.027961	-4.601965	0.159564
H	-2.622963	-2.676869	2.019419
H	0.450271	-2.456890	1.780337
H	1.186811	-2.953828	-1.176538
H	2.580532	-0.626871	-1.441784
C	-4.043979	-0.493706	0.411464
C	-4.192654	0.178106	1.634850
C	-5.148630	-0.570644	-0.452263
C	-5.405395	0.779108	1.970986
H	-3.368186	0.225388	2.334955
C	-6.359588	0.030253	-0.111876
H	-5.069959	-1.112364	-1.387064
C	-6.491258	0.712666	1.097977
H	-5.498476	1.294823	2.921738
H	-7.201373	-0.042441	-0.793670
H	-7.434774	1.180512	1.362113
C	-1.598189	1.174663	-0.901724

H	-2.527428	1.655942	-1.208108
N	-0.502764	1.819643	-0.753849
C	-0.349364	3.260722	-0.980687
H	-1.256834	3.800897	-0.695181
H	-0.177901	3.412476	-2.053140
C	0.904289	3.845877	-0.244743
O	0.933140	5.061173	-0.124294
O	1.801999	2.984580	0.104522
Pd	1.163934	0.937195	-0.041220
O	3.474065	-0.948077	-1.178984
C	3.688556	-0.587142	0.063014
O	2.938341	0.081826	0.762415
C	5.023337	-1.123236	0.617491
C	-2.744695	-1.174844	0.045240
C	-1.513307	-0.293448	-0.680480
B	-0.625935	-1.221591	-1.809240
B	0.070357	-0.812314	-0.209317
F	5.278284	-0.585461	1.806196
F	6.018689	-0.828636	-0.227565
F	4.938560	-2.456213	0.742716

4

Zero-point correction= 0.435418
Thermal correction to Energy= 0.467745
Thermal correction to Enthalpy= 0.468689
Thermal correction to Gibbs Free Energy= 0.367276
Sum of electronic and zero-point Energies= -1480.510869
Sum of electronic and thermal Energies= -1480.478542
Sum of electronic and thermal Enthalpies= -1480.477598
Sum of electronic and thermal Free Energies= -1480.579011

Cartesian coordinates

B	2.220856	-2.588268	0.982475
B	4.218070	-1.926414	-0.986289
B	2.485648	-2.287621	-0.756945
B	3.014154	-0.624671	-0.944286
B	3.725159	-3.147871	0.206664
B	3.794745	-2.395147	1.825658
B	5.023554	-1.994786	0.601374
B	4.321011	-0.724925	1.623321
H	2.829562	0.145542	-1.816327
H	4.912672	-0.028886	2.368204
H	2.084641	-0.630592	2.820061
H	4.083176	-2.984518	2.812131

H	6.185084	-2.203437	0.673619
H	3.974185	-4.293644	0.033313
H	4.842825	-2.083213	-1.977687
H	1.865316	-2.810085	-1.622258
H	1.392074	-3.336307	1.383305
C	5.547200	0.517062	-0.569038
C	5.545834	0.932361	-1.910152
C	6.533139	1.027001	0.290729
C	6.488801	1.849980	-2.371018
H	4.815740	0.530231	-2.601697
C	7.473372	1.946470	-0.173529
H	6.580548	0.698008	1.321432
C	7.452391	2.365538	-1.503856
H	6.469920	2.156242	-3.412432
H	8.227559	2.327658	0.508190
H	8.186458	3.080002	-1.863893
C	2.766686	1.437015	0.760508
H	3.522185	2.190038	0.989412
N	1.535238	1.721771	0.572263
C	0.982171	3.077435	0.651101
H	1.241752	3.604072	-0.275128
H	1.414835	3.628317	1.491343
C	-0.575449	3.086886	0.752410
O	-1.091446	4.150072	1.063058
O	-1.168511	1.978568	0.446026
Pd	0.139083	0.261163	0.239994
C	4.543682	-0.505467	-0.085422
C	3.118711	-0.003746	0.648590
B	2.589712	-1.093052	1.855804
B	1.761233	-1.014749	0.269665
C	-3.586682	-0.961220	-0.237475
C	-3.797061	0.387897	0.022770
C	-4.618258	-1.850672	-0.535744
C	-5.113142	0.857412	-0.020614
H	-2.980490	1.069826	0.247008
C	-5.920862	-1.359499	-0.572574
H	-4.423770	-2.898737	-0.735786
C	-6.174364	-0.006211	-0.315681
H	-5.307322	1.905198	0.177634
H	-6.754668	-2.014841	-0.800481
I	-1.583644	-1.786899	-0.184102
C	-7.592595	0.454978	-0.372540
O	-8.537125	-0.267058	-0.627337
O	-7.715322	1.772851	-0.108536

C	-9.056440	2.285624	-0.145822
H	-9.494818	2.142703	-1.136646
H	-9.682025	1.778427	0.592862
H	-8.971054	3.346763	0.086893

5-ts

Zero-point correction= 0.434282
Thermal correction to Energy= 0.465971
Thermal correction to Enthalpy= 0.466915
Thermal correction to Gibbs Free Energy= 0.369477
Sum of electronic and zero-point Energies= -1480.481656
Sum of electronic and thermal Energies= -1480.449967
Sum of electronic and thermal Enthalpies= -1480.449023
Sum of electronic and thermal Free Energies= -1480.546461

Cartesian coordinates

B	2.048400	-2.319422	-1.655602
B	3.014312	0.311296	-2.337940
B	1.568744	-0.734372	-2.323506
B	1.788876	0.476319	-1.067265
B	3.175928	-1.421707	-2.704289
B	3.792908	-2.239686	-1.240868
B	4.382789	-0.616430	-1.674101
B	4.006254	-1.017844	0.011428
H	1.173349	1.454603	-0.843572
H	4.761779	-0.985411	0.915937
H	2.420126	-2.754669	0.972580
H	4.512116	-3.180340	-1.268295
H	5.492761	-0.322286	-1.954270
H	3.461679	-1.779988	-3.796820
H	3.207629	1.231865	-3.053864
H	0.727898	-0.591858	-3.146452
H	1.535152	-3.333827	-1.984182
C	4.130424	1.766866	-0.197058
C	3.491686	3.003361	-0.379860
C	5.394036	1.746796	0.415076
C	4.089794	4.183175	0.061282
H	2.532013	3.052832	-0.878773
C	5.988822	2.928824	0.854460
H	5.924561	0.810302	0.536840
C	5.337288	4.150771	0.684642
H	3.578518	5.128700	-0.091053
H	6.967139	2.890888	1.323619
H	5.802243	5.070619	1.025990

C	2.037032	0.141183	1.602681
H	2.750709	0.651917	2.251353
N	0.821368	-0.068640	1.930308
C	0.220242	0.291150	3.207612
H	-0.230746	1.284533	3.091358
H	0.963454	0.336065	4.009054
C	-0.957589	-0.673088	3.596139
O	-1.294740	-0.654586	4.770410
O	-1.485489	-1.335332	2.622213
Pd	-0.420767	-1.218809	0.698622
C	3.506426	0.486580	-0.705178
C	2.447341	-0.372123	0.267479
B	2.559122	-2.065990	0.020551
B	1.174076	-1.142264	-0.635048
C	-2.147078	-0.287088	-0.379887
C	-3.132970	0.049614	0.546996
C	-1.881677	0.467389	-1.519986
C	-3.830090	1.241954	0.347796
H	-3.316334	-0.571649	1.414555
C	-2.591162	1.655361	-1.693958
H	-1.153053	0.148136	-2.252647
C	-3.563370	2.050595	-0.766308
H	-4.587676	1.540321	1.063657
H	-2.406871	2.283283	-2.559474
I	-1.939428	-2.798546	-0.795466
C	-4.287965	3.327403	-1.021913
O	-4.072294	4.060468	-1.968040
O	-5.219705	3.588156	-0.078954
C	-5.960171	4.804529	-0.267378
H	-5.289115	5.667087	-0.267525
H	-6.502862	4.780570	-1.215608
H	-6.654423	4.858270	0.570873

6

Zero-point correction= 0.435293
Thermal correction to Energy= 0.467437
Thermal correction to Enthalpy= 0.468381
Thermal correction to Gibbs Free Energy= 0.370223
Sum of electronic and zero-point Energies= -1480.491240
Sum of electronic and thermal Energies= -1480.459097
Sum of electronic and thermal Enthalpies= -1480.458153
Sum of electronic and thermal Free Energies= -1480.556311

Cartesian coordinates

B	2.022629	-2.164162	-1.789433
B	2.932938	0.509728	-2.378031
B	1.510792	-0.569607	-2.418407
B	1.685361	0.614557	-1.125924
B	3.143595	-1.207118	-2.787871
B	3.754170	-2.053606	-1.335898
B	4.310777	-0.403891	-1.712363
B	3.915907	-0.861740	-0.045971
H	1.045942	1.570049	-0.881114
H	4.652013	-0.837410	0.874099
H	2.340581	-2.652876	0.840376
H	4.495967	-2.975511	-1.374403
H	5.417956	-0.076358	-1.963641
H	3.455668	-1.527849	-3.884318
H	3.117848	1.454056	-3.064042
H	0.677774	-0.424019	-3.247679
H	1.539027	-3.179081	-2.151530
C	3.976567	1.930536	-0.174537
C	3.313371	3.157214	-0.334992
C	5.227860	1.920050	0.462778
C	3.875376	4.336207	0.153297
H	2.363481	3.201031	-0.852809
C	5.786119	3.101342	0.949386
H	5.777690	0.992754	0.568104
C	5.110108	4.312844	0.801959
H	3.345926	5.274224	0.018001
H	6.755127	3.071138	1.437898
H	5.546545	5.232126	1.180325
C	1.916224	0.211694	1.546539
H	2.624251	0.713081	2.208145
N	0.712238	-0.044166	1.883253
C	0.138520	0.182194	3.192086
H	-0.549472	1.032709	3.114748
H	0.900289	0.400664	3.945438
C	-0.744372	-1.055790	3.624957
O	-0.873475	-1.227987	4.825948
O	-1.280222	-1.704905	2.648381
Pd	-0.454319	-1.288495	0.616756
C	3.391945	0.651012	-0.730182
C	2.339066	-0.253895	0.198296
B	2.493544	-1.941442	-0.094315
B	1.109181	-1.033639	-0.752879
C	-1.750955	0.143075	-0.053099
C	-2.680815	0.501019	0.921106

C	-1.729401	0.719467	-1.317404
C	-3.577096	1.533791	0.630738
H	-2.725881	-0.020890	1.868911
C	-2.631344	1.751381	-1.585101
H	-1.054629	0.380582	-2.090227
C	-3.549243	2.170547	-0.615614
H	-4.304907	1.833108	1.376504
H	-2.639949	2.232663	-2.557593
I	-1.735228	-3.029574	-0.872273
C	-4.480829	3.279688	-0.971337
O	-4.476134	3.862603	-2.038039
O	-5.337639	3.572793	0.031008
C	-6.270980	4.628646	-0.248838
H	-5.743038	5.560502	-0.466123
H	-6.896752	4.370054	-1.106480
H	-6.876787	4.731029	0.651185

7

Zero-point correction= 0.463947
Thermal correction to Energy= 0.501020
Thermal correction to Enthalpy= 0.501965
Thermal correction to Gibbs Free Energy= 0.392236
Sum of electronic and zero-point Energies= -1995.229418
Sum of electronic and thermal Energies= -1995.192345
Sum of electronic and thermal Enthalpies= -1995.191401
Sum of electronic and thermal Free Energies= -1995.301129

Cartesian coordinates

B	0.009326	-1.773491	-2.039361
B	2.247228	-0.063816	-2.712700
B	0.527764	-0.061673	-2.226955
B	1.793590	0.267045	-1.037803
B	1.150468	-1.321610	-3.333670
B	1.429372	-2.818070	-2.395711
B	2.793208	-1.754087	-2.813363
B	2.679827	-2.475548	-1.200698
H	2.029798	1.243529	-0.436195
H	3.477264	-3.186922	-0.701976
H	0.638406	-3.272105	0.102990
H	1.337001	-3.907110	-2.850894
H	3.710176	-2.037732	-3.501957
H	0.852294	-1.343086	-4.479456
H	2.807398	0.785211	-3.313144
H	-0.192700	0.804788	-2.572127

H	-1.101098	-2.125199	-2.241883
C	4.521277	-0.397669	-1.044050
C	4.805783	0.875629	-0.526103
C	5.579867	-1.298011	-1.245828
C	6.116270	1.228214	-0.203264
H	4.016199	1.601958	-0.379558
C	6.887599	-0.938700	-0.925258
H	5.386174	-2.278683	-1.664090
C	7.160364	0.324360	-0.398667
H	6.316368	2.217547	0.196214
H	7.692208	-1.648275	-1.091726
H	8.179302	0.603994	-0.148780
C	2.346442	-1.248495	1.235135
H	3.169330	-1.868786	1.600736
N	1.465461	-0.729999	1.993764
C	1.222945	-1.200297	3.336616
H	0.998023	-0.360058	4.000403
H	2.039570	-1.795217	3.759751
C	-0.051572	-2.114780	3.225188
O	-0.284869	-2.905716	4.113313
O	-0.790231	-1.971257	2.139256
Pd	-0.563709	-0.189606	1.125783
C	3.115703	-0.804686	-1.425332
C	2.037458	-1.230375	-0.223934
B	0.959948	-2.492233	-0.721890
B	0.435008	-0.803150	-0.624481
C	-2.453018	-0.249797	0.406475
C	-2.903361	0.661808	-0.550706
C	-3.297946	-1.219091	0.955084
C	-4.237433	0.598915	-0.959962
H	-2.242558	1.406206	-0.976913
C	-4.628218	-1.262802	0.537299
H	-2.932314	-1.929193	1.686570
C	-5.105413	-0.356914	-0.417525
H	-4.602503	1.299350	-1.702578
H	-5.310162	-2.000789	0.946771
C	-6.539025	-0.455840	-0.816410
O	-7.321788	-1.272787	-0.371610
O	-6.884207	0.472954	-1.736889
C	-8.255343	0.433070	-2.160222
H	-8.362177	1.238015	-2.887261
H	-8.489150	-0.531714	-2.617413
H	-8.924956	0.590418	-1.310900
C	0.610181	3.967378	0.620946

C	-0.205232	2.762722	0.066744
O	-0.193200	1.799471	0.934179
O	-0.679371	2.824555	-1.051777
F	0.407249	5.072048	-0.101418
F	0.315385	4.237819	1.903404
F	1.934829	3.666056	0.558579

8-ts

Zero-point correction= 0.463291
Thermal correction to Energy= 0.499771
Thermal correction to Enthalpy= 0.500715
Thermal correction to Gibbs Free Energy= 0.393732
Sum of electronic and zero-point Energies= -1995.205134
Sum of electronic and thermal Energies= -1995.168654
Sum of electronic and thermal Enthalpies= -1995.167710
Sum of electronic and thermal Free Energies= -1995.274693

Cartesian coordinates

B	-0.730386	-2.223509	-1.447635
B	1.596865	-1.056623	-2.682617
B	-0.069634	-0.712410	-2.154203
B	1.291169	-0.201626	-1.152696
B	0.344887	-2.308992	-2.856641
B	0.537877	-3.471528	-1.513705
B	1.961678	-2.762926	-2.309498
B	1.899540	-2.938053	-0.549995
H	1.705281	0.868679	-0.928099
H	2.646131	-3.569337	0.110133
H	-0.085959	-3.051262	1.034217
H	0.297029	-4.628251	-1.596199
H	2.794502	-3.345395	-2.911880
H	-0.049785	-2.627857	-3.927035
H	2.181318	-0.490016	-3.538659
H	-0.711480	0.084192	-2.741737
H	-1.876230	-2.509652	-1.498798
C	3.948350	-1.146641	-1.128669
C	4.395428	0.183798	-1.097501
C	4.895347	-2.180415	-1.047002
C	5.755311	0.466826	-0.968777
H	3.695360	1.005872	-1.177040
C	6.253107	-1.891195	-0.923047
H	4.575066	-3.214629	-1.093541
C	6.688088	-0.566176	-0.878905
H	6.081020	1.502117	-0.945534

H	6.969206	-2.705199	-0.865239
H	7.745837	-0.340881	-0.782090
C	2.077921	-1.095385	1.392256
H	2.761557	-1.845944	1.800158
N	1.620045	-0.149099	2.111984
C	1.606322	-0.267100	3.554517
H	1.715401	0.714358	4.022763
H	2.360225	-0.954215	3.956083
C	0.185338	-0.847105	3.882701
O	-0.035557	-1.307651	4.981040
O	-0.701270	-0.827006	2.898161
Pd	-0.365184	0.516603	1.398143
C	2.485197	-1.491308	-1.294507
C	1.488069	-1.388263	0.044394
B	0.237621	-2.572921	0.002783
B	-0.222650	-0.883501	-0.387813
C	-2.010487	-0.134204	0.301243
C	-2.616515	0.727621	-0.638575
C	-2.796791	-1.120027	0.943962
C	-3.962204	0.570724	-0.961066
H	-2.025791	1.492123	-1.129916
C	-4.135096	-1.271004	0.612311
H	-2.354740	-1.755002	1.701669
C	-4.724454	-0.429845	-0.344103
H	-4.423217	1.225064	-1.691747
H	-4.746754	-2.029976	1.087943
C	-6.171009	-0.643806	-0.658875
O	-6.859369	-1.502431	-0.144085
O	-6.629612	0.225139	-1.582642
C	-8.014951	0.072201	-1.934539
H	-8.215324	0.843062	-2.678033
H	-8.196317	-0.921736	-2.350830
H	-8.650373	0.208474	-1.056109
C	1.225525	4.071581	-0.531315
C	0.176229	2.923474	-0.562718
O	0.197881	2.280605	0.558666
O	-0.457484	2.725983	-1.584847
F	1.030463	4.944774	-1.523310
F	1.219966	4.743285	0.631724
F	2.463159	3.530409	-0.688403

9

Zero-point correction= 0.466145

Thermal correction to Energy= 0.502939

Thermal correction to Enthalpy= 0.503883
Thermal correction to Gibbs Free Energy= 0.393467
Sum of electronic and zero-point Energies= -1995.292871
Sum of electronic and thermal Energies= -1995.256078
Sum of electronic and thermal Enthalpies= -1995.255134
Sum of electronic and thermal Free Energies= -1995.365549

