Supporting Information for Mechanistic study of the ligand controlled regioselectivity in Iridium catalyzed C-H borylation of aromatic imine

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I. Computational Details

The calculations were conducted using Gaussian 09 program [1]. Geometries were optimized using the B3LYP functional [2]. SDD [3] basis set was used for Ir, a standard 6-31G(d) [4] basis set was used for other atoms. Frequency analyses were carried out to ensure theses stationary points were at either a minimum or transition state. Solvation free energies are calculated with SMD[5] solvation model (solvent =tetrahydrofuran). Additional single point calculations were performed with M11L functional [6]. SDD basis set was employed for Ir while standard 6-311++G (d, p) [4] basis set level for other atoms. The solvation model for the single point calculation was the same as described above. The energies presented in this paper are the M11L-calculated single point energies added with B3LYP-optimized thermodynamic corrections.

II. Geometry and Mulliken charge for transition states

Table 1. Mulliken charge for transferring hydrogen, related carbon atom and iridium atom on transition states TS3a, TS3b, TS3a', TS3b'

atom	TS3a	TS3b	TS3a'	TS3b'
H	-0.013700	-0.178948	-0.191481	0.231294
Ir	0.213840	-0.260901	-0.401976	0.626415
C	0.150718	0.376478	0.239186	-0.574007

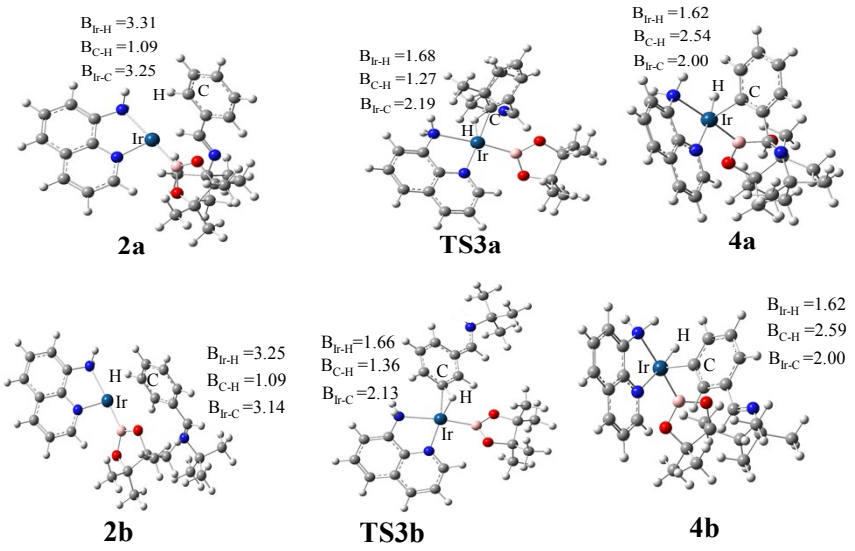

Fig. 1 Key transition states and intermediates in Ir(I)/AQ catalyzed C-H activation in path I

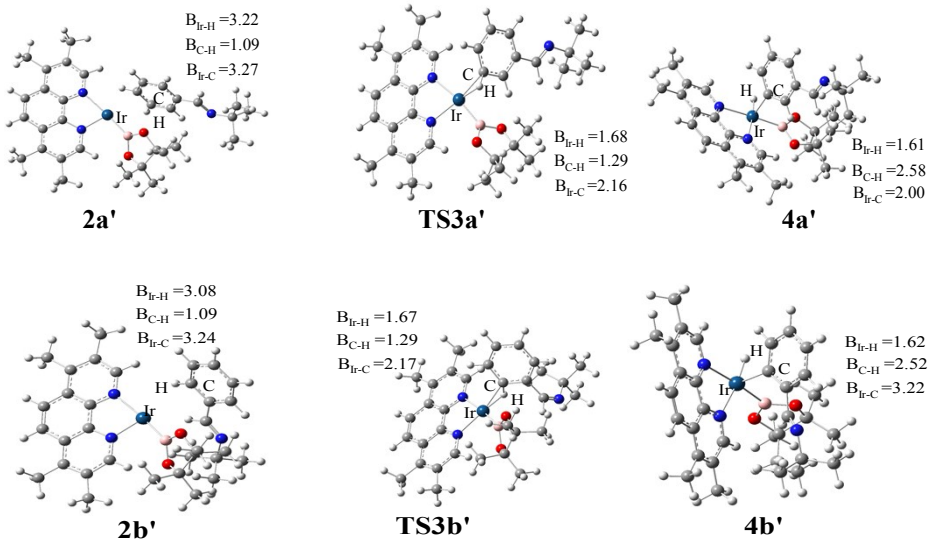

Fig. 2 Key transition states and intermediates in Ir(I)/TMP system catalyzed C-H activation in path I'