Cartesian coordinates

B	1.423798	-3.634342	-1.980785
B	3.022599	-1.255887	-2.312015
B	1.433574	-1.974484	-2.650177
B	1.618203	-0.853992	-1.299631
B	2.902447	-2.984998	-2.725597
B	3.010001	-3.917253	-1.206995
B	3.995986	-2.455296	-1.426058
B	3.174037	-2.762040	0.110733
H	1.181205	0.227171	-1.205414
H	3.702440	-2.892994	1.157711
H	1.129789	-4.153426	0.639885
H	3.511924	-4.986436	-1.117769
H	5.176662	-2.406101	-1.431212
H	3.336884	-3.387426	-3.751599
H	3.534454	-0.387020	-2.927862
H	0.818558	-1.649241	-3.608956
H	0.787548	-4.512077	-2.458144
C	3.931850	-0.087148	0.086578
C	3.576442	1.259254	-0.089199
C	5.039909	-0.395833	0.893105
C	4.300067	2.267237	0.548588
H	2.738488	1.533579	-0.716458
C	5.760971	0.615750	1.524508
H	5.351241	-1.426003	1.018478
C	5.390398	1.951232	1.359210
H	4.007596	3.302427	0.402146
H	6.616324	0.357058	2.141163
H	5.952543	2.739080	1.851593
C	1.341474	-1.371323	1.458422
H	1.681074	-2.046235	2.247316
N	0.645707	-0.359096	1.816277
C	0.307601	-0.239453	3.246364
H	0.820698	0.642267	3.646738
H	0.611552	-1.121199	3.817467
C	-1.213021	-0.006553	3.384991
O	-1.803288	-0.313084	4.397128

O	-1.762702	0.567731	2.334815
Pd	-0.490054	1.120956	0.918918
C	3.183714	-1.189997	-0.619238
C	1.730845	-1.819082	0.088306
B	1.592878	-3.490297	-0.225122
B	0.578096	-2.314806	-1.122455
C	-0.967228	-2.130124	-0.867650
C	-1.677875	-1.089099	-1.496866
C	-1.693324	-3.001127	-0.033713
C	-3.045401	-0.912232	-1.293532
H	-1.156617	-0.414577	-2.169932
C	-3.059407	-2.833932	0.174689
H	-1.187421	-3.829677	0.452900
C	-3.743722	-1.784549	-0.449784
H	-3.574293	-0.103768	-1.784785
H	-3.616754	-3.506239	0.818238
C	-5.206885	-1.650058	-0.187641
O	-5.852114	-2.414729	0.502082
O	-5.744076	-0.576704	-0.807701
C	-7.148477	-0.379329	-0.581399
H	-7.412536	0.518773	-1.139453
H	-7.720614	-1.238452	-0.940807
H	-7.349057	-0.242859	0.484028
C	-0.660744	4.201785	-1.640997
C	-0.578325	2.997331	-0.690098
O	0.478619	2.302828	-0.651880
O	-1.553342	2.728836	0.070855
F	-1.931107	4.527472	-1.893354
F	-0.048162	5.256845	-1.072579
F	-0.042419	3.923964	-2.797308

10

Zero-point correction= 0.322215
Thermal correction to Energy= 0.341482
Thermal correction to Enthalpy= 0.342426
Thermal correction to Gibbs Free Energy= 0.273945
Sum of electronic and zero-point Energies= -884.146043
Sum of electronic and thermal Energies= -884.126777
Sum of electronic and thermal Enthalpies= -884.125833
Sum of electronic and thermal Free Energies= -884.194313

Cartesian coordinates

B	-1.362530	-0.282798	1.439324
B	-3.837888	0.015464	0.020506

B	-1.373206	-0.235022	-1.424669
B	-2.584891	0.897411	0.921227
B	-2.591653	0.927276	-0.858275
B	-3.068194	-0.727913	1.452125
B	-3.078680	-0.679800	-1.440715
B	-1.859311	-1.893407	0.869618
B	-3.389295	-1.706776	-0.009700
B	-1.866184	-1.864217	-0.905271
H	-0.633610	-0.062455	-2.326521
H	-2.701588	1.952395	-1.437656
H	-3.642325	-0.807586	-2.475562
H	-1.450983	-2.778187	-1.527228
H	-1.441596	-2.827741	1.458213
H	-4.190154	-2.580606	-0.020860
H	-3.624254	-0.890328	2.486157
H	-4.961951	0.392128	0.030990
H	-2.689485	1.902807	1.535200
H	-0.618854	-0.141148	2.343081
C	-0.730095	-0.959144	-0.006550
C	-1.143999	0.692461	0.021883
C	-0.066370	1.754546	0.032840
C	0.440414	2.252448	1.243813
C	0.399809	2.313074	-1.168039
C	1.403481	3.260745	1.251291
H	0.077012	1.860459	2.185551
C	1.362262	3.321833	-1.157303
H	0.004080	1.968254	-2.115201
C	1.872390	3.796245	0.051465
H	1.781657	3.629553	2.199859
H	1.706574	3.739964	-2.098421
H	2.621139	4.582745	0.058827
C	0.739026	-1.272760	-0.022380
H	1.401232	-0.402984	-0.071321
N	1.118324	-2.479360	0.004810
C	2.526021	-2.847554	0.007918
H	2.702250	-3.477708	0.883968
H	2.695321	-3.473745	-0.877370
C	3.592282	-1.754799	0.028783
O	4.423174	-1.615092	0.895857
O	3.525025	-0.950721	-1.061366
H	4.239521	-0.297438	-0.964494

11

Zero-point correction= 0.447034

Thermal correction to Energy= 0.475856
Thermal correction to Enthalpy= 0.476800
Thermal correction to Gibbs Free Energy= 0.385490
Sum of electronic and zero-point Energies= -1342.963980
Sum of electronic and thermal Energies= -1342.935158
Sum of electronic and thermal Enthalpies= -1342.934214
Sum of electronic and thermal Free Energies= -1343.025524

Cartesian coordinates

B	-0.092140	-2.712381	-1.996345
B	-1.895980	-3.024193	0.221973
B	-0.194639	-3.148666	-0.263809
B	-0.750942	-1.728531	0.613097
B	-1.490502	-3.632190	-1.392547
B	-1.738593	-2.302627	-2.555047
B	-2.851358	-2.504373	-1.183430
B	-2.284217	-0.891079	-1.655247
H	-0.506315	-1.362776	1.709099
H	-2.978331	-0.013381	-2.015795
H	-0.178867	-0.192186	-2.890162
H	-2.106694	-2.463636	-3.669790
H	-4.011329	-2.726446	-1.239861
H	-1.686617	-4.767414	-1.671655
H	-2.402429	-3.627688	1.102234
H	0.529426	-3.925911	0.262811
H	0.724427	-3.174861	-2.720119
C	-3.283153	-0.684568	0.961217
C	-3.457511	-1.191024	2.259131
C	-3.993538	0.466230	0.587403
C	-4.330056	-0.573000	3.152870
H	-2.913133	-2.073519	2.572669
C	-4.858199	1.087006	1.489367
H	-3.867738	0.895671	-0.397692
C	-5.035034	0.569415	2.771917
H	-4.454055	-0.985950	4.149405
H	-5.393120	1.980164	1.181144
H	-5.712529	1.052790	3.469495
C	-0.856789	0.901442	-0.108518
H	-0.696892	1.035969	0.969531
N	-0.904626	1.856517	-0.937353
C	-0.727275	3.203249	-0.434394
H	0.175902	3.634224	-0.876730
H	-0.616058	3.256343	0.662445
C	-1.870143	4.137295	-0.814668

O	-1.752701	5.336480	-0.907350
O	-3.044357	3.491263	-0.985635
C	-2.338721	-1.384741	0.008619
C	-0.996699	-0.521533	-0.573668
B	-0.584756	-1.015263	-2.148320
B	0.402400	-1.535721	-0.746353
C	1.839926	-0.953595	-0.436569
C	2.595564	-1.461946	0.636811
C	2.422333	0.064734	-1.215466
C	3.870031	-0.980853	0.926042
H	2.181569	-2.255017	1.252407
C	3.693708	0.555693	-0.933414
H	1.875223	0.475650	-2.058108
C	4.427451	0.036774	0.140939
H	4.436416	-1.388776	1.755486
H	4.139950	1.339717	-1.536244
C	5.783719	0.597869	0.399008
O	6.295638	1.490499	-0.248895
O	6.398872	0.002687	1.447598
C	7.713434	0.496423	1.744528
H	8.059674	-0.083844	2.599841
H	8.380006	0.355799	0.889870
H	7.679420	1.560813	1.990806
H	-3.695781	4.177115	-1.212158

12-ts

Zero-point correction= 0.434527

Thermal correction to Energy= 0.478428

Thermal correction to Enthalpy= 0.479547

Thermal correction to Gibbs Free Energy= 0.350171

Sum of electronic and zero-point Energies= -1480.480267

Sum of electronic and thermal Energies= -1480.436367

Sum of electronic and thermal Enthalpies= -1480.435248

Sum of electronic and thermal Free Energies= -1480.564623

Cartesian coordinates

B	-0.374260	-2.646930	0.036118
B	-2.878393	-2.289999	1.417640
B	-1.129526	-1.945331	1.497923
B	-2.247241	-0.691955	0.979384
B	-1.715560	-3.503079	0.835775
B	-1.662764	-3.408178	-0.948618
B	-3.203589	-3.191808	-0.083660
B	-2.782950	-2.148788	-1.455814

H	-2.543161	0.321622	1.498384
H	-3.398353	-2.036653	-2.455087
H	-0.509898	-1.496498	-2.389724
H	-1.475959	-4.344655	-1.649484
H	-4.159690	-3.881688	-0.168336
H	-1.568267	-4.525194	1.416941
H	-3.622406	-2.368288	2.332766
H	-0.586021	-1.853485	2.546265
H	0.729748	-3.072767	0.021910
C	-4.856008	-0.914574	-0.056721
C	-5.283077	0.045136	0.874094
C	-5.765715	-1.359348	-1.029732
C	-6.576333	0.563776	0.815426
H	-4.613406	0.383264	1.654715
C	-7.058246	-0.839709	-1.083688
H	-5.471472	-2.121744	-1.740924
C	-7.467066	0.128041	-0.165627
H	-6.885810	1.306101	1.544676
H	-7.745850	-1.198373	-1.843446
H	-8.473724	0.532523	-0.208979
C	-2.387927	0.601203	-1.395869
H	-3.305301	0.820936	-1.945214
N	-1.422038	1.423265	-1.276609
C	-1.385899	2.758187	-1.863548
H	-1.864180	3.445454	-1.154548
H	-1.933641	2.800847	-2.809784
C	0.077536	3.276321	-2.051042
O	0.224433	4.220236	-2.812879
O	0.978853	2.683768	-1.338791
Pd	0.365459	0.865582	-0.278339
C	-3.465140	-1.505734	0.009447
C	-2.192336	-0.718651	-0.736564
B	-1.031831	-1.802568	-1.372859
B	-0.691619	-0.889953	0.129558
C	2.325835	0.390905	0.362793
C	2.628606	-0.925404	0.740550
C	3.263409	1.200908	-0.300138
C	3.843099	-1.479099	0.340972
H	1.935621	-1.508661	1.330856
C	4.472746	0.631369	-0.684288
H	3.017573	2.223697	-0.559692
C	4.769137	-0.704193	-0.369840
H	4.080153	-2.504803	0.598505
H	5.205515	1.214009	-1.232491

I	1.035998	1.501457	2.296969
C	6.094012	-1.242522	-0.798216
O	6.931140	-0.599940	-1.400221
O	6.263626	-2.534382	-0.440644
C	7.521061	-3.115306	-0.822689
H	7.641974	-3.087910	-1.908363
H	8.350179	-2.572581	-0.362043
H	7.489689	-4.144323	-0.465293

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Zero-point correction= 0.435953
Thermal correction to Energy= 0.480300
Thermal correction to Enthalpy= 0.481418
Thermal correction to Gibbs Free Energy= 0.351781
Sum of electronic and zero-point Energies= -1480.495254
Sum of electronic and thermal Energies= -1480.450907
Sum of electronic and thermal Enthalpies= -1480.449788
Sum of electronic and thermal Free Energies= -1480.579426

Cartesian coordinates

B	0.155162	2.342690	-0.831283
B	2.525708	2.637246	0.799531
B	0.801296	2.172794	0.836038
B	2.055634	0.931958	0.821659
B	1.356102	3.507238	-0.218519
B	1.501652	2.885724	-1.888684
B	2.949123	3.069883	-0.873149
B	2.740652	1.632088	-1.889842
H	2.352738	0.152464	1.644202
H	3.469406	1.280585	-2.747448
H	0.615252	0.538775	-2.772742
H	1.338933	3.551872	-2.853898
H	3.861818	3.789397	-1.085462
H	1.085645	4.637275	0.011448
H	3.160837	3.047822	1.707312
H	0.153388	2.346650	1.809599
H	-0.970550	2.628908	-1.049315
C	4.727326	1.053457	-0.035713
C	5.103255	0.329147	1.105901
C	5.714671	1.388412	-0.976464
C	6.428194	-0.066486	1.288640
H	4.370559	0.078830	1.862342
C	7.038078	0.994069	-0.787923
H	5.454356	1.968341	-1.853775

C	7.399404	0.260443	0.342628
H	6.697724	-0.626899	2.178500
H	7.785932	1.265568	-1.526564
H	8.430375	-0.047226	0.488486
C	2.456276	-1.001231	-1.104319
H	3.287968	-1.263625	-1.762959
N	1.578191	-1.837927	-0.714298
C	1.404656	-3.122619	-1.350832
H	1.210928	-3.891580	-0.597229
H	2.252929	-3.424128	-1.974750
C	0.128200	-2.986393	-2.261694
O	-0.056738	-3.830305	-3.116390
O	-0.644598	-1.957413	-2.020565
Pd	-0.454410	-1.070565	-0.090097
C	3.303340	1.517211	-0.248082
C	2.163171	0.430750	-0.817793
B	1.014187	1.184986	-1.869789
B	0.601701	0.745979	-0.199845
C	-2.339035	-0.336218	-0.116431
C	-2.774426	0.759056	0.636295
C	-3.203856	-0.999646	-0.992163
C	-4.087196	1.207314	0.491901
H	-2.113081	1.266203	1.326551
C	-4.519068	-0.549915	-1.116029
H	-2.854997	-1.830199	-1.594314
C	-4.967511	0.552867	-0.379906
H	-4.431199	2.061709	1.063705
H	-5.208857	-1.043845	-1.792404
I	-0.456507	-1.120169	2.567250
C	-6.381569	0.986520	-0.563310
O	-7.177927	0.444500	-1.304811
O	-6.693245	2.064931	0.192778
C	-8.043749	2.532648	0.060768
H	-8.250426	2.826980	-0.971356
H	-8.751867	1.752468	0.351325
H	-8.124423	3.391157	0.727541

14-ts

Zero-point correction= 0.461253

Thermal correction to Energy= 0.497760

Thermal correction to Enthalpy= 0.498704

Thermal correction to Gibbs Free Energy= 0.389145

Sum of electronic and zero-point Energies= -1995.275305

Sum of electronic and thermal Energies= -1995.238798

Sum of electronic and thermal Enthalpies= -1995.237854
Sum of electronic and thermal Free Energies= -1995.347413

Cartesian coordinates

B	-1.957053	2.101362	-1.673269
B	-1.625825	-0.432346	-3.026637
B	-0.759150	1.024332	-2.440925
B	-0.653149	-0.499629	-1.529820
B	-2.396217	1.174141	-3.131898
B	-3.551959	1.321021	-1.786415
B	-3.346331	-0.235952	-2.622186
H	-2.972919	1.695666	0.759247
H	-4.602746	1.861383	-1.771406
H	-4.257449	-0.744329	-3.176829
H	-2.607765	1.701206	-4.171205
H	-1.290451	-1.061698	-3.971950
H	0.202541	1.445982	-2.989874
H	-1.867024	3.279045	-1.658946
H	-0.148435	2.270530	-0.041403
C	-1.704392	-0.896761	1.055322
H	-2.350867	-1.711517	1.382910
N	-0.768532	-0.427918	1.784507
C	-0.419027	-0.931674	3.112250
H	-0.664170	-1.992005	3.219544
H	-0.993255	-0.360745	3.851833
C	1.083651	-0.673066	3.414494
O	1.596034	-1.261612	4.346135
O	1.660418	0.217974	2.652293
Pd	0.552883	0.931794	1.089590
O	0.383766	3.530926	-0.214733
C	1.595675	3.321433	0.051766
O	2.066662	2.264744	0.551186
C	2.603482	4.427819	-0.325136
C	-1.876026	-0.279924	-0.282205
B	-2.622985	1.266837	-0.279806
B	-0.881901	1.071828	-0.657294
B	-2.293147	-1.251529	-1.620406
H	-2.459224	-2.400703	-1.420543
C	-3.429328	-0.147538	-0.915704
C	-4.599994	-0.728342	-0.153857
C	-5.095524	-2.000499	-0.483205
C	-5.249369	0.006958	0.850371
C	-6.194986	-2.530614	0.190372
H	-4.633939	-2.574979	-1.277123

C	-6.347988	-0.527686	1.522678
H	-4.910830	1.004261	1.101850
C	-6.821928	-1.799363	1.199756
H	-6.563101	-3.515041	-0.081566
H	-6.836145	0.058139	2.295377
H	-7.678342	-2.212996	1.723388
F	2.073984	5.640561	-0.121980
F	3.730828	4.326776	0.383617
F	2.903826	4.304823	-1.631907
C	0.611802	-1.415226	-1.294516
C	1.900592	-0.856996	-1.399804
C	0.522876	-2.790485	-1.007171
C	3.046949	-1.627782	-1.217239
H	2.013679	0.198236	-1.627180
C	1.661377	-3.568220	-0.819756
H	-0.448545	-3.270854	-0.935639
C	2.932933	-2.991405	-0.921926
H	4.028115	-1.174394	-1.295915
H	1.589064	-4.627338	-0.596132
C	4.117881	-3.873152	-0.708527
O	4.049921	-5.061202	-0.458994
O	5.284617	-3.204588	-0.825431
C	6.467006	-3.991887	-0.613241
H	7.303588	-3.305691	-0.742839
H	6.469710	-4.415073	0.394226
H	6.521129	-4.807408	-1.338797

15

Zero-point correction= 0.466758

Thermal correction to Energy= 0.504067

Thermal correction to Enthalpy= 0.505011

Thermal correction to Gibbs Free Energy= 0.392153

Sum of electronic and zero-point Energies= -1995.288249

Sum of electronic and thermal Energies= -1995.250940

Sum of electronic and thermal Enthalpies= -1995.249996

Sum of electronic and thermal Free Energies= -1995.362854

Cartesian coordinates

B	-1.614469	1.585478	-2.208835
B	-1.838897	-1.213754	-2.914079
B	-0.687563	0.154424	-2.732688
B	-0.791477	-1.100681	-1.475852
B	-2.322360	0.441934	-3.385718
B	-3.331041	1.111852	-2.084283

B	-3.462455	-0.607974	-2.516300
H	-2.522474	1.954197	0.267135
H	-4.269583	1.825750	-2.171844
H	-4.484404	-1.048699	-2.914952
H	-2.523062	0.735428	-4.516648
H	-1.691585	-2.096315	-3.690945
H	0.286881	0.238597	-3.403797
H	-1.322345	2.701148	-2.487322
H	1.639750	5.192702	0.771121
C	-1.584989	-0.643930	1.147564
H	-2.229161	-1.287352	1.747105
N	-0.523487	-0.100052	1.613056
C	-0.031897	-0.264496	2.984824
H	0.554231	-1.190910	3.016730
H	-0.862496	-0.352933	3.691320
C	0.942560	0.889198	3.408795
O	1.090249	1.052514	4.612044
O	1.534126	1.504808	2.439739
Pd	0.609769	1.148119	0.516911
O	1.283672	4.306882	0.584838
C	2.082000	3.641742	-0.221021
O	1.906882	2.481744	-0.546882
C	3.285847	4.413190	-0.810723
C	-1.852942	-0.379185	-0.291074
B	-2.314907	1.233443	-0.640065
B	-0.668828	0.644645	-1.018039
B	-2.533668	-1.543428	-1.328241
H	-2.897298	-2.560097	-0.853315
C	-3.405897	-0.112038	-0.883017
C	-4.593557	-0.287739	0.036722
C	-5.406090	-1.426632	-0.084318
C	-4.932717	0.680160	0.994566
C	-6.518007	-1.597839	0.738466
H	-5.175548	-2.177829	-0.830137
C	-6.044044	0.503466	1.818917
H	-4.338272	1.579172	1.096047
C	-6.839441	-0.635656	1.696569
H	-7.133658	-2.485014	0.625738
H	-6.287689	1.264383	2.554070
H	-7.705230	-0.769950	2.337934
F	3.395171	5.617935	-0.195796
F	4.412511	3.734033	-0.627448
F	3.095542	4.621844	-2.115269
C	0.320303	-2.145877	-1.057088

C	1.678610	-1.776798	-1.104969
C	0.022514	-3.463575	-0.662529
C	2.691675	-2.669301	-0.762293
H	1.945964	-0.771651	-1.416061
C	1.025842	-4.362667	-0.312145
H	-1.009112	-3.801177	-0.634878
C	2.369358	-3.970800	-0.356160
H	3.730329	-2.361968	-0.804209
H	0.790581	-5.376396	-0.005275
C	3.402170	-4.972266	0.034034
O	3.157872	-6.109082	0.390614
O	4.658558	-4.478675	-0.048364
C	5.700341	-5.393765	0.322711
H	6.632432	-4.840609	0.207899
H	5.573590	-5.722363	1.357316
H	5.691779	-6.271894	-0.328074

16

Zero-point correction= 0.560313
Thermal correction to Energy= 0.602057
Thermal correction to Enthalpy= 0.603001
Thermal correction to Gibbs Free Energy= 0.481001
Sum of electronic and zero-point Energies= -1939.316459
Sum of electronic and thermal Energies= -1939.274716
Sum of electronic and thermal Enthalpies= -1939.273771
Sum of electronic and thermal Free Energies= -1939.395772

Cartesian coordinates

B	-0.110797	0.461144	-2.585765
B	0.649028	3.243154	-2.783687
B	-0.717133	2.116718	-2.939642
B	-0.536088	3.080581	-1.475240
B	0.916090	1.624695	-3.468412
B	1.623899	0.594639	-2.192941
B	2.091340	2.309481	-2.321982
B	1.779215	1.567385	-0.741533
H	-1.204213	3.958632	-1.059423
H	2.565901	1.495901	0.131466
H	2.424225	-0.246524	-2.424873
H	3.175667	2.726284	-2.541326
H	1.193802	1.497604	-4.613660
H	0.756466	4.287581	-3.327299
H	-1.608442	2.339068	-3.688131
H	-0.578251	-0.493881	-3.110831

C	1.689414	4.364582	-0.423015
C	1.050847	5.607061	-0.566405
C	2.844504	4.290594	0.370823
C	1.541956	6.737828	0.084308
H	0.174885	5.696476	-1.197601
C	3.331398	5.423676	1.022172
H	3.375142	3.352739	0.475123
C	2.680484	6.649802	0.886015
H	1.033592	7.688877	-0.041586
H	4.225818	5.343734	1.632344
H	3.061840	7.530801	1.393308
C	-0.087773	2.150209	1.111399
H	-0.273847	3.112767	1.589654
N	-0.136042	1.039812	1.741950
C	-0.450343	0.901827	3.166516
H	-1.542236	0.906479	3.269193
H	-0.046072	1.740438	3.741195
C	0.044674	-0.459246	3.760262
O	0.139362	-0.514978	4.976869
O	0.245792	-1.408967	2.903229
Pd	0.338114	-0.739685	0.845206
C	1.162654	3.152981	-1.157814
C	0.186063	2.040666	-0.344348
B	0.421875	0.408464	-0.883599
B	-1.052086	1.351380	-1.364649
C	-2.510713	1.057837	-0.818987
C	-2.869718	-0.215219	-0.336805
C	-3.518451	2.042015	-0.843779
C	-4.156212	-0.489280	0.123094
H	-2.132986	-1.011583	-0.324392
C	-4.806921	1.780408	-0.387422
H	-3.298670	3.030106	-1.235411
C	-5.135377	0.511930	0.105832
H	-4.403539	-1.475473	0.498981
H	-5.576127	2.545261	-0.407915
C	-6.528029	0.286550	0.587779
O	-7.397492	1.136307	0.598861
O	-6.727700	-0.980118	1.018767
C	-8.049854	-1.258209	1.505597
H	-8.036995	-2.304322	1.811249
H	-8.290892	-0.613399	2.354362
H	-8.791587	-1.095838	0.719508
C	1.582833	-2.784617	0.590437
C	0.304389	-3.046144	0.050963

C	0.153452	-3.245524	-1.343334
C	1.270539	-3.191109	-2.168798
C	2.544527	-2.928968	-1.643526
C	2.692668	-2.719955	-0.281015
H	1.715264	-2.772834	1.667299
H	-0.526103	-3.247546	0.719454
H	1.138160	-3.357505	-3.232514
H	3.402243	-2.892838	-2.305401
I	4.626850	-2.354153	0.536143
C	-1.162426	-3.562531	-1.971777
O	-1.318361	-3.760693	-3.159585
O	-2.164114	-3.610209	-1.067527
C	-3.463075	-3.918214	-1.607490
H	-3.431868	-4.858941	-2.161239
H	-4.126239	-3.998117	-0.746887
H	-3.794628	-3.119682	-2.275086

17-ts

Zero-point correction= 0.559080
Thermal correction to Energy= 0.600525
Thermal correction to Enthalpy= 0.601469
Thermal correction to Gibbs Free Energy= 0.480482
Sum of electronic and zero-point Energies= -1939.295186
Sum of electronic and thermal Energies= -1939.253742
Sum of electronic and thermal Enthalpies= -1939.252798
Sum of electronic and thermal Free Energies= -1939.373784

Cartesian coordinates

B	0.885258	-0.235790	-2.663775
B	3.601760	0.665265	-3.005462
B	1.898658	1.153889	-3.163072
B	2.831468	1.669592	-1.765254
B	2.396322	-0.514700	-3.562764
B	1.968952	-1.571813	-2.183094
B	3.647010	-1.007963	-2.400470
B	2.900479	-1.037953	-0.793301
H	3.182314	2.751294	-1.457115
H	3.305577	-1.644206	0.130151
H	1.701124	-2.718583	-2.309547
H	4.597897	-1.684101	-2.588321
H	2.412927	-0.914932	-4.677886
H	4.518120	1.111335	-3.604293
H	1.560288	1.947995	-3.974194
H	-0.177915	-0.420369	-3.151675

C	5.168550	0.606251	-0.665030
C	5.776807	1.867730	-0.764589
C	5.841279	-0.411210	0.029801
C	7.010090	2.110910	-0.161006
H	5.297751	2.660305	-1.326020
C	7.074863	-0.164360	0.631090
H	5.411135	-1.402965	0.092799
C	7.661230	1.098404	0.543929
H	7.462925	3.093577	-0.250527
H	7.577793	-0.965718	1.163525
H	8.621822	1.289056	1.012722
C	2.420954	0.998440	0.913085
H	3.165105	1.703693	1.287794
N	1.512264	0.479085	1.639653
C	1.321488	0.753612	3.061118
H	1.548475	1.796039	3.303605
H	2.011873	0.110273	3.620724
C	-0.116795	0.385277	3.549408
O	-0.444557	0.825118	4.641364
O	-0.801654	-0.387759	2.770875
Pd	0.059464	-0.818551	0.806725
C	3.846901	0.329953	-1.346907
C	2.410362	0.586414	-0.517568
B	1.188966	-0.568018	-0.935764
B	1.124020	1.133768	-1.551932
C	0.042269	2.155128	-1.014788
C	-1.324635	1.826005	-1.093716
C	0.376250	3.407377	-0.464550
C	-2.312488	2.699408	-0.640519
H	-1.624894	0.875331	-1.521737
C	-0.601401	4.284941	-0.007993
H	1.416579	3.712542	-0.398510
C	-1.955344	3.935469	-0.090167
H	-3.358417	2.423839	-0.708532
H	-0.339558	5.249571	0.413801
C	-2.959799	4.914232	0.417884
O	-2.681501	6.004716	0.877667
O	-4.226639	4.456611	0.311583
C	-5.241122	5.348569	0.799009
H	-6.187313	4.830525	0.643543
H	-5.088444	5.559689	1.860268
H	-5.222964	6.291158	0.246117
C	-2.704261	-1.708760	0.986785
C	-3.976551	-1.582977	0.435737

C	-4.170421	-1.717794	-0.948285
C	-3.078868	-1.985379	-1.786214
C	-1.799481	-2.118439	-1.253830
C	-1.615834	-1.919945	0.123821
H	-2.539489	-1.584472	2.050674
H	-4.823811	-1.380822	1.080875
H	-3.251910	-2.104770	-2.850526
H	-0.965236	-2.367288	-1.895780
I	0.171315	-3.552787	0.955491
C	-5.517533	-1.607284	-1.581951
O	-5.722587	-1.722171	-2.774608
O	-6.491816	-1.362440	-0.680197
C	-7.816285	-1.245357	-1.225110
H	-8.107321	-2.170986	-1.727696
H	-8.467372	-1.049285	-0.373633
H	-7.863728	-0.423941	-1.944298

18

Zero-point correction= 0.559990
Thermal correction to Energy= 0.601861
Thermal correction to Enthalpy= 0.602805
Thermal correction to Gibbs Free Energy= 0.481412
Sum of electronic and zero-point Energies= -1939.306327
Sum of electronic and thermal Energies= -1939.264456
Sum of electronic and thermal Enthalpies= -1939.263512
Sum of electronic and thermal Free Energies= -1939.384905

Cartesian coordinates

B	0.639292	-0.407083	-2.489274
B	3.371164	0.328317	-3.047062
B	1.693059	0.901552	-3.120462
B	2.742068	1.426454	-1.805045
B	2.073796	-0.806851	-3.468575
B	1.693029	-1.776724	-2.016788
B	3.379375	-1.315968	-2.375328
B	2.758211	-1.231445	-0.724428
H	3.173853	2.496920	-1.568821
H	3.183925	-1.814600	0.198397
H	1.352750	-2.907009	-2.070295
H	4.278684	-2.052147	-2.587354
H	1.989717	-1.258394	-4.560275
H	4.260345	0.700840	-3.729996
H	1.342629	1.676938	-3.943564
H	-0.461992	-0.571670	-2.887413

C	5.088446	0.325264	-0.819183
C	5.799898	1.469760	-1.214534
C	5.697273	-0.571485	0.072180
C	7.077357	1.718925	-0.715992
H	5.362645	2.163809	-1.922348
C	6.974544	-0.316496	0.570992
H	5.185652	-1.476976	0.372382
C	7.667677	0.829954	0.183059
H	7.610767	2.608567	-1.036322
H	7.427295	-1.022885	1.259882
H	8.662591	1.025245	0.571445
C	2.437487	0.924228	0.920863
H	3.054289	1.793811	1.157819
N	1.648327	0.372389	1.755163
C	1.270767	0.991005	3.003723
H	1.868667	1.873417	3.255221
H	1.342574	0.258041	3.813353
C	-0.238124	1.410014	2.874901
O	-0.686070	2.180793	3.701760
O	-0.903397	0.870747	1.888464
Pd	-0.064221	-0.878837	0.989033
C	3.716063	0.056221	-1.395177
C	2.348836	0.425469	-0.479905
B	1.069578	-0.654785	-0.786136
B	1.022006	1.013154	-1.472551
C	0.046613	2.154505	-0.989184
C	-1.333755	2.021293	-1.221471
C	0.494347	3.345239	-0.387589
C	-2.230047	3.025243	-0.864642
H	-1.717270	1.116110	-1.680494
C	-0.393152	4.352299	-0.023907
H	1.554523	3.504278	-0.209908
C	-1.764131	4.198950	-0.261172
H	-3.290908	2.900710	-1.048089
H	-0.045964	5.268951	0.440653
C	-2.669345	5.312953	0.142473
O	-2.292505	6.362189	0.627468
O	-3.970493	5.032926	-0.094492
C	-4.895284	6.063707	0.283305
H	-5.883378	5.679595	0.030007
H	-4.825539	6.268284	1.354555
H	-4.689257	6.986484	-0.265109
C	-2.957390	-0.911396	0.842045
C	-4.231206	-1.215561	0.357206

C	-4.385842	-2.069305	-0.742257
C	-3.253188	-2.621955	-1.353601
C	-1.977164	-2.339264	-0.869499
C	-1.837913	-1.470798	0.218873
H	-2.842117	-0.223573	1.671500
H	-5.104856	-0.782961	0.831590
H	-3.388101	-3.284329	-2.202333
H	-1.115964	-2.794211	-1.341586
I	0.639069	-3.427337	1.284537
C	-5.721354	-2.427537	-1.298300
O	-5.895323	-3.156709	-2.255696
O	-6.737108	-1.849263	-0.616980
C	-8.052041	-2.161004	-1.100758
H	-8.236174	-3.237063	-1.048725
H	-8.740477	-1.622525	-0.449511
H	-8.168667	-1.834988	-2.137440

19

Zero-point correction= 0.588844
Thermal correction to Energy= 0.635571
Thermal correction to Enthalpy= 0.636515
Thermal correction to Gibbs Free Energy= 0.504782
Sum of electronic and zero-point Energies= -2454.039182
Sum of electronic and thermal Energies= -2453.992455
Sum of electronic and thermal Enthalpies= -2453.991511
Sum of electronic and thermal Free Energies= -2454.123244

Cartesian coordinates

B	0.197336	-0.016129	2.509439
B	2.759122	-1.162794	3.190230
B	1.011954	-1.477993	3.165144
B	2.043156	-2.135290	1.894461
B	1.623388	0.148197	3.570454
B	1.472778	1.185474	2.123841
B	3.050514	0.470267	2.557276
B	2.518085	0.499969	0.876753
H	2.322197	-3.255369	1.658190
H	3.070709	1.021470	-0.013012
H	1.307011	2.350593	2.180582
H	4.037126	1.058960	2.830397
H	1.549869	0.591897	4.665709
H	3.541113	-1.674915	3.912703
H	0.507386	-2.206068	3.950575
H	-0.889000	0.309354	2.845168

C	4.579321	-1.380900	1.049419
C	5.097951	-2.619130	1.461543
C	5.352502	-0.572900	0.200666
C	6.349092	-3.046265	1.020651
H	4.531647	-3.247862	2.138353
C	6.602906	-1.006870	-0.239557
H	4.994211	0.399456	-0.113501
C	7.104233	-2.244145	0.164305
H	6.733153	-4.005871	1.352727
H	7.185776	-0.367597	-0.895295
H	8.079037	-2.577276	-0.178707
C	1.924626	-1.579339	-0.827440
H	2.295436	-2.586368	-1.031689
N	1.329143	-0.860573	-1.693232
C	0.769996	-1.396782	-2.909922
H	1.104864	-2.411834	-3.148720
H	0.990073	-0.730754	-3.750228
C	-0.783510	-1.418731	-2.696017
O	-1.467984	-2.091917	-3.436042
O	-1.257774	-0.685875	-1.706161
Pd	-0.046706	0.825772	-1.005916
C	3.234142	-0.923351	1.565337
C	1.876863	-1.072231	0.574268
B	0.767277	0.183075	0.847924
B	0.419979	-1.465499	1.484065
C	-0.684004	-2.443877	0.923650
C	-2.039412	-2.082929	1.024769
C	-0.386200	-3.704506	0.372876
C	-3.052242	-2.932522	0.588106
H	-2.308184	-1.115683	1.436635
C	-1.390567	-4.558087	-0.072409
H	0.644062	-4.041672	0.301795
C	-2.732852	-4.176575	0.031055
H	-4.090539	-2.632483	0.669401
H	-1.157645	-5.527722	-0.499369
C	-3.767204	-5.129308	-0.465696
O	-3.522334	-6.227201	-0.927048
O	-5.020649	-4.638811	-0.347277
C	-6.062463	-5.503257	-0.826017
H	-6.993218	-4.960085	-0.663255
H	-5.923810	-5.718700	-1.888362
H	-6.065286	-6.446014	-0.273055
C	-2.896557	1.343375	-0.554062
C	-4.021403	2.021605	-0.080537

C	-3.877403	3.198286	0.665268
C	-2.596264	3.696805	0.929661
C	-1.459758	3.035900	0.459858
C	-1.627813	1.859256	-0.273873
H	-3.012001	0.430775	-1.125426
H	-5.011745	1.634063	-0.291548
H	-2.498493	4.610643	1.506473
H	-0.476273	3.440348	0.663847
C	-5.046692	3.955178	1.198152
O	-4.965963	4.977499	1.850469
O	-6.226318	3.375666	0.876092
C	-7.393534	4.057143	1.360051
H	-7.441449	5.072158	0.957725
H	-8.242741	3.467472	1.014792
H	-7.382345	4.112606	2.451546
C	3.021977	3.864606	-1.589818
C	1.800538	3.399029	-0.743016
O	1.507600	4.000985	0.272059
O	1.290185	2.337391	-1.285125
F	3.513903	5.023503	-1.145957
F	4.009429	2.934350	-1.507602
F	2.704879	4.006573	-2.888778

20-ts

Zero-point correction= 0.588029
Thermal correction to Energy= 0.634142
Thermal correction to Enthalpy= 0.635086
Thermal correction to Gibbs Free Energy= 0.505803
Sum of electronic and zero-point Energies= -2454.011921
Sum of electronic and thermal Energies= -2453.965809
Sum of electronic and thermal Enthalpies= -2453.964865
Sum of electronic and thermal Free Energies= -2454.094148

Cartesian coordinates

B	-0.302174	0.214161	2.488052
B	1.677492	-1.673942	3.385884
B	-0.061964	-1.422158	3.150421
B	0.847824	-2.358115	1.976435
B	0.975856	-0.080306	3.688049
B	1.307864	0.961272	2.272599
B	2.524875	-0.211145	2.827486
B	2.189680	-0.007365	1.095906
H	0.760192	-3.505874	1.720680
H	3.011154	0.295062	0.322082