II. Cartesian coordinates and energies from the B3LYP-D3 method and electronic energies for the M11Ls method.

1

Number of Negative Frequencies = 0

B	-1.64742	-0.25456	-0.0008	C	3.25729	-0.83196	0.00227
C	0.7816	1.84085	-0.00191	C	4.62887	-0.99251	-0.00586
H	-0.2965	1.91587	-0.01007	N	1.27877	0.5848	-0.00191
C	1.58439	2.99195	-0.01293	N	2.34279	-1.95329	0.0189
C	3.53839	1.60184	-0.01899	O	-2.08245	1.04382	-0.36048
C	2.68092	0.45947	-0.0058	O	-2.7928	-1.00788	0.3461

C	4.9442	1.40273	-0.02802
C	5.48019	0.13341	-0.02214
H	5.58929	2.27714	-0.03948
H	6.55683	-0.00841	-0.02918
C	2.95702	2.8943	-0.02267
C	-3.9866	-0.27554	-0.01305
C	-3.47356	1.20614	-0.00012
Ir	0.22059	-1.054	0.01377
C	-4.41508	-0.74884	-1.40873
H	-4.57027	-1.83306	-1.38553
H	-5.34919	-0.27588	-1.73149
H	-3.63842	-0.533	-2.14961
C	-5.08349	-0.58742	1.00215
H	-5.97638	0.01991	0.81203
H	-5.37045	-1.64268	0.92775
H	-4.74844	-0.40309	2.02617
C	-4.14341	2.13108	-1.01294
H	-5.21975	2.20746	-0.81846
H	-3.71469	3.13702	-0.93846
H	-3.99862	1.7791	-2.03754
C	-3.5128	1.84186	1.39614
H	-2.96457	2.79022	1.37281
H	-4.53819	2.04725	1.72285
H	-3.03338	1.19225	2.13558
H	3.59441	3.77347	-0.03336
H	1.08678	3.95683	-0.01548
H	5.04542	-1.99627	0.00059
H	2.51571	-2.53522	0.84077
H	2.50572	-2.55029	-

0.79429Thermal correction to Energy= 0.367027

Thermal correction to Enthalpy= 0.368177

Thermal correction to Gibbs Free Energy= 0.273881

Sum of electronic and zero-point Energies= -972.679637

Sum of electronic and thermal Energies=-972.650864

Sum of electronic and thermal Enthalpies=-972.649714

Sum of electronic and thermal Free Energies= -972.744010

SCF Done: E(RM11L) = -973.143151045

2a

Number of Negative Frequencies = 0

Ir	-0.64772	-0.32544	-0.38174
B	0.80916	1.0778	-0.57534
O	1.64722	1.2093	-1.70302
O	1.16483	2.08917	0.3525
C	-4.52398	1.16517	0.48253
C	-3.04141	3.03875	0.70657
C	-1.95706	2.19813	0.41361
H	-0.94623	2.57873	0.39766
C	-4.83941	-1.59427	0.02654
N	-2.3831	-1.83627	-0.21503
N	-2.08643	0.8799	0.14301
C	-3.57286	-1.04362	0.00713
C	-3.38682	0.34441	0.21331
C	-5.96937	-0.78149	0.26154
C	-5.81212	0.56773	0.49288
H	-6.95929	-1.22812	0.26736
H	-6.67344	1.20111	0.68769
C	-4.32736	2.54766	0.72868
C	2.72455	2.12521	-1.39458
C	2.08479	3.01444	-0.2755
C	3.90689	1.28759	-0.88888
H	3.6381	0.74026	0.01953
H	4.17552	0.55554	-1.65773
H	4.78764	1.90636	-0.68302
C	3.12071	2.87343	-2.66448
H	3.86546	3.64766	-2.44463
H	3.56206	2.17589	-3.38559
H	2.25729	3.34533	-3.14076
C	1.25204	4.17616	-0.83577
H	0.68067	4.63298	-0.01989
H	1.88291	4.95141	-1.28479
H	0.54186	3.82344	-1.59089
C	3.06302	3.53669	0.77314
H	3.81833	4.18432	0.3119
H	2.52417	4.12734	1.52295
H	3.57279	2.72239	1.29234
C	0.54783	-3.31751	-0.81244
C	1.64022	-2.58807	-0.30849
C	0.50753	-3.70279	-2.15612
C	2.69701	-2.25845	-1.17697
C	1.56055	-3.36564	-3.00808
H	-0.33985	-4.27062	-2.53145
C	2.6569	-2.64618	-2.51226
H	3.53482	-1.69196	-0.78665
H	1.53303	-3.66364	-4.05278
H	3.478	-2.38456	-3.17454
C	1.63388	-2.1726	1.1116
H	0.72269	-2.44416	1.65689