H	1.523486	2.114440	2.386378
H	3.607122	0.051983	3.220645
H	0.922075	0.369683	4.782375
H	2.177888	-2.414029	4.159167
H	-0.862700	-1.961239	3.836549
H	-1.265909	0.852275	2.741295
C	3.573611	-2.426539	1.445586
C	3.612608	-3.786054	1.795943
C	4.679878	-1.866397	0.786450
C	4.720876	-4.569557	1.479143
H	2.783576	-4.233077	2.331668
C	5.784586	-2.656594	0.468935
H	4.693983	-0.816839	0.520429
C	5.809171	-4.008954	0.809684
H	4.732343	-5.617597	1.762376
H	6.629398	-2.205372	-0.042025
H	6.672617	-4.619305	0.562871
C	1.333720	-1.958598	-0.669229
H	1.293195	-3.050401	-0.702900
N	1.323200	-1.256533	-1.732841
C	0.787162	-1.777940	-2.969606
H	0.765675	-2.872394	-3.027165
H	1.332463	-1.374180	-3.826612
C	-0.692163	-1.248060	-3.005291
O	-1.479314	-1.727780	-3.790657
O	-1.001883	-0.298572	-2.135672
Pd	0.552024	0.789184	-1.383913
C	2.377692	-1.588181	1.835609
C	1.176528	-1.306253	0.671913
B	0.411029	0.336201	0.858344
B	-0.417491	-1.202392	1.399533
C	-1.731789	-1.837129	0.782228
C	-2.978531	-1.306875	1.166298
C	-1.749848	-2.966662	-0.056072
C	-4.177941	-1.854597	0.716661
H	-3.012848	-0.451873	1.833400
C	-2.939990	-3.521341	-0.514740
H	-0.821669	-3.443673	-0.353319
C	-4.166625	-2.966571	-0.133633
H	-5.124476	-1.426931	1.027173
H	-2.941469	-4.387494	-1.167498
C	-5.412360	-3.605107	-0.646287
O	-5.437165	-4.604784	-1.337189
O	-6.527926	-2.948508	-0.254478

C	-7.763296	-3.514782	-0.718358
H	-8.548939	-2.871570	-0.322113
H	-7.792803	-3.529801	-1.810660
H	-7.880842	-4.536912	-0.349589
C	-2.029715	1.605550	-0.207532
C	-2.964784	2.563217	0.165760
C	-2.538362	3.804996	0.660519
C	-1.168850	4.081826	0.767727
C	-0.225128	3.127999	0.402299
C	-0.646430	1.861593	-0.063031
H	-2.363808	0.665271	-0.625539
H	-4.024162	2.360045	0.060587
H	-0.859732	5.054400	1.135367
H	0.832528	3.347684	0.490259
C	-3.500106	4.874886	1.069441
O	-3.168369	5.963942	1.492726
O	-4.786153	4.495545	0.915228
C	-5.764041	5.482430	1.284054
H	-5.640713	6.386556	0.683021
H	-6.732657	5.021800	1.091882
H	-5.664026	5.744433	2.340208
C	4.495676	2.618013	-1.443229
C	3.072263	2.609421	-0.815695
O	2.868626	3.239165	0.207454
O	2.301195	1.826684	-1.496915
F	5.250372	3.600406	-0.943932
F	5.103480	1.436227	-1.153702
F	4.466554	2.743273	-2.780353

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Zero-point correction= 0.591292
Thermal correction to Energy= 0.637669
Thermal correction to Enthalpy= 0.638613
Thermal correction to Gibbs Free Energy= 0.506469
Sum of electronic and zero-point Energies= -2454.102611
Sum of electronic and thermal Energies= -2454.056234
Sum of electronic and thermal Enthalpies= -2454.055290
Sum of electronic and thermal Free Energies= -2454.187434

Cartesian coordinates

B	-1.280436	-1.737152	3.106786
B	0.048145	-4.110876	2.158085
B	-1.541030	-3.377810	2.446553
B	-0.865042	-3.392544	0.822308

B	-0.199123	-3.067727	3.575260
B	0.478821	-1.467844	3.195229
B	1.297497	-2.931232	2.619042
B	1.116981	-1.518767	1.554667
H	-1.232227	-3.984878	-0.129010
H	2.022455	-0.913532	1.126979
H	0.997068	-0.787066	4.013601
H	2.391563	-3.270872	2.907512
H	-0.173906	-3.518522	4.670474
H	0.278576	-5.269173	2.121319
H	-2.484946	-4.045217	2.703179
H	-2.038604	-1.233380	3.865540
C	1.753281	-3.736434	-0.037815
C	1.379573	-4.903574	-0.724565
C	3.015422	-3.176490	-0.290753
C	2.238593	-5.483244	-1.656202
H	0.423566	-5.371549	-0.522277
C	3.869658	-3.759634	-1.226956
H	3.342279	-2.288684	0.234538
C	3.484750	-4.910194	-1.915383
H	1.933516	-6.387463	-2.173999
H	4.840944	-3.310312	-1.409484
H	4.153477	-5.362757	-2.641425
C	-0.261605	-1.444402	-0.893415
H	-1.097208	-1.890723	-1.435139
N	0.512078	-0.670047	-1.556906
C	0.159473	-0.410043	-2.964693
H	-0.789356	-0.875174	-3.246242
H	0.958634	-0.811895	-3.597584
C	0.096871	1.117696	-3.188896
O	-0.595726	1.594880	-4.061019
O	0.868287	1.807339	-2.375278
Pd	2.005214	0.715694	-1.170009
C	0.835839	-3.140726	0.999191
C	-0.222070	-1.819300	0.551529
B	-0.471252	-0.724123	1.869526
B	-1.742288	-1.942584	1.399337
C	-3.126517	-1.548433	0.735116
C	-3.911262	-0.537627	1.323415
C	-3.661473	-2.205497	-0.390374
C	-5.158303	-0.188640	0.810678
H	-3.539608	-0.014093	2.198084
C	-4.902664	-1.859014	-0.916756
H	-3.116438	-3.023029	-0.853741

C	-5.660242	-0.844696	-0.320331
H	-5.744738	0.591952	1.281492
H	-5.308467	-2.369239	-1.783926
C	-6.984488	-0.515289	-0.923368
O	-7.448483	-1.069039	-1.901128
O	-7.620484	0.475387	-0.260812
C	-8.902910	0.843456	-0.793490
H	-9.270269	1.642046	-0.149359
H	-8.804388	1.194531	-1.823669
H	-9.585330	-0.009913	-0.776144
C	-1.290464	1.409601	0.556379
C	-1.340074	2.787904	0.359537
C	-0.670819	3.643707	1.241814
C	0.043506	3.098973	2.315465
C	0.093948	1.720299	2.497164
C	-0.569494	0.836151	1.621783
H	-1.836082	0.776844	-0.135641
H	-1.890664	3.201214	-0.477232
H	0.555896	3.772746	2.994073
H	0.658326	1.323618	3.334437
C	-0.681349	5.127756	1.086467
O	-0.113882	5.898985	1.835619
O	-1.398004	5.527277	0.013871
C	-1.430025	6.945246	-0.209190
H	-0.419523	7.332307	-0.361572
H	-2.033734	7.087777	-1.105203
H	-1.879252	7.459140	0.644512
C	5.600056	1.538351	0.393985
C	4.211677	1.200509	-0.171128
O	3.575952	2.069074	-0.838167
O	3.728421	0.044090	0.001249
F	5.742986	2.855344	0.558727
F	5.785233	0.925896	1.570967
F	6.541858	1.104826	-0.465165

22

Zero-point correction= 0.571592

Thermal correction to Energy= 0.610008

Thermal correction to Enthalpy= 0.610952

Thermal correction to Gibbs Free Energy= 0.498116

Sum of electronic and zero-point Energies= -1801.773469

Sum of electronic and thermal Energies= -1801.735054

Sum of electronic and thermal Enthalpies= -1801.734110

Sum of electronic and thermal Free Energies= -1801.846946

Cartesian coordinates

B	-0.933410	0.558433	-2.942771
B	-3.594828	-0.383193	-2.383790
B	-1.966766	-0.890725	-2.863078
B	-2.480979	-1.089494	-1.192653
B	-2.632403	0.647194	-3.465788
B	-1.933911	1.963500	-2.486716
B	-3.574709	1.379355	-2.153704
B	-2.452731	1.720485	-0.820709
H	-2.678220	-2.083799	-0.592398
H	-2.635013	2.526555	0.020114
H	-1.745462	3.060355	-2.892320
H	-4.569265	2.014376	-2.220994
H	-2.946293	0.798096	-4.598309
H	-4.604030	-0.956332	-2.608021
H	-1.806039	-1.838968	-3.554231
H	-0.035345	0.640294	-3.711948
C	-4.545730	0.193066	0.185217
C	-5.064149	-1.058754	0.552860
C	-5.126014	1.348061	0.734918
C	-6.117330	-1.152042	1.461715
H	-4.654300	-1.964327	0.123463
C	-6.179736	1.250902	1.642451
H	-4.764853	2.327316	0.445227
C	-6.675981	0.000890	2.013886
H	-6.502329	-2.130257	1.732669
H	-6.614580	2.156577	2.053982
H	-7.496256	-0.073670	2.721307
C	-1.612199	0.032247	1.146290
H	-2.499652	0.263350	1.749144
N	-0.516916	-0.353724	1.650695
C	-0.420427	-0.504116	3.089454
H	-1.381249	-0.474779	3.619754
H	0.201130	0.315504	3.475233
C	0.304595	-1.805403	3.469423
O	0.234061	-2.265905	4.581730
O	1.042633	-2.358185	2.496932
C	-3.436174	0.307703	-0.834778
C	-1.778075	0.219047	-0.332984
B	-0.786645	1.252538	-1.305908
B	-0.800052	-0.551189	-1.545280
C	0.372786	-1.569727	-1.219616
C	1.639568	-1.170092	-0.748128

C	0.184903	-2.944396	-1.463996
C	2.660860	-2.091925	-0.525229
H	1.834139	-0.123462	-0.548778
C	1.197542	-3.873674	-1.242772
H	-0.769519	-3.297425	-1.840999
C	2.445185	-3.454954	-0.769507
H	3.626162	-1.759894	-0.160305
H	1.040138	-4.930476	-1.430473
C	3.494242	-4.490623	-0.544675
O	3.342254	-5.678403	-0.754018
O	4.648047	-3.963249	-0.077659
C	5.694467	-4.912666	0.176827
H	6.537569	-4.329130	0.546386
H	5.376227	-5.643548	0.924350
H	5.965467	-5.442337	-0.740019
C	1.549241	2.328402	-1.533721
C	2.618639	3.106502	-1.095993
C	2.586623	3.688705	0.177225
C	1.467455	3.486038	0.993765
C	0.405365	2.707103	0.545958
C	0.419772	2.099607	-0.723879
H	1.593093	1.888706	-2.525147
H	3.478021	3.266022	-1.737193
H	1.449682	3.951278	1.973776
H	-0.452103	2.580470	1.199194
C	3.698455	4.527014	0.708719
O	3.700291	5.051305	1.805935
O	4.721899	4.643266	-0.167476
C	5.829200	5.436565	0.286614
H	6.263237	5.008280	1.193638
H	6.553451	5.423956	-0.527739
H	5.508537	6.459342	0.499991
H	0.936266	-1.842019	1.673925

23-ts

Zero-point correction= 0.462331
Thermal correction to Energy= 0.498918
Thermal correction to Enthalpy= 0.499863
Thermal correction to Gibbs Free Energy= 0.393791
Sum of electronic and zero-point Energies= -1995.188525
Sum of electronic and thermal Energies= -1995.151938
Sum of electronic and thermal Enthalpies= -1995.150994
Sum of electronic and thermal Free Energies= -1995.257065

Cartesian coordinates

B	-1.200762	-2.160754	-1.672857
B	1.263711	-1.846314	-3.130636
B	-0.040039	-0.932011	-2.287765
B	-0.384518	-2.465622	-3.204042
B	-0.530367	-3.764827	-1.986381
B	0.955088	-3.594795	-2.939012
B	1.041461	-3.907713	-1.194470
H	1.469018	-4.859779	-0.634943
H	-0.643620	-3.425363	0.646305
H	-1.247171	-4.702824	-2.087321
H	1.314002	-4.383534	-3.746923
H	-0.997942	-2.438253	-4.217375
H	1.847915	-1.321171	-4.012642
H	-0.307181	0.130594	-2.726986
H	-2.365491	-1.965881	-1.614857
C	2.041195	-2.431154	0.842317
H	2.466099	-3.400812	1.122736
N	1.938030	-1.488124	1.694294
C	1.995833	-1.777851	3.113127
H	2.452063	-0.946936	3.658032
H	2.522835	-2.707710	3.357117
C	0.503065	-1.927588	3.543128
O	0.215053	-2.425011	4.608701
O	-0.402178	-1.511800	2.664678
Pd	0.222148	-0.140908	1.282100
C	1.360164	-2.390494	-0.490111
B	-0.271167	-2.982444	-0.384897
B	-0.309058	-1.196519	-0.542559
C	-1.656418	-0.064930	0.377705
C	-2.051377	1.015999	-0.440065
C	-2.646600	-0.836661	1.034014
C	-3.403462	1.270995	-0.650756
H	-1.303498	1.636545	-0.918632
C	-3.990843	-0.572340	0.817714
H	-2.354873	-1.636494	1.702765
C	-4.376728	0.477197	-0.029909
H	-3.705127	2.089616	-1.293619
H	-4.760857	-1.163373	1.301492
C	-5.843269	0.708674	-0.224401
O	-6.710128	0.043240	0.305513
O	-6.093291	1.739398	-1.055247
C	-7.485157	2.017444	-1.288220
H	-7.503727	2.863441	-1.974384

H	-7.978758	1.149313	-1.731474
H	-7.986210	2.269273	-0.350504
C	1.925786	3.782350	0.526151
C	1.009986	2.631653	0.010490
O	0.287232	2.849988	-0.946154
O	1.157945	1.571115	0.735346
F	3.050922	3.336456	1.109459
F	2.274312	4.594254	-0.482838
F	1.245537	4.510608	1.436279
B	2.173081	-2.797921	-1.948868
C	1.503272	-1.214484	-1.567865
H	3.347897	-2.894749	-1.918103
C	2.558752	-0.133648	-1.471199
C	2.413600	1.029599	-2.241222
C	3.749699	-0.307291	-0.749079
C	3.407783	2.006891	-2.252710
H	1.514913	1.188663	-2.821398
C	4.742929	0.669757	-0.762612
H	3.928304	-1.210543	-0.180712
C	4.573514	1.836823	-1.507173
H	3.257953	2.907178	-2.839529
H	5.652493	0.512070	-0.191053
H	5.344473	2.601008	-1.511932

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Zero-point correction= 0.258185
Thermal correction to Energy= 0.270645
Thermal correction to Enthalpy= 0.271589
Thermal correction to Gibbs Free Energy= 0.220604
Sum of electronic and zero-point Energies= -562.903835
Sum of electronic and thermal Energies= -562.891375
Sum of electronic and thermal Enthalpies= -562.890431
Sum of electronic and thermal Free Energies= -562.941415

Cartesian coordinates

B	2.405080	0.337784	1.479046
B	0.945303	-1.541947	-0.146703
B	0.933922	-0.666306	1.402448
B	2.461156	-1.286867	0.738044
B	3.325290	0.067688	-0.031506
B	2.414916	-1.097590	-1.040638
B	2.336847	0.640159	-1.390628
H	2.675245	1.191397	-2.381262

H	2.659120	2.658674	0.189087
H	4.507760	0.141759	-0.068168
H	2.929258	-1.860630	-1.787588
H	3.015831	-2.197695	1.256052
H	0.358663	-2.560435	-0.265219
H	0.304673	-1.079473	2.314534
H	2.912964	0.603068	2.516511
C	0.886022	1.143667	-0.661292
B	2.324573	1.524327	0.155447
B	0.862186	1.071279	1.053412
B	0.871411	-0.364048	-1.471051
C	0.053339	-0.087515	0.043882
H	0.191287	-0.472789	-2.429215
H	0.185212	1.841710	1.636101
H	0.277303	1.914310	-1.115219
C	-1.457389	-0.034709	0.016827
C	-2.200416	-1.222988	0.019559
C	-2.143552	1.188260	0.005647
C	-3.594286	-1.186755	0.004576
H	-1.690616	-2.178167	0.036060
C	-3.537412	1.221238	-0.016327
H	-1.598996	2.125997	0.032823
C	-4.269191	0.033781	-0.017388
H	-4.150847	-2.119064	0.009287
H	-4.048408	2.179250	-0.025301
H	-5.354563	0.059828	-0.030736

25-ts

Zero-point correction= 0.494826

Thermal correction to Energy= 0.534076

Thermal correction to Enthalpy= 0.535020

Thermal correction to Gibbs Free Energy= 0.422680

Sum of electronic and zero-point Energies= -2109.681050

Sum of electronic and thermal Energies= -2109.641800

Sum of electronic and thermal Enthalpies= -2109.640856

Sum of electronic and thermal Free Energies= -2109.753196

Cartesian coordinates

B	-1.831005	-2.044155	-1.752602
B	0.678042	-2.083184	-3.162206
B	-0.500979	-1.003887	-2.345990
B	-1.040983	-2.456584	-3.279468
B	-1.406402	-3.731517	-2.086823

B	0.117836	-3.767755	-2.998124
B	0.107169	-4.111958	-1.259939
H	0.389528	-5.121297	-0.708704
H	-1.541954	-3.405414	0.550187
H	-2.249069	-4.553435	-2.220330
H	0.388469	-4.592001	-3.805043
H	-1.620924	-2.328107	-4.304723
H	1.363173	-1.641691	-4.017087
H	-0.609767	0.096469	-2.757664
H	-2.952163	-1.672660	-1.710402
C	1.262705	-2.864328	0.828295
H	1.524562	-3.901457	1.062120
N	1.282330	-1.962187	1.728419
C	1.229425	-2.324112	3.130085
H	1.793153	-1.609472	3.735601
H	1.578552	-3.341480	3.342099
C	-0.288608	-2.234155	3.494961
O	-0.701165	-2.724986	4.522114
O	-1.068636	-1.628962	2.608083
Pd	-0.147264	-0.337726	1.316178
C	0.619475	-2.663267	-0.512021
B	-1.081091	-3.025431	-0.469576
B	-0.766176	-1.268713	-0.604241
C	-1.920393	0.086812	0.302410
C	-2.063793	1.261214	-0.468510
C	-3.069676	-0.500056	0.888111
C	-3.328363	1.796921	-0.694791
H	-1.190953	1.748445	-0.885144
C	-4.324850	0.042658	0.657632
H	-2.968129	-1.375491	1.517092
C	-4.462195	1.189457	-0.139440
H	-3.436514	2.691625	-1.296624
H	-5.213894	-0.402216	1.091225
C	-5.843239	1.726782	-0.351009
O	-6.844919	1.228192	0.121585
O	-5.850881	2.828891	-1.126643
C	-7.148093	3.399878	-1.370200
H	-6.971303	4.268759	-2.003265
H	-7.794118	2.678280	-1.875966
H	-7.617693	3.696577	-0.429301
C	2.319337	3.201502	0.913418
C	1.202037	2.312859	0.286127
O	0.538917	2.770198	-0.627514
O	1.144232	1.170316	0.889351