N	2.60863	-1.54655	1.64521
C	2.54635	-1.0891	3.04589
C	2.94452	0.39953	3.01523
H	2.23503	0.97481	2.41153
H	2.96235	0.81367	4.03087
H	3.94201	0.51944	2.57762
C	3.60527	-1.89572	3.82108
H	3.68638	-1.53195	4.85238
H	3.33914	-2.95939	3.85118
H	4.58735	-1.8034	3.34345
C	1.17457	-1.2299	3.7286
H	0.3991	-0.69147	3.16918
H	0.86624	-2.27761	3.82967
H	1.22167	-0.80535	4.73761
H	-0.25705	-3.60217	-0.14035
H	-4.95633	-2.66218	-0.13803
H	-2.49158	-2.42014	-1.04524
H	-2.23537	-2.47088	0.57212
H	-5.18105	3.18604	0.93544
H	-2.83304	4.08604	0.9027

Thermal correction to Energy= 0.623526

Thermal correction to Enthalpy= 0.624676

Thermal correction to Gibbs Free Energy=0.488120

Sum of electronic and zero-point Energies=-1455.442485

Sum of electronic and thermal Energies=-1455.394594

Sum of electronic and thermal Enthalpies=-1455.393444

Sum of electronic and thermal Free Energies=-1455.530000

SCF Done: E(RM11L) = -1456.13739528

TS3a

Number of Negative Frequencies = 1

Ir	-0.03311	-0.04061	0.13176
B	1.2587	-1.64948	0.09934
O	2.32854	-1.85463	0.9874
O	1.1282	-2.8094	-0.69972
C	-4.22957	-1.01361	-0.32788
C	-3.11115	-3.13273	-0.61847
C	-1.89486	-2.44807	-0.43887
H	-0.95276	-2.97472	-0.51289
C	-4.01767	1.82032	0.09297
N	-1.60794	1.51319	0.213
N	-1.79356	-1.13406	-0.20777
C	-2.86265	1.00439	0.0635
C	-2.96291	-0.41104	-0.15092
C	-5.29086	1.18032	-0.07769
C	-5.38917	-0.16652	-0.275
H	-6.19403	1.77983	-0.05403
H	-6.36948	-0.61077	-0.40449
C	-4.30727	-2.41709	-0.56011
C	2.9861	-3.11315	0.70685
C	1.89021	-3.89013	-0.10424
C	4.246	-2.81857	-0.11659
H	3.99634	-2.4027	-1.09694
H	4.86044	-2.08712	0.41903
H	4.84442	-3.72338	-0.27079
C	3.38576	-3.75342	2.03524
H	3.80915	-4.75273	1.87974
H	4.1471	-3.13642	2.52578
H	2.5336	-3.8355	2.71465
C	0.9316	-4.68301	0.79636
H	0.10776	-5.07898	0.19267
H	1.43348	-5.52934	1.27747
H	0.50413	-4.04318	1.57551
C	2.41805	-4.79394	-1.21527
H	3.04948	-5.59017	-0.80361
H	1.57801	-5.26572	-1.73764
H	2.99887	-4.23479	-1.95295
C	1.61185	1.1446	0.91839
C	2.97507	1.19687	0.53317
C	1.25343	1.76212	2.13911
C	3.94224	1.69558	1.41191
C	2.22415	2.25966	3.00962
H	0.20821	1.81272	2.42793
C	3.57598	2.21072	2.65723
H	4.98742	1.68656	1.11461
H	1.92315	2.68328	3.9649
H	4.33586	2.59296	3.33375
H	0.97154	1.24659	-0.1986
C	3.38108	0.70859	-0.82223
H	3.44349	-0.378	-0.89765
N	3.67022	1.34643	-1.88789
C	3.63127	2.81773	-2.06345
C	2.47044	3.54654	-1.35581
H	2.59314	3.57829	-0.27136
H	2.41695	4.58065	-1.71736
H	1.51466	3.06021	-1.58327
C	3.48074	3.02732	-3.58331
H	3.50264	4.09417	-3.83627

H	4.29045	2.52451	-4.1241
H	2.52958	2.6105	-3.93672
C	4.9842	3.39273	-1.60448
H	5.09167	3.32228	-0.51786
H	5.8146	2.84866	-2.06949
H	5.06483	4.44886	-1.88868
H	-3.94471	2.87801	0.23747
H	-1.61878	2.49217	0.0093
H	-1.30091	1.37193	1.15415
H	-5.25975	-2.8864	-0.6921
H	-3.07276	-4.18612	-0.80232

Thermal correction to Energy= 0.619602

Thermal correction to Enthalpy=0.620752

Thermal correction to Gibbs Free Energy=0.487396

Sum of electronic and zero-point Energies=-1455.417355

Sum of electronic and thermal Energies=-1455.370574

Sum of electronic and thermal Enthalpies=-1455.369424

Sum of electronic and thermal Free Energies=-1455.502779

SCF Done: E(RM11L) = -1456.10596565

4a

Number of Negative Frequencies = 0

Ir	0.06967	-1.62392	-0.18977
B	-1.82894	-0.93326	-0.34887
C	3.40511	0.84365	-1.81427
C	1.3949	1.88611	-2.64818
C	0.65128	0.89105	-1.98124
H	-0.432	0.8953	-2.01233
C	4.56881	-1.33519	-0.48133
N	2.33122	-2.34391	-0.1167
N	1.20763	-0.0835	-1.2688
O	-2.56812	-1.03999	-1.54354
O	-2.6108	-0.30653	0.62578
C	3.1942	-1.28079	-0.59002
C	2.5822	-0.16359	-1.22291
C	5.38238	-0.30512	-1.00889
C	4.81456	0.75627	-1.67797
H	6.46085	-0.37187	-0.90157
H	5.43205	1.53547	-2.11603
C	2.76629	1.88296	-2.53795
C	-3.98097	-0.2438	0.16002
C	-3.80795	-0.29939	-1.3997
H	-0.66516	-2.90199	0.47763
C	-4.62577	1.03227	0.69316
H	-5.64205	1.1509	0.29972
H	-4.68817	0.98567	1.78612
H	-4.04472	1.91976	0.42995
C	-4.70343	-1.4723	0.72874
H	-4.25263	-2.39888	0.35849
H	-4.60994	-1.46485	1.81989
H	-5.76894	-1.47373	0.47412
C	-4.91596	-1.03903	-2.14417
H	-5.88502	-0.55201	-1.98334
H	-4.70919	-1.03303	-3.22043
H	-4.99174	-2.0806	-1.82187
C	-3.58141	1.07935	-2.031
H	-4.49112	1.68942	-2.019
H	-2.79099	1.62476	-1.50807
H	-3.27196	0.94806	-3.07376
C	0.49066	0.42701	2.07586
C	0.41722	-0.93709	1.66305
C	0.79614	-1.90293	2.63592
C	1.26049	-1.56273	3.90518
C	1.35689	-0.21806	4.27834
C	0.96356	0.75155	3.36637
H	0.72775	-2.95731	2.38225
H	1.53724	-2.34999	4.60404
H	1.00059	1.80342	3.63513
H	1.70995	0.06417	5.26704
C	0.04031	1.55942	1.23154
N	0.43484	2.75324	1.46598
C	-0.09573	3.92207	0.75
C	-0.64995	4.8593	1.84243
H	-1.50098	4.39367	2.35411
H	0.11988	5.07479	2.59191
H	-0.98712	5.80802	1.40711
C	1.10463	4.59591	0.05789
H	1.51985	3.94279	-0.71762
H	0.80375	5.54104	-0.41018
H	1.89747	4.80516	0.78501
C	-1.20365	3.6406	-0.27843
H	-1.556	4.58237	-0.71456
H	-0.84646	3.01087	-1.09818
H	-2.06235	3.14607	0.18846
H	-0.67922	1.30671	0.45124
H	3.37042	2.65623	-3.00428
H	0.87004	2.65337	-3.20685
H	5.02783	-2.19187	0.00488