F	3.382352	2.484972	1.334225
F	2.756431	4.109871	0.033824
F	1.818222	3.854391	1.983226
B	1.403398	-3.156344	-1.960509
C	0.958865	-1.491644	-1.579297
H	2.551907	-3.416224	-1.893609
C	2.142853	-0.568490	-1.434514
C	2.194706	0.609439	-2.200948
C	3.267914	-0.893738	-0.667625
C	3.300066	1.444745	-2.160305
H	1.356866	0.891896	-2.824380
C	4.381547	-0.058937	-0.609626
H	3.303282	-1.813708	-0.098734
C	4.398297	1.131535	-1.346807
H	3.321557	2.365213	-2.732844
H	5.221395	-0.344450	0.011738
O	5.417370	2.025729	-1.350805
C	6.474373	1.849647	-0.415636
H	7.131931	2.710410	-0.542530
H	6.091491	1.831193	0.611372
H	7.042686	0.932109	-0.613511

26-ts

Zero-point correction= 0.495687
Thermal correction to Energy= 0.534873
Thermal correction to Enthalpy= 0.535817
Thermal correction to Gibbs Free Energy= 0.422401
Sum of electronic and zero-point Energies= -2109.697996
Sum of electronic and thermal Energies= -2109.658810
Sum of electronic and thermal Enthalpies= -2109.657865
Sum of electronic and thermal Free Energies= -2109.771281

Cartesian coordinates

B	-1.025371	-2.227605	-1.437445
B	1.300426	-0.993657	-2.608450
B	-0.388580	-0.697983	-2.127571
B	0.929630	-0.147839	-1.087841
B	0.091197	-2.282762	-2.814623
B	0.282937	-3.436238	-1.464075
B	1.706137	-2.686626	-2.221227
B	1.599073	-2.856955	-0.462927
H	1.304947	0.934047	-0.850831
H	2.341892	-3.467453	0.220768

H	-0.428077	-3.035722	1.062776
H	0.079749	-4.600082	-1.549786
H	2.572564	-3.246730	-2.797366
H	-0.263239	-2.614972	-3.895091
H	1.889528	-0.409658	-3.449583
H	-1.037721	0.077425	-2.735205
H	-2.160477	-2.547697	-1.519992
C	3.606395	-1.006078	-0.994001
C	4.024402	0.338965	-1.014875
C	4.584920	-1.996480	-0.835218
C	5.361828	0.670181	-0.862145
H	3.308552	1.139792	-1.153382
C	5.933055	-1.674507	-0.685708
H	4.302768	-3.042968	-0.841930
C	6.331158	-0.331437	-0.694654
H	5.682798	1.706094	-0.877527
H	6.655770	-2.472969	-0.570729
C	1.663495	-1.008819	1.479565
H	2.355293	-1.738831	1.910212
N	1.162007	-0.071192	2.181610
C	1.111849	-0.183863	3.623679
H	1.182256	0.801714	4.090713
H	1.872592	-0.849205	4.048565
C	-0.301389	-0.800617	3.916459
O	-0.539415	-1.260603	5.011665
O	-1.160985	-0.810663	2.908302
Pd	-0.822054	0.533469	1.408912
C	2.165967	-1.398433	-1.197799
C	1.118681	-1.323517	0.118066
B	-0.090031	-2.546119	0.041153
B	-0.586591	-0.872569	-0.366249
C	-2.414982	-0.173828	0.270187
C	-3.021940	0.664591	-0.690008
C	-3.188228	-1.179271	0.898020
C	-4.354109	0.467096	-1.044796
H	-2.441833	1.443578	-1.171099
C	-4.512886	-1.370943	0.534139
H	-2.746965	-1.797162	1.670100
C	-5.102516	-0.551761	-0.440963
H	-4.815337	1.104185	-1.790441
H	-5.113930	-2.145018	0.998835
C	-6.534347	-0.807927	-0.788952
O	-7.210696	-1.683397	-0.286639
O	-6.995408	0.044146	-1.727352

C	-8.367359	-0.148757	-2.110129
H	-8.571716	0.612691	-2.862218
H	-8.511790	-1.149310	-2.525044
H	-9.026498	-0.025867	-1.247312
C	0.713840	4.123895	-0.501076
C	-0.299886	2.944818	-0.551375
O	-0.289901	2.309305	0.574262
O	-0.899585	2.722978	-1.588941
F	0.506425	4.994210	-1.493479
F	0.671755	4.791879	0.663421
F	1.968885	3.620764	-0.642205
O	7.609499	0.098595	-0.556284
C	8.641243	-0.868840	-0.402484
H	9.569786	-0.303724	-0.316531
H	8.497572	-1.469016	0.504395
H	8.701019	-1.533995	-1.272521

27

Zero-point correction= 0.290605
Thermal correction to Energy= 0.305764
Thermal correction to Enthalpy= 0.306708
Thermal correction to Gibbs Free Energy= 0.248719
Sum of electronic and zero-point Energies= -677.395927
Sum of electronic and thermal Energies= -677.380768
Sum of electronic and thermal Enthalpies= -677.379823
Sum of electronic and thermal Free Energies= -677.437813

Cartesian coordinates

B	-3.219846	-0.443994	1.395990
B	-1.631461	1.558197	0.065794
B	-1.704911	0.489857	1.487652
B	-3.183689	1.263166	0.873902
B	-4.084170	0.062538	-0.087374
B	-3.094006	1.305070	-0.913593
B	-3.081862	-0.375056	-1.486558
H	-3.416265	-0.776502	-2.548146
H	-3.534771	-2.562751	-0.190797
H	-5.267335	0.048859	-0.159555
H	-3.552298	2.182927	-1.565014
H	-3.712017	2.125102	1.493491
H	-1.001007	2.556911	0.100663
H	-1.086596	0.752669	2.460939
H	-3.768868	-0.819363	2.377155

C	-1.675599	-1.035076	-0.796290
B	-3.151132	-1.449936	-0.070233
B	-1.697176	-1.185390	0.913523
B	-1.573011	0.560955	-1.399754
C	-0.807991	0.053785	0.084825
H	-0.861432	0.761814	-2.319347
H	-1.080137	-2.059463	1.409474
H	-1.084326	-1.767477	-1.330025
C	0.696648	-0.065908	0.061747
C	1.500134	1.078466	0.062439
C	1.335034	-1.318480	0.032737
C	2.892422	0.991928	0.035259
H	1.041008	2.059159	0.083893
C	2.717911	-1.418703	-0.002365
H	0.753030	-2.233663	0.049037
C	3.512517	-0.262442	-0.001116
H	3.475488	1.904807	0.039201
H	3.207963	-2.386155	-0.025708
O	4.855832	-0.465575	-0.035860
C	5.711454	0.669625	-0.038282
H	6.728818	0.277865	-0.069473
H	5.539799	1.301280	-0.918746
H	5.583440	1.272384	0.869368

28-ts

Zero-point correction= 0.467313

Thermal correction to Energy= 0.507459

Thermal correction to Enthalpy= 0.508403

Thermal correction to Gibbs Free Energy= 0.394009

Sum of electronic and zero-point Energies= -2332.215146

Sum of electronic and thermal Energies= -2332.175000

Sum of electronic and thermal Enthalpies= -2332.174056

Sum of electronic and thermal Free Energies= -2332.288450

Cartesian coordinates

B	-2.133132	-1.718446	-1.951490
B	0.455372	-1.904188	-3.203249
B	-0.645037	-0.779161	-2.322800
B	-1.282193	-2.053589	-3.457006
B	-1.865459	-3.397616	-2.434000
B	-0.303767	-3.519404	-3.265714
B	-0.460484	-4.038494	-1.576024
H	-0.343683	-5.126255	-1.122972

H	-2.128978	-3.344525	0.205842
H	-2.784805	-4.095307	-2.700988
H	-0.085210	-4.276373	-4.150217
H	-1.771444	-1.750317	-4.492421
H	1.231349	-1.452109	-3.970491
H	-0.589476	0.357892	-2.634211
H	-3.210351	-1.231063	-1.939227
C	0.678629	-3.117380	0.698003
H	0.825368	-4.188703	0.871137
N	0.713695	-2.284842	1.663228
C	0.547724	-2.739590	3.029569
H	1.136741	-2.124265	3.715179
H	0.797475	-3.796141	3.180517
C	-0.971702	-2.541524	3.326945
O	-1.486750	-3.070971	4.285696
O	-1.645948	-1.795835	2.458004
Pd	-0.551994	-0.499943	1.318036
C	0.168000	-2.749504	-0.660174
B	-1.563349	-2.895719	-0.730355
B	-1.152467	-1.148797	-0.647403
C	-2.248439	0.204395	0.333799
C	-2.257600	1.433960	-0.359289
C	-3.468021	-0.337536	0.807337
C	-3.466253	2.068899	-0.630566
H	-1.327902	1.875078	-0.698438
C	-4.666054	0.305148	0.531269
H	-3.467042	-1.254673	1.382935
C	-4.672673	1.507159	-0.192742
H	-3.474421	3.003677	-1.178731
H	-5.610395	-0.103144	0.874563
C	-5.998762	2.150486	-0.458605
O	-7.059942	1.692375	-0.086003
O	-5.880738	3.295223	-1.158644
C	-7.118077	3.968780	-1.450193
H	-6.840293	4.861960	-2.008679
H	-7.770203	3.326815	-2.047156
H	-7.634105	4.236031	-0.525064
C	2.196405	2.863792	1.209862
C	1.071078	2.068437	0.480743
O	0.541697	2.569922	-0.495751
O	0.855944	0.936209	1.068399
F	3.075765	2.065698	1.836481
F	2.870086	3.625324	0.336606
F	1.635085	3.672803	2.131906

B	0.981890	-3.190822	-2.107089
C	0.699708	-1.540248	-1.560355
H	2.086578	-3.594418	-2.019644
C	1.980355	-0.793354	-1.254854
C	2.219874	0.435446	-1.888141
C	3.005531	-1.346084	-0.472746
C	3.423020	1.110681	-1.706151
H	1.460747	0.884256	-2.513506
C	4.208671	-0.672060	-0.285651
H	2.890386	-2.316576	-0.009561
C	4.418163	0.564832	-0.894733
H	3.581008	2.066324	-2.192828
H	4.988176	-1.114592	0.323954
C	5.688081	1.335758	-0.646212
F	5.524055	2.257119	0.326441
F	6.091089	1.996026	-1.753495
F	6.699406	0.525314	-0.262704

29-ts

Zero-point correction= 0.467880
Thermal correction to Energy= 0.508066
Thermal correction to Enthalpy= 0.509010
Thermal correction to Gibbs Free Energy= 0.392470
Sum of electronic and zero-point Energies= -2332.230694
Sum of electronic and thermal Energies= -2332.190509
Sum of electronic and thermal Enthalpies= -2332.189565
Sum of electronic and thermal Free Energies= -2332.306105

Cartesian coordinates

B	-1.420710	-2.201737	-1.458579
B	0.941118	-1.003173	-2.592323
B	-0.745928	-0.677609	-2.122830
B	0.571509	-0.168516	-1.064250
B	-0.292657	-2.262986	-2.827342
B	-0.141319	-3.439790	-1.490812
B	1.305641	-2.711797	-2.224704
B	1.179094	-2.907965	-0.470317
H	0.971804	0.900356	-0.810833
H	1.907074	-3.540660	0.209151
H	-0.861810	-3.053444	1.036817
H	-0.369585	-4.597120	-1.595109
H	2.166770	-3.279752	-2.800721
H	-0.643480	-2.572541	-3.915350

H	1.555218	-0.422060	-3.417359
H	-1.371005	0.120665	-2.725627
H	-2.561343	-2.496277	-1.555159
C	3.232189	-1.093454	-0.959083
C	3.669398	0.239750	-0.914415
C	4.183276	-2.120030	-0.850492
C	5.020353	0.533946	-0.743922
H	2.968596	1.058241	-1.018054
C	5.533389	-1.824978	-0.683587
H	3.874237	-3.156480	-0.911747
C	5.954617	-0.495825	-0.624684
H	5.346147	1.567959	-0.717896
H	6.259112	-2.627207	-0.611220
C	1.268240	-1.083587	1.500225
H	1.934599	-1.836944	1.931274
N	0.778727	-0.143084	2.206504
C	0.709128	-0.269152	3.646753
H	0.796697	0.709998	4.124235
H	1.448966	-0.956117	4.073829
C	-0.721695	-0.855299	3.917161
O	-0.982373	-1.322168	5.003729
O	-1.571142	-0.833247	2.900070
Pd	-1.186376	0.517422	1.419278
C	1.777676	-1.448247	-1.175529
C	0.734229	-1.366776	0.126610
B	-0.504532	-2.560491	0.023640
B	-0.964872	-0.869640	-0.365396
C	-2.785051	-0.143469	0.264037
C	-3.366616	0.718625	-0.690808
C	-3.581370	-1.144226	0.870318
C	-4.697703	0.547757	-1.063204
H	-2.768248	1.494605	-1.154161
C	-4.904431	-1.309097	0.488352
H	-3.159462	-1.779311	1.639245
C	-5.469105	-0.467170	-0.482210
H	-5.140387	1.202519	-1.804739
H	-5.523441	-2.079323	0.935537
C	-6.901026	-0.696002	-0.850294
O	-7.595624	-1.567845	-0.367268
O	-7.337315	0.175558	-1.781857
C	-8.708021	0.009778	-2.183080
H	-8.891245	0.784214	-2.927210
H	-8.863093	-0.982871	-2.612735
H	-9.374764	0.131964	-1.326098

C	0.462140	4.078326	-0.449575
C	-0.589718	2.933876	-0.513759
O	-0.600484	2.286178	0.605287
O	-1.195516	2.741275	-1.553489
F	0.300623	4.952608	-1.445938
F	0.425290	4.747714	0.713599
F	1.702317	3.531419	-0.570693
C	7.407183	-0.171330	-0.383678
F	7.770021	0.974252	-0.996133
F	8.218830	-1.153061	-0.829177
F	7.658617	-0.014069	0.935407

30

Zero-point correction= 0.262816
Thermal correction to Energy= 0.278981
Thermal correction to Enthalpy= 0.279925
Thermal correction to Gibbs Free Energy= 0.218615
Sum of electronic and zero-point Energies= -899.930234
Sum of electronic and thermal Energies= -899.914069
Sum of electronic and thermal Enthalpies= -899.913125
Sum of electronic and thermal Free Energies= -899.974436

Cartesian coordinates

B	-3.746540	-0.334103	1.494056
B	-2.315688	1.539266	-0.165145
B	-2.283385	0.679378	1.393237
B	-3.820878	1.282847	0.736566
B	-4.682514	-0.085361	-0.011090
B	-3.789468	1.075676	-1.040685
B	-3.702576	-0.665640	-1.373744
H	-4.045429	-1.229152	-2.355616
H	-3.997193	-2.670023	0.229717
H	-5.864473	-0.167512	-0.036201
H	-4.315254	1.827270	-1.790827
H	-4.376258	2.195143	1.250556
H	-1.734713	2.558967	-0.299788
H	-1.646203	1.105518	2.293709
H	-4.242404	-0.591545	2.538968
C	-2.242464	-1.152780	-0.652472
B	-3.671322	-1.533931	0.181496
B	-2.203848	-1.063031	1.061639
B	-2.244974	0.348018	-1.478612
C	-1.414074	0.091863	0.032022

H	-1.572753	0.450910	-2.442980
H	-1.513422	-1.821372	1.644553
H	-1.633985	-1.924414	-1.105173
C	0.096390	0.051260	-0.001949
C	0.829531	1.245708	-0.000920
C	0.793597	-1.165131	-0.016437
C	2.221586	1.224511	-0.017218
H	0.313416	2.197131	0.013370
C	2.185572	-1.188583	-0.039156
H	0.259586	-2.108406	0.007226
C	2.904321	0.007446	-0.039138
H	2.775791	2.156667	-0.021546
H	2.711495	-2.136654	-0.057727
C	4.409908	-0.016023	0.000925
F	4.908426	-1.117791	-0.600494
F	4.942858	1.062893	-0.611038
F	4.868890	-0.017076	1.272558

31-ts

Zero-point correction= 0.372998
Thermal correction to Energy= 0.405792
Thermal correction to Enthalpy= 0.406736
Thermal correction to Gibbs Free Energy= 0.308624
Sum of electronic and zero-point Energies= -1863.457424
Sum of electronic and thermal Energies= -1863.424630
Sum of electronic and thermal Enthalpies= -1863.423685
Sum of electronic and thermal Free Energies= -1863.521798

Cartesian coordinates

B	-0.471230	-2.252539	-1.687034
B	1.748862	-1.297553	-3.278245
B	0.275639	-0.775731	-2.378727
B	0.312457	-2.333708	-3.280312
B	0.571478	-3.631326	-2.081294
B	1.917183	-3.071314	-3.110069
B	2.172842	-3.385199	-1.376858
H	2.865242	-4.197765	-0.865707
H	0.505426	-3.352293	0.567500
H	0.118253	-4.720670	-2.181073
H	2.417640	-3.735018	-3.953396
H	-0.340441	-2.461998	-4.259985
H	2.140908	-0.597941	-4.144898
H	-0.224272	0.218094	-2.760653

H	-1.639217	-2.372111	-1.547138
C	2.927443	-1.645046	0.592120
H	3.595133	-2.469296	0.862340
N	2.695350	-0.686607	1.399649
C	2.944521	-0.863719	2.817541
H	3.211513	0.087013	3.285632
H	3.711368	-1.612941	3.045265
C	1.575471	-1.368068	3.384853
O	1.514747	-1.858909	4.489385
O	0.529341	-1.254374	2.573696
Pd	0.682461	0.167662	1.111071
C	2.124363	-1.861009	-0.648485
B	0.707087	-2.831911	-0.474024
B	0.266213	-1.082236	-0.624438
C	-1.232099	-0.195238	0.383666
C	-1.902469	0.763891	-0.406348
C	-1.983354	-1.119572	1.146440
C	-3.292446	0.761875	-0.467973
H	-1.333984	1.474544	-0.994424
C	-3.369531	-1.114678	1.073714
H	-1.477165	-1.827190	1.791742
C	-4.030271	-0.176479	0.267243
H	-3.808449	1.488096	-1.085034
H	-3.961482	-1.823067	1.642994
C	-5.526819	-0.219206	0.237553
O	-6.193404	-1.021490	0.859563
O	-6.050290	0.734578	-0.556659
C	-7.486968	0.753580	-0.630371
H	-7.734602	1.576195	-1.300274
H	-7.861097	-0.193470	-1.026427
H	-7.917504	0.918333	0.360157
C	1.595625	4.139117	-0.418835
C	0.913327	2.757633	-0.642974
O	0.330476	2.524118	-1.685918
O	1.088417	2.015561	0.404007
F	2.920203	3.983831	-0.223601
F	1.417897	4.939593	-1.473866
F	1.082692	4.749530	0.667127
B	2.931028	-2.000271	-2.161258
C	1.831333	-0.706685	-1.699162
H	4.077677	-1.720898	-2.163187
F	2.462936	0.457144	-1.472487