H	2.55215	-2.57413	0.8535
H	2.49292	-3.19291	-0.66153

Thermal correction to Energy=0.620307

Thermal correction to Enthalpy= 0.621457

Thermal correction to Gibbs Free Energy=0.50931

Sum of electronic and zero-point Energies=-1455.479463

Sum of electronic and thermal Energies=-1455.431765

Sum of electronic and thermal Enthalpies=-1455.430615

Sum of electronic and thermal Free Energies=-1455.565424

SCF Done: E(RM11L) = -1456.16218799

TS5a

Number of Negative Frequencies = 1

Ir	0.24336	0.26635	0.55529
B	1.03778	-1.38066	-0.61011
C	-4.12675	-0.21922	0.66629
C	-3.39487	-2.44767	1.23161
C	-2.0732	-1.97583	1.10217
H	-1.25156	-2.66834	1.22105
C	-3.38383	2.43367	-0.16128
N	-1.05577	1.72264	0.01949
N	-1.73961	-0.72368	0.79618
O	0.20119	-2.52808	-0.72736
O	1.63164	-1.11684	-1.87055
C	-2.39992	1.46538	0.14063
C	-2.76455	0.14672	0.55575
C	-4.75937	2.04609	-0.00885
C	-5.11182	0.78692	0.38343
H	-5.53722	2.77101	-0.22053
H	-6.16319	0.53687	0.47329
C	-4.45079	-1.55593	1.03229
C	0.8788	-1.83937	-2.8637
C	0.36053	-3.07715	-2.04684
H	1.50008	1.22511	0.28705
C	1.80504	-2.17854	-4.02892
H	1.29258	-2.8078	-4.76614
H	2.12168	-1.25765	-4.53144
H	2.70375	-2.69955	-3.68822
C	-0.2582	-0.92443	-3.34233
H	-0.92486	-0.6703	-2.51258
H	0.17447	0.00834	-3.72012
H	-0.84326	-1.38513	-4.14596
C	-0.98141	-3.63985	-2.50978
H	-0.92491	-3.99048	-3.54705
H	-1.26402	-4.49147	-1.8798
H	-1.77418	-2.89097	-2.43504
C	1.40229	-4.20075	-1.95102
H	1.53358	-4.72501	-2.90424
H	2.3717	-3.80381	-1.63236
H	1.07086	-4.92841	-1.20192
C	1.47655	-1.89745	1.95267
C	1.95294	-1.28029	0.77439
C	3.31397	-0.82497	0.78884
C	4.12279	-1.07554	1.89437
C	3.60148	-1.66017	3.0588
C	2.27014	-2.0503	3.10039
H	5.17241	-0.79799	1.85876
H	1.85451	-2.51047	3.99311
H	4.24812	-1.8138	3.91922
C	3.94122	-0.21518	-0.42384
H	3.91255	-0.88712	-1.28619
N	4.51427	0.90213	-0.63845
C	4.63584	2.08825	0.22881
C	6.14675	2.38388	0.30782
H	6.58154	2.46744	-0.69457
H	6.32643	3.32277	0.84513
H	6.67068	1.58039	0.84031
C	4.05033	2.06575	1.65496
H	3.00468	1.74783	1.65678
H	4.61485	1.41311	2.32491
H	4.09687	3.08066	2.07006
C	3.93535	3.21199	-0.56813
H	4.33127	3.26865	-1.58789
H	2.85829	3.01736	-0.62954
H	4.08653	4.18216	-0.07977
H	0.48377	-2.32801	1.95726
H	-5.47451	-1.85203	1.12836
H	-3.54343	-3.4789	1.4753
H	-3.11556	3.41591	-0.49013
H	-0.85072	2.53017	0.57252
H	-0.87613	1.95208	-0.93711