32-ts

Zero-point correction= 0.373681
Thermal correction to Energy= 0.406217
Thermal correction to Enthalpy= 0.407162
Thermal correction to Gibbs Free Energy= 0.309509
Sum of electronic and zero-point Energies= -1863.459367
Sum of electronic and thermal Energies= -1863.426830
Sum of electronic and thermal Enthalpies= -1863.425886
Sum of electronic and thermal Free Energies= -1863.523539

Cartesian coordinates

B	-0.395505	-2.349640	-1.556230
B	1.734500	-1.285535	-3.173704
B	0.199016	-0.867680	-2.371529
B	1.725959	-0.410499	-1.616316
B	0.417044	-2.478829	-3.133229
B	0.770277	-3.666002	-1.842035
B	2.076342	-3.025484	-2.870852
B	2.301982	-3.226803	-1.123780
H	2.306631	0.601592	-1.486397
H	3.165210	-3.861043	-0.629243
H	0.610699	-3.229791	0.778443
H	0.452564	-4.805535	-1.884117
H	2.799515	-3.616790	-3.593390
H	-0.170244	-2.767552	-4.119846
H	2.225139	-0.749836	-4.104358
H	-0.502649	-0.048345	-2.845391
H	-1.545772	-2.579712	-1.412275
C	2.924583	-1.377264	0.738609
H	3.634875	-2.160100	1.020193
N	2.645736	-0.411833	1.521672
C	2.884186	-0.540505	2.944167
H	3.104681	0.432590	3.389487
H	3.673817	-1.254891	3.204405
C	1.522992	-1.083289	3.511962
O	1.482662	-1.542635	4.631545
O	0.483541	-1.036258	2.691792
Pd	0.585546	0.339179	1.179102
C	2.759974	-1.791259	-1.939407
C	2.072223	-1.641072	-0.468687
B	0.785046	-2.766131	-0.293593
B	0.350458	-1.041177	-0.598256
C	-1.253379	-0.200566	0.380013
C	-1.947317	0.685747	-0.471910

C	-1.984970	-1.120113	1.167301
C	-3.334539	0.620747	-0.564416
H	-1.397444	1.390396	-1.083884
C	-3.367807	-1.178574	1.066226
H	-1.465994	-1.772025	1.859414
C	-4.049898	-0.311109	0.199743
H	-3.864884	1.293405	-1.228352
H	-3.942125	-1.883068	1.658040
C	-5.540931	-0.420486	0.139101
O	-6.189786	-1.219507	0.784212
O	-6.085742	0.470320	-0.713358
C	-7.519124	0.423474	-0.818658
H	-7.785353	1.198066	-1.537098
H	-7.844685	-0.558271	-1.170839
H	-7.980090	0.621995	0.151876
C	1.407027	4.219008	-0.627493
C	0.776424	2.801901	-0.760190
O	0.933133	2.151276	0.346785
O	0.256595	2.460613	-1.808661
F	1.192388	4.947342	-1.727520
F	0.890973	4.880140	0.425632
F	2.739968	4.115787	-0.443035
F	4.077268	-1.517923	-1.965759

33

Zero-point correction= 0.168517
Thermal correction to Energy= 0.177176
Thermal correction to Enthalpy= 0.178120
Thermal correction to Gibbs Free Energy= 0.136656
Sum of electronic and zero-point Energies= -431.160020
Sum of electronic and thermal Energies= -431.151362
Sum of electronic and thermal Enthalpies= -431.150417
Sum of electronic and thermal Free Energies= -431.191881

Cartesian coordinates

B	1.069474	1.458223	0.442350
B	-0.419082	-0.883417	1.272522
B	-0.418897	0.910707	1.254113
B	1.095921	0.016050	1.504179
B	1.991698	-0.000287	-0.037089
B	1.069518	-1.448352	0.473210
B	1.026810	-0.906245	-1.223101
H	1.388703	-1.505054	-2.176241

H	1.387860	1.459681	-2.207416
H	3.174975	-0.000470	-0.091286
H	1.581448	-2.470615	0.782855
H	1.630143	0.027017	2.561833
H	-1.083801	-1.452856	2.066318
H	-1.084654	1.496710	2.034828
H	1.581047	2.487132	0.729657
C	-0.413641	-0.014555	-1.342644
B	1.026043	0.879868	-1.242600
B	-0.451582	1.453295	-0.440431
B	-0.451344	-1.462615	-0.410174
C	-1.222295	0.000546	0.074668
H	-1.159338	-2.326606	-0.789025
F	-2.565943	-0.000241	-0.022712
H	-1.041039	-0.023816	-2.225420
H	-1.159032	2.308963	-0.838729

34-ts

Zero-point correction= 0.371349
Thermal correction to Energy= 0.404552
Thermal correction to Enthalpy= 0.405496
Thermal correction to Gibbs Free Energy= 0.306629
Sum of electronic and zero-point Energies= -2223.807982
Sum of electronic and thermal Energies= -2223.774780
Sum of electronic and thermal Enthalpies= -2223.773835
Sum of electronic and thermal Free Energies= -2223.872702

Cartesian coordinates

B	-0.703881	-2.076702	-1.664577
B	1.655583	-1.503065	-3.236674
B	0.295291	-0.718976	-2.316868
B	0.074780	-2.286240	-3.229727
B	0.125148	-3.597777	-2.009679
B	1.535383	-3.278173	-3.037501
B	1.741618	-3.582161	-1.294699
H	2.286256	-4.487473	-0.760530
H	0.107425	-3.279978	0.625178
H	-0.494752	-4.604245	-2.085929
H	1.920045	-4.028470	-3.869189
H	-0.583898	-2.323687	-4.213390
H	2.133468	-0.901115	-4.132490
H	-0.045293	0.327042	-2.742205
H	-1.879835	-2.016132	-1.550855
C	2.704322	-1.923050	0.663023

H	3.284254	-2.802518	0.961254
N	2.524864	-0.946297	1.463095
C	2.733383	-1.134666	2.886003
H	3.084891	-0.209625	3.350864
H	3.423138	-1.950232	3.131662
C	1.320672	-1.498924	3.440569
O	1.194641	-1.980553	4.543714
O	0.297017	-1.280471	2.620348
Pd	0.580700	0.124630	1.161800
C	1.934840	-2.047944	-0.609234
B	0.376599	-2.789217	-0.416174
B	0.070220	-1.017124	-0.555264
C	-1.370436	-0.054130	0.474323
C	-1.971058	0.922320	-0.348573
C	-2.180740	-0.946872	1.213696
C	-3.356923	0.955688	-0.478260
H	-1.355054	1.614186	-0.911247
C	-3.560703	-0.902305	1.074195
H	-1.725548	-1.664142	1.885365
C	-4.154908	0.044955	0.226842
H	-3.821317	1.689518	-1.126540
H	-4.199349	-1.587701	1.620751
C	-5.649163	0.040814	0.122856
O	-6.366619	-0.731485	0.725805
O	-6.106421	0.990851	-0.714938
C	-7.536739	1.044277	-0.862517
H	-7.728239	1.855484	-1.563936
H	-7.915127	0.097066	-1.254003
H	-8.012084	1.245163	0.100458
C	1.879910	4.020317	-0.279945
C	0.956412	2.783217	-0.481515
O	0.258877	2.702500	-1.475213
O	1.121346	1.955840	0.502704
F	3.169493	3.650663	-0.445108
F	1.602349	4.977661	-1.168754
F	1.751477	4.537426	0.955149
B	2.720800	-2.368899	-2.109679
C	1.872413	-0.898856	-1.683180
H	3.899094	-2.317175	-2.126935
Cl	2.949981	0.479561	-1.500540

35-ts

Zero-point correction= 0.371880

Thermal correction to Energy= 0.404921

Thermal correction to Enthalpy= 0.405865
Thermal correction to Gibbs Free Energy= 0.306730
Sum of electronic and zero-point Energies= -2223.818615
Sum of electronic and thermal Energies= -2223.785574
Sum of electronic and thermal Enthalpies= -2223.784630
Sum of electronic and thermal Free Energies= -2223.883765

Cartesian coordinates

B	-0.369303	-2.381769	-1.422378
B	1.806379	-1.314085	-2.975067
B	0.221385	-0.915212	-2.267575
B	1.692454	-0.373877	-1.455548
B	0.526687	-2.547446	-2.947035
B	0.853423	-3.664501	-1.590107
B	2.186903	-3.024889	-2.581273
B	2.333569	-3.142610	-0.815802
H	2.215012	0.670680	-1.343606
H	3.173193	-3.741568	-0.243644
H	0.550511	-3.130658	0.994104
H	0.579087	-4.816174	-1.596210
H	2.954005	-3.630683	-3.243322
H	0.001831	-2.896240	-3.949550
H	2.312852	-0.798128	-3.907844
H	-0.474943	-0.137251	-2.814198
H	-1.517209	-2.646344	-1.326308
C	2.781648	-1.201652	1.007425
H	3.492196	-1.951565	1.366971
N	2.429279	-0.212627	1.729214
C	2.587843	-0.274231	3.167237
H	2.750039	0.723848	3.581233
H	3.384420	-0.948417	3.502587
C	1.215555	-0.840416	3.680058
O	1.123566	-1.253255	4.814640
O	0.225813	-0.865366	2.799615
Pd	0.369172	0.450474	1.239013
C	2.804854	-1.727419	-1.669864
C	2.021294	-1.539614	-0.241464
B	0.758745	-2.698874	-0.085877
B	0.274919	-1.007976	-0.485470
C	-1.403988	-0.194947	0.368312
C	-2.088622	0.631259	-0.549462
C	-2.138288	-1.115890	1.151765
C	-3.465357	0.503505	-0.709780

H	-1.537742	1.338123	-1.158223
C	-3.510215	-1.237291	0.982722
H	-1.629366	-1.720363	1.892462
C	-4.180880	-0.431281	0.050515
H	-3.987264	1.129523	-1.424126
H	-4.085295	-1.944599	1.570412
C	-5.660731	-0.607991	-0.082908
O	-6.309323	-1.408872	0.560155
O	-6.195599	0.223640	-0.999004
C	-7.617897	0.108877	-1.177400
H	-7.876929	0.840031	-1.942480
H	-7.882121	-0.900304	-1.502345
H	-8.139005	0.327392	-0.242227
C	1.191805	4.265498	-0.699674
C	0.583385	2.835503	-0.789506
O	0.708796	2.236885	0.350487
O	0.109433	2.439225	-1.840224
F	0.978692	4.951754	-1.826756
F	0.658913	4.957384	0.324663
F	2.524415	4.184721	-0.500225
Cl	4.518938	-1.324163	-1.680852

36

Zero-point correction= 0.166959
Thermal correction to Energy= 0.176027
Thermal correction to Enthalpy= 0.176972
Thermal correction to Gibbs Free Energy= 0.134241
Sum of electronic and zero-point Energies= -791.519580
Sum of electronic and thermal Energies= -791.510511
Sum of electronic and thermal Enthalpies= -791.509567
Sum of electronic and thermal Free Energies= -791.552297

Cartesian coordinates

B	1.383079	1.454141	0.445365
B	-0.098481	-0.890203	1.273177
B	-0.098598	0.901356	1.265666
B	1.419560	0.006636	1.497202
B	2.304017	0.000004	-0.048788
B	1.383226	-1.450072	0.458166
B	1.329539	-0.897099	-1.232901
H	1.680079	-1.493187	-2.192171
H	1.679519	1.474395	-2.205077
H	3.487066	-0.000114	-0.112131

H	1.893145	-2.476604	0.757301
H	1.958668	0.011089	2.552594
H	-0.747290	-1.470573	2.071530
H	-0.748076	1.488177	2.058735
H	1.892644	2.483443	0.735429
C	-0.111882	-0.006051	-1.339718
B	1.329027	0.886307	-1.240870
B	-0.145839	1.456587	-0.427669
B	-0.145487	-1.460464	-0.415296
C	-0.928986	0.000394	0.080784
H	-0.837233	-2.334690	-0.798446
H	-0.837113	2.327521	-0.819094
H	-0.732099	-0.010095	-2.227131
Cl	-2.690842	-0.000081	-0.008129

37-ts

Zero-point correction= 0.370650
Thermal correction to Energy= 0.404171
Thermal correction to Enthalpy= 0.405115
Thermal correction to Gibbs Free Energy= 0.305082
Sum of electronic and zero-point Energies= -4335.020108
Sum of electronic and thermal Energies= -4334.986587
Sum of electronic and thermal Enthalpies= -4334.985643
Sum of electronic and thermal Free Energies= -4335.085676

Cartesian coordinates

B	-0.871983	-2.057710	-1.639946
B	1.573999	-1.572322	-3.104181
B	0.213768	-0.735699	-2.230473
B	-0.037882	-2.286703	-3.171461
B	-0.094044	-3.608860	-1.962937
B	1.368909	-3.341914	-2.928035
B	1.490116	-3.666923	-1.181863
H	1.971002	-4.599521	-0.633551
H	-0.205577	-3.312181	0.670269
H	-0.753374	-4.586965	-2.072399
H	1.755593	-4.101560	-3.750370
H	-0.655396	-2.286139	-4.182280
H	2.109406	-0.988792	-3.979186
H	-0.064897	0.325525	-2.663406
H	-2.048206	-1.946805	-1.577044
C	2.432942	-2.063224	0.832355

H	2.965215	-2.965821	1.149764
N	2.251443	-1.086507	1.632076
C	2.390578	-1.291785	3.061122
H	2.754764	-0.383038	3.548051
H	3.039444	-2.133188	3.330023
C	0.943967	-1.607688	3.552215
O	0.752440	-2.091961	4.644793
O	-0.035298	-1.345642	2.691436
Pd	0.358010	0.063058	1.261106
C	1.720871	-2.146457	-0.476148
B	0.126314	-2.821121	-0.353038
B	-0.116563	-1.040033	-0.484162
C	-1.567495	-0.043288	0.494938
C	-2.100755	0.953995	-0.349053
C	-2.436157	-0.919319	1.186324
C	-3.476768	1.021756	-0.550291
H	-1.440566	1.633724	-0.875163
C	-3.805586	-0.839524	0.976554
H	-2.032519	-1.652448	1.873535
C	-4.331911	0.126230	0.105442
H	-3.888988	1.770424	-1.216614
H	-4.488002	-1.512089	1.484837
C	-5.818168	0.157489	-0.078525
O	-6.585043	-0.597589	0.484003
O	-6.206877	1.117207	-0.939557
C	-7.625188	1.202628	-1.166488
H	-7.758377	2.011867	-1.883510
H	-8.003732	0.261015	-1.571025
H	-8.148094	1.423259	-0.232898
C	1.766554	3.982226	-0.017266
C	0.859115	2.749759	-0.303778
O	0.223930	2.694233	-1.340041
O	0.963896	1.897557	0.667294
F	3.064447	3.626310	-0.148170
F	1.517021	4.972497	-0.878026
F	1.589249	4.449547	1.231237
B	2.554923	-2.491080	-1.944254
C	1.755973	-0.991387	-1.539539
H	3.733826	-2.501581	-1.916308
Br	3.005814	0.451056	-1.308924

38-ts

Zero-point correction= 0.371275

Thermal correction to Energy= 0.404633

Thermal correction to Enthalpy= 0.405577
Thermal correction to Gibbs Free Energy= 0.304680
Sum of electronic and zero-point Energies= -4335.031891
Sum of electronic and thermal Energies= -4334.998534
Sum of electronic and thermal Enthalpies= -4334.997590
Sum of electronic and thermal Free Energies= -4335.098487

Cartesian coordinates

B	-0.363438	-2.454071	-1.166207
B	1.828204	-1.344007	-2.665926
B	0.174437	-1.015956	-2.093522
B	1.544146	-0.298932	-1.241473
B	0.643501	-2.668394	-2.612486
B	0.960269	-3.645150	-1.148596
B	2.306103	-2.981613	-2.106200
B	2.342809	-2.945301	-0.332536
H	1.970943	0.792290	-1.186431
H	3.180422	-3.431843	0.339973
H	0.443945	-2.931134	1.358600
H	0.774578	-4.812137	-1.074770
H	3.156963	-3.577861	-2.666806
H	0.216216	-3.136351	-3.612901
H	2.354016	-0.865782	-3.608040
H	-0.538485	-0.342377	-2.746771
H	-1.492888	-2.799622	-1.120608
C	2.519960	-0.836099	1.342258
H	3.257157	-1.496171	1.808215
N	2.049249	0.178279	1.952555
C	2.117922	0.245942	3.397616
H	2.180051	1.283696	3.733892
H	2.938273	-0.334668	3.835345
C	0.760884	-0.382731	3.876000
O	0.623958	-0.704013	5.035504
O	-0.162920	-0.561892	2.943379
Pd	-0.019705	0.631774	1.287065
C	2.763084	-1.571403	-1.272183
C	1.873674	-1.333801	0.082414
B	0.692140	-2.574338	0.259778
B	0.114536	-0.964225	-0.309820
C	-1.673303	-0.227228	0.368635
C	-2.353849	0.465298	-0.656311
C	-2.386424	-1.142595	1.177764
C	-3.701367	0.210624	-0.894067
H	-1.816937	1.164700	-1.285874

C	-3.729128	-1.391509	0.931156
H	-1.884561	-1.644428	1.996025
C	-4.392942	-0.719780	-0.106583
H	-4.219230	0.732619	-1.690195
H	-4.287074	-2.097378	1.536845
C	-5.840278	-1.032230	-0.322097
O	-6.469206	-1.829413	0.344658
O	-6.370007	-0.329307	-1.343163
C	-7.760532	-0.582795	-1.607693
H	-8.017243	0.050249	-2.456449
H	-7.917311	-1.636578	-1.850039
H	-8.368360	-0.325892	-0.736789
C	0.544235	4.365564	-0.891324
C	0.134577	2.863888	-0.907040
O	0.218850	2.376381	0.288182
O	-0.187468	2.328728	-1.953866
F	0.418018	4.911874	-2.104662
F	-0.222767	5.062920	-0.031781
F	1.829940	4.493935	-0.502396
Br	4.591606	-0.985436	-1.206869

39

Zero-point correction= 0.166411
Thermal correction to Energy= 0.175740
Thermal correction to Enthalpy= 0.176684
Thermal correction to Gibbs Free Energy= 0.132639
Sum of electronic and zero-point Energies= -2902.732317
Sum of electronic and thermal Energies= -2902.722988
Sum of electronic and thermal Enthalpies= -2902.722044
Sum of electronic and thermal Free Energies= -2902.766089

Cartesian coordinates

B	1.884280	1.459101	0.425350
B	0.404940	-0.874098	1.284789
B	0.405269	0.915696	1.256663
B	1.925371	0.024309	1.494065
B	2.804066	-0.000607	-0.054411
B	1.884563	-1.444346	0.472250
B	1.825839	-0.911501	-1.224520
H	2.171388	-1.519765	-2.178017
H	2.170942	1.449023	-2.225680
H	3.987025	-0.001407	-0.121845
H	2.393576	-2.468185	0.782237

H	2.466804	0.040868	2.548237
H	-0.237357	-1.446902	2.093731
H	-0.238091	1.513497	2.046421
H	2.392659	2.492850	0.701609
C	0.383309	-0.021917	-1.336713
B	1.825033	0.871220	-1.253549
B	0.350759	1.449770	-0.442551
B	0.351433	-1.463835	-0.396034
C	-0.427840	0.001523	0.086006
H	-0.336061	-2.346468	-0.766975
H	-0.335965	2.320068	-0.842999
H	-0.238584	-0.036161	-2.222592
Br	-2.349626	-0.000103	-0.003433

40-ts

Zero-point correction= 0.410417
Thermal correction to Energy= 0.443606
Thermal correction to Enthalpy= 0.444550
Thermal correction to Gibbs Free Energy= 0.345828
Sum of electronic and zero-point Energies= -1803.516602
Sum of electronic and thermal Energies= -1803.483414
Sum of electronic and thermal Enthalpies= -1803.482470
Sum of electronic and thermal Free Energies= -1803.581192

Cartesian coordinates

B	-0.387455	-2.607301	-1.299185
B	1.684398	-1.933124	-3.171153
B	0.244369	-1.299250	-2.335217
B	0.311287	-3.009711	-2.880390
B	0.694944	-4.005545	-1.454045
B	1.964450	-3.613192	-2.641821
B	2.306354	-3.543196	-0.902772
H	3.075104	-4.190082	-0.276558
H	0.725570	-3.161646	1.079238
H	0.295665	-5.108427	-1.287625
H	2.480705	-4.409987	-3.350224
H	-0.377422	-3.377570	-3.771349
H	2.011436	-1.444008	-4.196905
H	-0.353337	-0.429981	-2.863954
H	-1.539904	-2.726116	-1.065325
C	3.061447	-1.438247	0.637951
H	3.752200	-2.199446	1.015225
N	2.864885	-0.351958	1.277453

C	3.193829	-0.300377	2.690527
H	3.458692	0.715819	2.992433
H	3.992330	-0.990662	2.987336
C	1.874720	-0.741273	3.407561
O	1.885530	-1.036716	4.581396
O	0.788277	-0.807804	2.645600
Pd	0.782972	0.390083	0.994268
C	2.201068	-1.885182	-0.501713
B	0.864880	-2.887315	-0.061520
B	0.422667	-1.221496	-0.568260
C	-1.084413	-0.270612	0.358428
C	-1.848883	0.504324	-0.542460
C	-1.749903	-1.086842	1.305506
C	-3.237059	0.415664	-0.534453
H	-1.355393	1.145080	-1.263463
C	-3.134832	-1.165579	1.307149
H	-1.176226	-1.647621	2.032779
C	-3.885297	-0.420588	0.385259
H	-3.821232	0.996690	-1.238386
H	-3.657698	-1.793516	2.020307
C	-5.375803	-0.551208	0.436738
O	-5.966477	-1.260813	1.225790
O	-5.988616	0.207519	-0.492744
C	-7.425004	0.129299	-0.500474
H	-7.749697	0.789772	-1.303703
H	-7.750109	-0.896746	-0.688217
H	-7.830231	0.459361	0.459021
C	0.931275	4.385283	-0.730533
C	0.582967	2.883356	-0.944329
O	0.022236	2.526831	-1.968967
O	0.994813	2.186841	0.062511
F	2.261369	4.541888	-0.572953
F	0.543073	5.124918	-1.773462
F	0.321547	4.856501	0.374016
B	2.939708	-2.306801	-1.984050
C	1.828278	-0.953078	-1.778626
H	4.078913	-2.019018	-2.105636
C	2.484259	0.407611	-1.980599
H	1.748932	1.092189	-2.401561
H	2.859264	0.830537	-1.050363
H	3.313640	0.308007	-2.682209

41-ts

Zero-point correction= 0.410079

Thermal correction to Energy= 0.443482
Thermal correction to Enthalpy= 0.444426
Thermal correction to Gibbs Free Energy= 0.344666
Sum of electronic and zero-point Energies= -1803.525555
Sum of electronic and thermal Energies= -1803.492152
Sum of electronic and thermal Enthalpies= -1803.491207
Sum of electronic and thermal Free Energies= -1803.590968

Cartesian coordinates

B	-0.542241	-2.172168	-1.706895
B	1.683918	-1.123144	-3.189755
B	0.162376	-0.669889	-2.391578
B	1.703242	-0.372582	-1.577747
B	0.298910	-2.229483	-3.270672
B	0.556881	-3.526829	-2.068199
B	1.921972	-2.881066	-3.013390
B	2.095577	-3.223774	-1.290338
H	2.310676	0.608822	-1.356450
H	2.884855	-3.967202	-0.820925
H	0.362726	-3.275668	0.574883
H	0.178663	-4.640903	-2.203372
H	2.607027	-3.473249	-3.774400
H	-0.281746	-2.408442	-4.287427
H	2.206411	-0.542810	-4.077604
H	-0.474277	0.228695	-2.812593
H	-1.707232	-2.342993	-1.599509
C	2.746695	-1.587271	0.741042
H	3.368614	-2.450167	1.000456
N	2.520726	-0.656254	1.581392
C	2.703955	-0.900988	2.996723
H	2.992756	0.017827	3.512987
H	3.424453	-1.695208	3.225058
C	1.291157	-1.363147	3.502353
O	1.188644	-1.888185	4.589191
O	0.277716	-1.176687	2.671259
Pd	0.521812	0.262803	1.240559
C	2.698836	-1.766624	-1.985620
C	1.949186	-1.694711	-0.525381
B	0.586524	-2.746762	-0.458229
B	0.255001	-0.986366	-0.641913
C	-1.320185	-0.138745	0.366365
C	-1.955233	0.848464	-0.417929
C	-2.109693	-1.086618	1.059739

C	-3.341889	0.854184	-0.541957
H	-1.359354	1.579609	-0.951457
C	-3.490372	-1.075466	0.925124
H	-1.636830	-1.816873	1.704840
C	-4.114054	-0.107515	0.122831
H	-3.827356	1.605345	-1.153992
H	-4.108010	-1.802248	1.441584
C	-5.606116	-0.145623	0.022166
O	-6.304279	-0.967642	0.581407
O	-6.093058	0.838345	-0.760810
C	-7.523854	0.861245	-0.899380
H	-7.741647	1.707801	-1.549782
H	-7.879728	-0.070302	-1.346132
H	-8.000388	0.990326	0.075378
C	1.921092	4.019041	-0.457181
C	0.953255	2.805586	-0.562560
O	1.068076	2.064394	0.491181
O	0.278243	2.658879	-1.566801
F	1.661656	4.932202	-1.398123
F	1.849667	4.618654	0.744204
F	3.191166	3.584565	-0.630745
C	4.203770	-1.539302	-2.020751
H	4.745089	-2.438576	-1.719392
H	4.498492	-1.283826	-3.039883
H	4.493157	-0.711487	-1.369121

42

Zero-point correction= 0.204705
Thermal correction to Energy= 0.213458
Thermal correction to Enthalpy= 0.214402
Thermal correction to Gibbs Free Energy= 0.172813
Sum of electronic and zero-point Energies= -371.225677
Sum of electronic and thermal Energies= -371.216925
Sum of electronic and thermal Enthalpies= -371.215981
Sum of electronic and thermal Free Energies= -371.257570

Cartesian coordinates

B	1.111967	1.431787	0.512348
B	-0.382197	-0.933685	1.221993
B	-0.382870	0.844992	1.284478
B	1.134854	-0.056275	1.505278
B	2.036092	-0.003436	-0.031517
B	1.105350	-1.468991	0.406661

B	1.067495	-0.847952	-1.259339
H	1.427088	-1.403787	-2.239891
H	1.437506	1.554156	-2.133488
H	3.220198	-0.004346	-0.085864
H	1.609446	-2.509407	0.667547
H	1.666402	-0.094560	2.564399
H	-1.034952	-1.547401	1.995519
H	-1.031004	1.406248	2.100715
H	1.621818	2.447201	0.849496
C	-0.373861	0.051277	-1.336858
B	1.073481	0.932595	-1.194920
B	-0.407428	1.466416	-0.375580
B	-0.418171	-1.430399	-0.477653
C	-1.225274	0.001287	0.064102
H	-1.098419	-2.295228	-0.907627
H	-1.084188	2.363233	-0.740154
H	-0.968361	0.085738	-2.241463
C	-2.746511	0.002755	-0.013828
H	-3.152894	-0.354404	0.934219
H	-3.131090	1.007706	-0.197671
H	-3.100535	-0.662321	-0.804978

43-ts

Zero-point correction= 0.467350
Thermal correction to Energy= 0.503275
Thermal correction to Enthalpy= 0.504219
Thermal correction to Gibbs Free Energy= 0.399811
Sum of electronic and zero-point Energies= -1882.079697
Sum of electronic and thermal Energies= -1882.043771
Sum of electronic and thermal Enthalpies= -1882.042827
Sum of electronic and thermal Free Energies= -1882.147235

Cartesian coordinates

B	-0.908160	-2.394629	-1.382174
B	1.425630	-2.070408	-3.033565
B	0.064521	-1.186330	-2.272253
B	-0.151290	-2.864123	-2.908001
B	-0.098481	-3.964917	-1.506701
B	1.319778	-3.788685	-2.558978
B	1.510690	-3.826028	-0.794993
H	2.084051	-4.625074	-0.135579
H	-0.130861	-3.223330	1.056588
H	-0.711862	-4.975141	-1.423693

H	1.737949	-4.650734	-3.255890
H	-0.811860	-3.058346	-3.872226
H	1.908502	-1.655600	-4.028259
H	-0.350127	-0.231460	-2.826404
H	-2.080009	-2.292606	-1.268268
C	2.495988	-1.952168	0.900238
H	3.021138	-2.834901	1.280400
N	2.407983	-0.888529	1.598375
C	2.614909	-0.965912	3.032543
H	3.016029	-0.025206	3.418139
H	3.260158	-1.794893	3.346887
C	1.186177	-1.210147	3.618341
O	1.045735	-1.568220	4.766152
O	0.170282	-1.042774	2.777395
Pd	0.503225	0.223104	1.215043
C	1.688639	-2.183532	-0.339563
B	0.149933	-2.939610	-0.055095
B	0.035321	-1.216479	-0.492368
C	-1.375651	-0.107064	0.387160
C	-1.939106	0.818641	-0.519913
C	-2.235090	-0.873517	1.214723
C	-3.321275	0.918643	-0.646373
H	-1.298290	1.449120	-1.122883
C	-3.610585	-0.760501	1.085588
H	-1.816759	-1.548519	1.950507
C	-4.161270	0.127599	0.148455
H	-3.750294	1.616022	-1.356216
H	-4.279963	-1.347171	1.705269
C	-5.653927	0.197369	0.052692
O	-6.407793	-0.462927	0.738800
O	-6.066578	1.075018	-0.882246
C	-7.492809	1.191725	-1.029084
H	-7.646500	1.926573	-1.818524
H	-7.927677	0.228758	-1.307108
H	-7.946423	1.528515	-0.093894
C	1.889813	4.094753	-0.266586
C	0.878513	2.922324	-0.431139
O	0.033093	2.981390	-1.305641
O	1.168356	1.977742	0.407262
F	3.088101	3.716284	-0.776458
F	1.484737	5.183955	-0.924177
F	2.077777	4.421870	1.023221
B	2.467971	-2.723399	-1.771149
C	1.656155	-1.168166	-1.607301

H	3.643627	-2.732030	-1.780488
C	2.567875	0.094244	-1.631491
H	2.335792	0.662520	-0.734245
C	2.267508	1.008698	-2.834613
H	1.219515	1.300770	-2.888030
H	2.854457	1.923985	-2.721512
H	2.552562	0.538122	-3.779391
C	4.080685	-0.190082	-1.588671
H	4.431871	-0.685772	-2.498152
H	4.597359	0.770934	-1.509367
H	4.384262	-0.792858	-0.728954

44-ts

Zero-point correction= 0.467189
Thermal correction to Energy= 0.503151
Thermal correction to Enthalpy= 0.504095
Thermal correction to Gibbs Free Energy= 0.398616
Sum of electronic and zero-point Energies= -1882.094872
Sum of electronic and thermal Energies= -1882.058910
Sum of electronic and thermal Enthalpies= -1882.057966
Sum of electronic and thermal Free Energies= -1882.163446

Cartesian coordinates

B	-0.359322	-2.399386	-1.298178
B	1.872988	-1.303965	-2.729887
B	0.238593	-0.937661	-2.144513
B	1.646401	-0.331827	-1.257753
B	0.645279	-2.577632	-2.749319
B	0.922911	-3.635230	-1.341408
B	2.300674	-2.964390	-2.253532
B	2.322250	-3.020377	-0.488909
H	2.093737	0.748755	-1.140320
H	3.098707	-3.605014	0.177181
H	0.422122	-3.039263	1.197063
H	0.695476	-4.797458	-1.327372
H	3.107636	-3.583335	-2.856787
H	0.202929	-2.976686	-3.773208
H	2.373329	-0.801349	-3.671245
H	-0.444180	-0.199738	-2.760282
H	-1.501501	-2.703660	-1.268333
C	2.555543	-1.041104	1.308234
H	3.225062	-1.777481	1.764455
N	2.150273	-0.023619	1.960712

C	2.208166	-0.036122	3.407893
H	2.327791	0.977262	3.798512
H	2.990146	-0.685254	3.819419
C	0.815894	-0.609553	3.850916
O	0.656628	-0.977302	4.994197
O	-0.109686	-0.692438	2.908812
Pd	0.102297	0.564546	1.308747
C	2.848619	-1.617166	-1.359590
C	1.919298	-1.434991	0.008223
B	0.685996	-2.631185	0.119223
B	0.181524	-0.976507	-0.368061
C	-1.575089	-0.196818	0.349632
C	-2.231665	0.572080	-0.636508
C	-2.321346	-1.126593	1.111251
C	-3.587519	0.377714	-0.883982
H	-1.672131	1.286099	-1.229117
C	-3.671716	-1.315641	0.854306
H	-1.838150	-1.687537	1.901493
C	-4.311832	-0.567552	-0.145280
H	-4.086159	0.959458	-1.650471
H	-4.253736	-2.032533	1.423238
C	-5.769285	-0.815811	-0.373014
O	-6.426236	-1.626347	0.249364
O	-6.275730	-0.037060	-1.350496
C	-7.674646	-0.225119	-1.623048
H	-7.912550	0.470703	-2.427038
H	-7.868703	-1.254629	-1.933574
H	-8.270617	-0.005836	-0.733834
C	1.020452	4.299569	-0.736467
C	0.385335	2.879915	-0.795648
O	0.456348	2.323114	0.369299
O	-0.050000	2.453391	-1.851179
F	0.823862	4.966238	-1.878622
F	0.508525	5.028529	0.272080
F	2.353121	4.191523	-0.537021
C	4.328932	-1.148543	-1.256172
H	4.365380	-0.468304	-0.395671
C	5.321549	-2.294842	-0.994935
H	6.334799	-1.885147	-0.953381
H	5.134947	-2.812328	-0.051916
H	5.292057	-3.035180	-1.799452
C	4.778416	-0.337563	-2.482873
H	5.792174	0.033354	-2.306139
H	4.799603	-0.955322	-3.385129

H	4.132985	0.522781	-2.669280

45

Zero-point correction= 0.262325
Thermal correction to Energy= 0.274307
Thermal correction to Enthalpy= 0.275251
Thermal correction to Gibbs Free Energy= 0.226201
Sum of electronic and zero-point Energies= -449.794380
Sum of electronic and thermal Energies= -449.782399
Sum of electronic and thermal Enthalpies= -449.781455
Sum of electronic and thermal Free Energies= -449.830505

Cartesian coordinates

B	1.641037	1.450369	0.548296
B	0.071341	-0.886723	1.177359
B	0.071565	0.890797	1.174443
B	1.551824	0.002595	1.593837
B	2.619962	0.000127	0.168978
B	1.640771	-1.448701	0.553181
B	1.795147	-0.890735	-1.127460
H	2.257037	-1.488564	-2.038067
H	2.257263	1.481524	-2.042972
H	3.802705	0.000170	0.249385
H	2.107439	-2.478888	0.908101
H	1.959924	0.004396	2.707149
H	-0.635620	-1.485456	1.911196
H	-0.635279	1.492086	1.906266
H	2.107903	2.481674	0.899701
C	0.375519	-0.002361	-1.398796
B	1.795266	0.886758	-1.130415
B	0.226623	1.439598	-0.505359
B	0.226485	-1.441277	-0.500577
C	-0.655433	-0.000015	-0.095360
H	-0.371105	-2.336215	-0.983804
H	-0.370856	2.332965	-0.991681
H	-0.110981	-0.003881	-2.366222
C	-2.182632	-0.000055	-0.398934
H	-2.262891	-0.000003	-1.493753
C	-2.907520	1.254206	0.119331
H	-3.947831	1.228400	-0.218745
H	-2.912934	1.282902	1.212368
H	-2.457913	2.179959	-0.243761

C	-2.907797	-1.254140	0.119338
H	-2.912415	-1.283282	1.212366
H	-3.948349	-1.227630	-0.217943
H	-2.459016	-2.180004	-0.244473

46-ts

Zero-point correction= 0.495241
Thermal correction to Energy= 0.532240
Thermal correction to Enthalpy= 0.533184
Thermal correction to Gibbs Free Energy= 0.426961
Sum of electronic and zero-point Energies= -1921.356829
Sum of electronic and thermal Energies= -1921.319830
Sum of electronic and thermal Enthalpies= -1921.318886
Sum of electronic and thermal Free Energies= -1921.425110

Cartesian coordinates

B	-0.529134	-2.739619	-0.669653
B	1.724229	-2.684040	-2.448977
B	0.318404	-1.691909	-1.879042
B	0.252381	-3.531375	-2.008292
B	0.467260	-4.155864	-0.345479
B	1.813410	-4.188350	-1.487736
B	2.070076	-3.645683	0.183578
H	2.716551	-4.157033	1.034401
H	0.448216	-2.710097	1.856620
H	-0.033644	-5.141217	0.082281
H	2.273923	-5.188270	-1.926166
H	-0.402853	-4.063207	-2.840613
H	2.056226	-2.580475	-3.576163
H	-0.200678	-1.049199	-2.723859
H	-1.706732	-2.749597	-0.552489
C	2.801731	-1.266772	1.224553
H	3.545443	-1.864971	1.761061
N	2.381308	-0.165403	1.713368
C	2.543211	0.157361	3.117066
H	2.738581	1.226049	3.243809
H	3.323596	-0.424161	3.620355
C	1.164830	-0.188175	3.760627
O	1.054977	-0.324461	4.958106
O	0.150810	-0.345961	2.915403
Pd	0.377971	0.472659	1.070498
C	2.107021	-1.942027	0.081124