Thermal correction to Energy= 0.619050

Thermal correction to Enthalpy=0.620200

Thermal correction to Gibbs Free Energy= 0.488082

Sum of electronic and zero-point Energies=-1455.428902

Sum of electronic and thermal Energies=-1455.382164

Sum of electronic and thermal Enthalpies=-1455.381014

Sum of electronic and thermal Free Energies=-1455.513132

SCF Done: E(RM11L) = -1456.11612317

6a

Number of Negative Frequencies = 0

Ir	-0.17491	-1.15634	-0.27306
B	0.579	1.44174	-0.56093
C	-4.51857	-0.56589	0.27261
C	-4.06381	0.71235	-1.71348
C	-2.70764	0.33444	-1.6027
H	-1.98749	0.71544	-2.31174
C	-3.5204	-2.24049	2.29968
N	-1.25012	-2.10205	1.30874
N	-2.23164	-0.44608	-0.63761
O	-0.44573	2.16956	-1.15176
O	0.98133	2.00185	0.64335
C	-2.66476	-1.76161	1.33161
C	-3.13462	-0.91265	0.30132
C	-4.88977	-1.88935	2.27585
C	-5.37951	-1.07007	1.28152
H	-5.55165	-2.27411	3.04574
H	-6.43148	-0.79962	1.25202
C	-4.9704	0.27382	-0.77872
C	-0.04817	2.94465	1.04015
C	-0.66792	3.35761	-0.34464
H	1.17688	-1.89487	0.18557
C	0.60529	4.08126	1.8188
H	-0.12797	4.86071	2.05535
H	1.01055	3.69796	2.76174
H	1.42798	4.53226	1.25857
C	-1.03426	2.1859	1.93815
H	-1.51673	1.37119	1.38988
H	-0.48169	1.74605	2.77537
H	-1.80529	2.84954	2.34443
C	-2.16167	3.66458	-0.31189
H	-2.36427	4.51372	0.35072
H	-2.50906	3.92889	-1.31694
H	-2.74466	2.80697	0.03017
C	0.09445	4.49983	-1.02472
H	-0.0673	5.45522	-0.51445
H	1.16955	4.29413	-1.05015
H	-0.25684	4.59753	-2.05736
C	0.55389	-0.53633	-2.2348
C	1.27384	0.22906	-1.23616
C	2.69997	-0.05689	-1.06176
C	3.30274	-1.04359	-1.8074
C	2.56283	-1.84306	-2.72571
C	1.23541	-1.5843	-2.95126
H	4.37377	-1.19864	-1.72437
H	0.68776	-2.13531	-3.71309
H	3.075	-2.6253	-3.28066
C	3.52488	0.88538	-0.25616
H	3.30179	1.93073	-0.50513
N	4.44542	0.75064	0.61869
C	4.91297	-0.48236	1.28041
C	6.22289	-0.91664	0.59478
H	6.93403	-0.08349	0.55393
H	6.68846	-1.73866	1.15188
H	6.04164	-1.2604	-0.42896
C	3.92192	-1.65902	1.35458
H	2.94105	-1.31619	1.69951
H	3.77837	-2.15816	0.39527
H	4.29581	-2.40412	2.06779
C	5.2336	-0.03771	2.72536
H	5.93695	0.80229	2.72258
H	4.32004	0.28739	3.2384
H	5.67478	-0.86144	3.29956
H	-0.29743	-0.09126	-2.74571
H	-6.0188	0.55428	-0.82767
H	-4.36109	1.35723	-2.534
H	-3.13637	-2.89209	3.07997
H	-1.13216	-3.11666	1.24243
H	-0.80099	-1.82463	2.18539

Thermal correction to Energy=0.620800

Thermal correction to Enthalpy=0.621950

Thermal correction to Gibbs Free Energy=0.487730

Sum of electronic and zero-point Energies= -1455.444831

Sum of electronic and thermal Energies=-1455.397446

Sum of electronic and thermal Enthalpies=-1455.396296

Sum of electronic and thermal Free Energies= -1455.530515

SCF Done: E(RM11L) = -1456.13739036

7

Number of Negative Frequencies = 0

C	2.60547	-1.92103	-1.79857
H	1.95144	-2.2444	-2.59691
C	4.00066	-2.05898	-1.9035
C	4.2345	-1.07325	0.2769
C	2.81476	-0.96017	0.32894