B	0.636425	-2.690697	0.689380
B	0.035112	-1.218267	-0.142809
C	-1.502887	-0.117355	0.391989
C	-2.102494	0.487020	-0.733356
C	-2.314022	-0.749093	1.360320
C	-3.474288	0.379827	-0.931758
H	-1.490402	1.014956	-1.453590
C	-3.685500	-0.840396	1.161305
H	-1.860895	-1.168252	2.251377
C	-4.269161	-0.286704	0.012809
H	-3.936015	0.817973	-1.808741
H	-4.324644	-1.333039	1.885937
C	-5.751691	-0.424727	-0.147067
O	-6.470337	-0.983428	0.656460
O	-6.198550	0.140360	-1.285931
C	-7.617044	0.041065	-1.505100
H	-7.801287	0.535313	-2.458331
H	-7.923818	-1.006657	-1.547062
H	-8.163199	0.538278	-0.699993
C	0.845805	4.104284	-0.883842
C	0.679954	2.918801	0.091215
O	0.745244	3.065994	1.309531
O	0.513058	1.785607	-0.514720
F	-0.149396	4.117686	-1.789508
F	0.850735	5.269912	-0.235388
F	2.013847	3.977556	-1.549068
B	2.900543	-2.841061	-1.127739
C	1.987201	-1.390259	-1.420906
H	4.075154	-2.789464	-1.198472
C	2.836394	-0.183816	-2.055584
C	4.031776	-0.700917	-2.907311
H	3.731646	-1.409524	-3.678802
H	4.478645	0.163503	-3.407286
H	4.810952	-1.160396	-2.296825
C	1.939869	0.621250	-3.024173
H	1.069140	1.043146	-2.529051
H	2.526572	1.450635	-3.430710
H	1.610297	0.003926	-3.863873
C	3.474575	0.765626	-1.023732
H	2.752372	1.234588	-0.365257
H	4.227493	0.254633	-0.416104
H	3.990034	1.561152	-1.569270

47-ts

Zero-point correction= 0.495719

Thermal correction to Energy= 0.532755

Thermal correction to Enthalpy= 0.533699

Thermal correction to Gibbs Free Energy= 0.427293

Sum of electronic and zero-point Energies= -1921.373158

Sum of electronic and thermal Energies= -1921.336123

Sum of electronic and thermal Enthalpies= -1921.335178

Sum of electronic and thermal Free Energies= -1921.441584

Cartesian coordinates

B	-0.551053	-2.291321	-1.347886
B	1.727636	-1.180714	-2.695749
B	0.088331	-0.809497	-2.127719
B	1.488825	-0.263453	-1.193376
B	0.475955	-2.433872	-2.784973
B	0.710330	-3.541319	-1.408423
B	2.111116	-2.870057	-2.275369
B	2.108831	-2.980510	-0.517089
H	1.912700	0.816041	-1.044223
H	2.849353	-3.615844	0.140942
H	0.188053	-3.019001	1.138174
H	0.468153	-4.700441	-1.437036
H	2.902169	-3.500270	-2.887103
H	0.046505	-2.786987	-3.831105
H	2.231024	-0.646406	-3.617275
H	-0.562926	-0.032338	-2.731296
H	-1.697418	-2.579872	-1.345697
C	2.310814	-1.107693	1.388308
H	2.951977	-1.879176	1.825331
N	1.872147	-0.142065	2.094887
C	1.859445	-0.248410	3.539342
H	1.994497	0.734670	3.997561
H	2.601478	-0.947503	3.942786
C	0.431756	-0.793092	3.887131
O	0.210005	-1.235167	4.993011
O	-0.461386	-0.765382	2.909819
Pd	-0.107227	0.540951	1.383570
C	2.697921	-1.559353	-1.336876
C	1.743397	-1.408702	0.031088
B	0.469592	-2.579727	0.076849
B	-0.018985	-0.907440	-0.362698
C	-1.774173	-0.116487	0.321352

C	-2.380150	0.737353	-0.626290
C	-2.568976	-1.073574	0.996750
C	-3.733279	0.599032	-0.924669
H	-1.783945	1.480370	-1.143218
C	-3.914612	-1.207057	0.688386
H	-2.126873	-1.701760	1.759751
C	-4.503758	-0.374522	-0.275537
H	-4.193581	1.247021	-1.661419
H	-4.532038	-1.945385	1.188386
C	-5.959004	-0.567695	-0.563168
O	-6.654360	-1.403384	-0.020846
O	-6.416515	0.291766	-1.496195
C	-7.810003	0.158160	-1.822973
H	-8.008338	0.918803	-2.577455
H	-8.016281	-0.839724	-2.217669
H	-8.428362	0.322364	-0.937180
C	1.463273	4.066854	-0.623922
C	0.429082	2.904787	-0.628532
O	0.471799	2.276413	0.500635
O	-0.214170	2.685871	-1.640321
F	1.235287	4.931139	-1.617369
F	1.468457	4.746486	0.535042
F	2.703372	3.542713	-0.801072
C	4.239014	-1.191334	-1.293654
C	5.050025	-2.269712	-0.540574
H	6.110473	-2.007711	-0.594673
H	4.788212	-2.336068	0.518798
H	4.926990	-3.259853	-0.985966
C	4.790601	-1.124620	-2.738586
H	5.870064	-0.955419	-2.684902
H	4.623582	-2.052380	-3.289734
H	4.353357	-0.301269	-3.305017
C	4.515753	0.179574	-0.636192
H	4.059267	1.006360	-1.182554
H	4.179138	0.234033	0.401728
H	5.597542	0.343004	-0.632700

48

Zero-point correction= 0.290672

Thermal correction to Energy= 0.303687

Thermal correction to Enthalpy= 0.304631

Thermal correction to Gibbs Free Energy= 0.254229

Sum of electronic and zero-point Energies= -489.077372

Sum of electronic and thermal Energies= -489.064357
Sum of electronic and thermal Enthalpies= -489.063413
Sum of electronic and thermal Free Energies= -489.113816

Cartesian coordinates

B	1.901794	1.447784	0.464264
B	0.418396	-0.891461	1.259549
B	0.418304	0.882894	1.265518
B	1.936498	-0.005002	1.503391
B	2.832519	0.000168	-0.032376
B	1.901896	-1.450646	0.454416
B	1.861981	-0.885322	-1.226328
H	2.213515	-1.478214	-2.188233
H	2.214110	1.492748	-2.178002
H	4.016593	0.000342	-0.090272
H	2.403509	-2.483440	0.749042
H	2.466544	-0.008605	2.564218
H	-0.183696	-1.497375	2.074275
H	-0.183512	1.483175	2.084580
H	2.403532	2.478508	0.765864
C	0.423950	0.004393	-1.331502
B	1.862211	0.893439	-1.220210
B	0.370670	1.438633	-0.417522
B	0.370915	-1.435739	-0.426853
C	-0.466570	-0.000116	0.081731
H	-0.273378	-2.333350	-0.841773
C	-2.044946	-0.000053	0.003755
C	-2.628747	-1.248471	0.702174
H	-2.394249	-1.261303	1.768350
H	-3.718233	-1.230302	0.600406
H	-2.266184	-2.179192	0.260026
C	-2.628944	1.244705	0.708644
H	-2.266813	2.177895	0.271287
H	-3.718504	1.226842	0.607112
H	-2.394151	1.252149	1.774841
C	-2.529223	0.003784	-1.462196
H	-2.200507	0.896757	-2.003041
H	-2.200696	-0.886209	-2.008117
H	-3.622799	0.003963	-1.472924
H	-0.150346	0.007730	-2.245582
H	-0.273779	2.338687	-0.826942

49-ts

Zero-point correction= 0.382527

Thermal correction to Energy= 0.414042

Thermal correction to Enthalpy= 0.414986

Thermal correction to Gibbs Free Energy= 0.319279

Sum of electronic and zero-point Energies= -1764.246071

Sum of electronic and thermal Energies= -1764.214556

Sum of electronic and thermal Enthalpies= -1764.213612

Sum of electronic and thermal Free Energies= -1764.309319

Cartesian coordinates

B	-0.510342	-2.027977	-1.933905
B	1.724448	-0.893330	-3.364244
B	0.243972	-0.492590	-2.454222
B	0.291770	-1.931300	-3.522487
B	0.536038	-3.356634	-2.479317
B	1.904349	-2.670483	-3.401339
B	2.122085	-3.196688	-1.717288
H	2.815400	-4.060616	-1.299920
H	0.409302	-3.390275	0.193342
H	0.088898	-4.427700	-2.716989
H	2.431930	-3.230031	-4.302016
H	-0.344122	-1.954588	-4.521647
H	2.141028	-0.110536	-4.145460
H	-0.278739	0.538668	-2.693747
H	-1.679914	-2.153090	-1.814601
C	2.854708	-1.703678	0.451255
H	3.493573	-2.571284	0.642151
N	2.677372	-0.803801	1.335788
C	2.952359	-1.092741	2.730436
H	3.284141	-0.191725	3.252271
H	3.685279	-1.893412	2.880939
C	1.576176	-1.561778	3.308645
O	1.522664	-2.116618	4.383114
O	0.515456	-1.340369	2.540944
Pd	0.706945	0.116990	1.135660
C	2.046051	-1.772496	-0.806196
B	0.641525	-2.766574	-0.783869
B	0.298885	-1.000149	-0.756364
C	-1.193920	-0.196165	0.339680
C	-1.852059	0.879832	-0.294087
C	-1.958763	-1.203815	0.969444
C	-3.240356	0.908536	-0.355798

H	-1.272785	1.683640	-0.730382
C	-3.345224	-1.166928	0.905897
H	-1.460832	-2.004008	1.504099
C	-3.991547	-0.117178	0.237563
H	-3.747904	1.728065	-0.850857
H	-3.947960	-1.937466	1.374145
C	-5.488073	-0.132879	0.204903
O	-6.167682	-1.000773	0.714495
O	-5.997202	0.926068	-0.455028
C	-7.433380	0.974519	-0.523374
H	-7.669331	1.876235	-1.087372
H	-7.821354	0.088237	-1.030918
H	-7.861597	1.023601	0.480620
C	1.658012	4.001040	-0.462944
C	1.901398	2.492726	-0.181034
O	3.009790	2.002482	-0.330609
O	0.796725	1.920829	0.187289
F	1.364746	4.645254	0.682814
F	2.737404	4.571334	-1.004726
F	0.621931	4.161871	-1.310825
B	2.881221	-1.705544	-2.300332
C	1.772249	-0.487130	-1.715913
H	4.032906	-1.452476	-2.245801
H	2.270719	0.419924	-1.389780

50-ts

Zero-point correction= 0.382322

Thermal correction to Energy= 0.413878

Thermal correction to Enthalpy= 0.414822

Thermal correction to Gibbs Free Energy= 0.318987

Sum of electronic and zero-point Energies= -1764.234502

Sum of electronic and thermal Energies= -1764.202946

Sum of electronic and thermal Enthalpies= -1764.202002

Sum of electronic and thermal Free Energies= -1764.297837

Cartesian coordinates

B	-0.481206	-2.289603	-1.723090
B	1.615349	-1.247345	-3.393278
B	0.149928	-0.794173	-2.491821
B	1.741218	-0.456071	-1.797255
B	0.239941	-2.372096	-3.345457
B	0.601774	-3.644199	-2.138629

B	1.883498	-3.004092	-3.198334
B	2.192463	-3.314912	-1.482350
H	2.355486	0.531611	-1.634275
H	3.027474	-4.032981	-1.055979
H	0.594305	-3.338009	0.507882
H	0.223231	-4.762960	-2.222994
H	2.525018	-3.600176	-3.992301
H	-0.415723	-2.578025	-4.309972
H	2.071176	-0.681241	-4.324783
H	-0.533523	0.084023	-2.879565
H	-1.633514	-2.467875	-1.527152
C	2.979307	-1.617162	0.452982
H	3.640414	-2.462884	0.669102
N	2.805226	-0.677047	1.295291
C	3.102412	-0.898813	2.695289
H	3.401517	0.033883	3.179419
H	3.860125	-1.670005	2.876986
C	1.742395	-1.395564	3.305112
O	1.732850	-1.913302	4.400051
O	0.668447	-1.245263	2.545697
Pd	0.771893	0.202390	1.100433
C	2.682984	-1.860605	-2.235556
C	2.075079	-1.762551	-0.735589
B	0.739959	-2.832031	-0.549538
B	0.384004	-1.074134	-0.744114
C	-1.124057	-0.210606	0.361687
C	-1.812663	0.757471	-0.401014
C	-1.862589	-1.136179	1.135532
C	-3.204232	0.768064	-0.421563
H	-1.257517	1.468023	-1.001178
C	-3.249945	-1.119302	1.106149
H	-1.344745	-1.852075	1.762277
C	-3.928194	-0.169171	0.327887
H	-3.731583	1.504229	-1.016928
H	-3.829910	-1.827293	1.688207
C	-5.423859	-0.197617	0.344570
O	-6.081081	-1.000253	0.976701
O	-5.963820	0.771603	-0.421528
C	-7.401001	0.804209	-0.448438
H	-7.662877	1.637298	-1.099940
H	-7.797355	-0.134273	-0.843555
H	-7.798695	0.960472	0.557201
C	1.677703	4.140123	-0.528765
C	0.988655	2.756597	-0.714664

O	1.162892	2.039725	0.347602
O	0.412220	2.496236	-1.756673
F	1.480410	4.925323	-1.592476
F	1.197838	4.772691	0.558756
F	3.007926	3.979756	-0.364583
H	3.748811	-1.682322	-2.311874

51

Zero-point correction= 0.177396
Thermal correction to Energy= 0.185090
Thermal correction to Enthalpy= 0.186034
Thermal correction to Gibbs Free Energy= 0.146630
Sum of electronic and zero-point Energies= -331.935142
Sum of electronic and thermal Energies= -331.927448
Sum of electronic and thermal Enthalpies= -331.926504
Sum of electronic and thermal Free Energies= -331.965908

Cartesian coordinates

B	1.452861	-0.030438	0.910335
B	-0.860024	1.458932	0.023928
B	0.923631	1.420114	0.024603
B	0.019603	0.893044	1.461153
B	-0.019216	-0.889010	1.463740
B	-1.452559	0.033165	0.910914
B	-0.923591	-1.419883	0.028927
H	-1.532142	-2.420736	-0.135834
H	1.425629	-2.484695	-0.136828
H	-0.032793	-1.531288	2.459904
H	-2.478638	0.057064	1.503164
H	0.033601	1.538168	2.455479
H	-1.424462	2.484880	-0.143374
H	1.532945	2.419936	-0.143497
H	2.479049	-0.052554	1.502469
C	-0.018564	-0.813782	-1.273872
B	0.860045	-1.458931	0.027666
B	1.455400	-0.032648	-0.853634
B	-1.455856	0.030268	-0.853316
C	0.017999	0.809956	-1.276202
H	-2.332055	0.049602	-1.644515
H	0.028066	1.285194	-2.248765
H	2.331810	-0.053157	-1.644603
H	-0.029090	-1.292516	-2.244747

AgI

Zero-point correction= 0.003057
Thermal correction to Energy= 0.020049
Thermal correction to Enthalpy= 0.020994
Thermal correction to Gibbs Free Energy= -0.054089
Sum of electronic and zero-point Energies= -628.976681
Sum of electronic and thermal Energies= -628.959689
Sum of electronic and thermal Enthalpies= -628.958744
Sum of electronic and thermal Free Energies= -629.033827
Cartesian coordinates

Ag	0.000000	1.580685	-1.118369
I	0.000000	2.459335	1.738001
I	2.459432	0.000000	-1.737978
Ag	1.580756	0.000000	1.118343
Ag	-1.580756	0.000000	1.118343
I	0.000000	-2.459335	1.738001
I	-2.459432	0.000000	-1.737978
Ag	0.000000	-1.580685	-1.118369

AgTFA

Zero-point correction= 0.027548
Thermal correction to Energy= 0.035539
Thermal correction to Enthalpy= 0.036483
Thermal correction to Gibbs Free Energy= -0.008875
Sum of electronic and zero-point Energies= -671.933428
Sum of electronic and thermal Energies= -671.925438
Sum of electronic and thermal Enthalpies= -671.924494
Sum of electronic and thermal Free Energies= -671.969852
Cartesian coordinates

C	-2.219714	0.002921	0.000081
C	-0.671858	0.038699	-0.000163
O	-0.107965	1.161172	-0.000205
O	-0.108147	-1.088797	-0.000176
F	-2.664650	-0.652401	1.088657
F	-2.664880	-0.646917	-1.091763
F	-2.757072	1.229633	0.003259
Ag	1.954420	-0.004288	0.000046

ArI

Zero-point correction= 0.133099
Thermal correction to Energy= 0.143563
Thermal correction to Enthalpy= 0.144508
Thermal correction to Gibbs Free Energy= 0.094559
Sum of electronic and zero-point Energies= -470.774245

Sum of electronic and thermal Energies= -470.763781
Sum of electronic and thermal Enthalpies= -470.762836
Sum of electronic and thermal Free Energies= -470.812785
Cartesian coordinates

C	-0.083130	-1.130892	0.000004
C	1.308233	-1.049137	-0.000001
C	1.942947	0.199501	-0.000003
C	1.171056	1.367893	-0.000014
C	-0.220243	1.298323	-0.000013
C	-0.834524	0.044865	0.000001
H	-0.570898	-2.098723	0.000013
H	1.903698	-1.954905	0.000001
H	1.678079	2.327109	-0.000025
H	-0.812765	2.206181	-0.000013
I	-2.972701	-0.082047	0.000001
C	3.426560	0.343953	-0.000005
O	4.012529	1.408935	0.000027
O	4.059653	-0.850761	-0.000005
C	5.494333	-0.784144	-0.000005
H	5.855028	-0.259931	0.888474
H	5.836152	-1.818966	-0.000051
H	5.855026	-0.259849	-0.888436

HTFA

Zero-point correction= 0.039253
Thermal correction to Energy= 0.045499
Thermal correction to Enthalpy= 0.046444
Thermal correction to Gibbs Free Energy= 0.007745
Sum of electronic and zero-point Energies= -526.742319
Sum of electronic and thermal Energies= -526.736072
Sum of electronic and thermal Enthalpies= -526.735128
Sum of electronic and thermal Free Energies= -526.773827
Cartesian coordinates

C	0.600745	-0.000690	0.000015
C	-0.934489	0.159693	0.000009
O	-1.497497	1.222466	-0.000060
O	-1.520401	-1.045515	-0.000012
H	-2.481712	-0.897412	-0.000027
F	1.188198	1.196203	-0.000271
F	0.996319	-0.679636	1.090375
F	0.996301	-0.680146	-1.090054