C	2.19939	-0.39818	1.47143
C	2.96287	0.04033	2.53518
N	1.99054	-1.3881	-0.72301
N	0.75306	-0.30024	1.44329
C	4.99255	-0.61492	1.38662
C	4.37089	-0.07095	2.49132
H	6.07498	-0.70266	1.34729
H	4.96043	0.27654	3.33476
C	4.82546	-1.64202	-0.88186
C	-4.35016	-0.66783	0.34751
Ir	0.06092	-1.14345	-0.47639
H	-0.35426	-1.7725	-1.92772
C	-5.00251	-0.73815	-1.03551
H	-5.51911	-1.69153	-1.18313
H	-5.73622	0.06953	-1.12184
H	-4.26101	-0.61296	-1.83122
C	-5.39099	-0.84004	1.44615
H	-6.22785	-0.15627	1.26976
H	-5.77976	-1.86411	1.44333
H	-4.97657	-0.62518	2.43414
O	-2.03663	-0.69825	-0.0363
B	-2.46216	0.6212	0.11278
C	0.03232	3.3993	-1.12726
C	0.24503	3.46679	0.43198
B	-1.35793	1.89668	-0.10072
O	-0.48283	2.28167	0.89929
O	-1.21189	2.63262	-1.24505
C	1.69431	3.34319	0.88885
H	2.29085	4.17659	0.50245
H	1.74058	3.37176	1.98306
H	2.14481	2.40666	0.55305
C	1.10772	2.58857	-1.85706
H	0.80855	2.46323	-2.90293
H	2.07686	3.09754	-1.83358
H	1.2106	1.5884	-1.42079
C	-0.16997	4.75081	-1.80324
H	-0.32712	4.6051	-2.87713
H	-1.03802	5.27936	-1.40192
H	0.71655	5.38077	-1.67098
C	-0.42945	4.67001	1.09524
H	-0.39666	4.54239	2.18239
H	0.08241	5.60397	0.84225
H	-1.47873	4.75188	0.7939
O	-3.776	0.68099	0.46249
C	-3.09501	-1.59562	0.49253
C	-2.70447	-1.89332	1.94027
H	-1.71294	-2.35769	1.94348
H	-2.66158	-0.97673	2.53762
H	-3.41547	-2.58326	2.40479
C	-3.1289	-2.86951	-0.33564
H	-3.22816	-2.6574	-1.4017
H	-2.19881	-3.42743	-0.1876
H	-3.97058	-3.49487	-0.01734
H	4.40539	-2.50043	-2.80885
H	5.90519	-1.73958	-0.94422
H	2.47171	0.47293	3.40276
H	0.35354	-0.7567	2.26631
H	0.46492	0.68538	1.48155

Thermal correction to Energy= 0.561167

Thermal correction to Enthalpy= 0.562111

Thermal correction to Gibbs Free Energy= 0.470423

Sum of electronic and zero-point Energies= -1384.405361

Sum of electronic and thermal Energies= -1384.374970

Sum of electronic and thermal Enthalpies= -1384.374025

Sum of electronic and thermal Free Energies= -1384.465713

E(RM11L) = -1385.05611278

TS8

Number of Negative Frequencies = 1

Ir	0.08355	-0.41387	-1.31294
B	1.27404	-1.13049	0.93896
B	2.70471	-0.53355	0.18922
C	-3.94629	0.44317	-0.43181
C	-2.54759	0.45524	-0.60721
C	-1.75743	1.5523	-0.16292
C	-2.34741	2.67212	0.45981
C	-0.12385	3.58379	0.70962
C	0.36528	2.4168	0.0871
H	1.43198	2.26199	-0.031
N	-1.85703	-0.60055	-1.17044
N	-0.41107	1.42652	-0.35255
O	1.0702	-2.50894	1.12837
O	0.69365	-0.40545	1.99177
C	-4.53279	1.60075	0.18994
C	-3.77629	2.65789	0.61259
H	-5.60728	1.63002	0.33315
H	-4.26626	3.50423	1.0814
C	-1.5017	3.72804	0.9032

C	0.50649	-2.70389	2.44578
C	-0.14061	-1.30575	2.75726
H	0.31781	-1.83584	-2.12458
C	4.47353	0.87267	-0.25994
O	3.57543	-1.27739	-0.58617
O	3.13973	0.77592	0.32021
C	4.48431	-0.3463	-1.24482
C	1.67909	-3.03909	3.37893
H	1.34316	-3.26121	4.39786
H	2.20293	-3.9184	2.98922
C	-0.47483	-3.87252	2.39988
H	0.06407	-4.79887	2.17107
H	-0.97455	-4.00142	3.36734
H	-1.2366	-3.72886	1.62926
C	-1.57792	-1.18668	2.23874
H	-2.2726	-1.78174	2.8419
H	-1.89067	-0.13886	2.28674
H	-1.64485	-1.51299	1.19972
C	-0.0856	-0.88165	4.22342
H	-0.56679	0.09606	4.34267
H	-0.61739	-1.59992	4.85831
H	0.94361	-0.7938	4.58121
C	5.83959	-1.01905	-1.42508
H	5.74739	-1.85867	-2.12239
H	6.56787	-0.312	-1.83842
H	6.22567	-1.4054	-0.47874
C	3.86234	-0.02171	-2.6092
H	4.50692	0.63457	-3.20352
H	3.71173	-0.95348	-3.16338
H	2.88425	0.46183	-2.49363
C	4.61932	2.24005	-0.91882
H	4.58837	3.02468	-0.15458
H	5.5786	2.31571	-1.4434
H	3.81618	2.43235	-1.63468
C	5.4684	0.7263	0.89617
H	6.50184	0.85004	0.5559
H	5.25816	1.49481	1.64742
H	5.37138	-0.25301	1.37603
H	2.39365	-2.21016	3.41793
H	-1.92791	4.58891	1.37452
H	0.58415	4.32324	1.02084
H	-4.45593	-0.33521	-0.71901
H	-2.47419	-0.58455	-1.95711
H	-2.46473	-1.24535	-0.70681

Thermal correction to Energy=0.573134

Thermal correction to Enthalpy=0.574284

Thermal correction to Gibbs Free Energy= 0.450609

Sum of electronic and zero-point Energies=-1384.383945

Sum of electronic and thermal Energies= -1384.340651

Sum of electronic and thermal Enthalpies= -1384.339501

Sum of electronic and thermal Free Energies= -1384.463175

SCF Done: E(RM11L) = -1385.03185484

9

Number of Negative Frequencies = 0

Ir	0.19283	-0.31284	-1.14007
B	-1.66473	-0.80172	-0.51004
H	-0.54252	0.27116	-2.46218
C	4.68105	-0.68785	-0.95784
C	3.32088	-0.57863	-0.74796
C	2.71837	-1.25559	0.35179
C	3.54996	-1.9694	1.26836
C	1.56717	-2.48939	2.53817
C	0.80707	-1.80754	1.5646
N	2.46617	0.20775	-1.59453
N	1.34605	-1.21757	0.50016
O	1.05784	2.14236	0.23574
O	-1.19833	2.25353	-0.17703
C	5.49547	-1.4369	-0.07701
C	4.9467	-2.04917	1.02737
H	6.56223	-1.50482	-0.26909
H	5.56716	-2.60549	1.72447
C	2.93007	-2.58638	2.38494
C	-0.88563	3.37809	0.68144
C	0.66713	3.51657	0.4959
C	-3.73011	-1.86516	-0.42299
B	-0.06002	1.46001	-0.29661
H	-0.27147	-1.73357	1.6467
C	-3.4987	-1.05996	0.90316
O	-2.08175	-0.77438	0.83704
O	-2.71015	-1.32057	-1.29329
C	-4.23297	0.28703	0.92581
H	-3.88926	0.8642	1.79042
H	-4.01157	0.86803	0.02585
H	-5.3178	0.15788	1.00927
C	-3.7865	-1.83281	2.188
H	-3.58145	-1.19614	3.05625
H	-4.83828	-2.13873	2.23384

H	-3.16145	-2.726	2.27123
C	-3.44	-3.36459	-0.26986
H	-4.20191	-3.87069	0.3332
H	-3.42476	-3.82758	-1.2625
H	-2.46123	-3.52774	0.19417
C	-5.09516	-1.66128	-1.0739
H	-5.15837	-2.25179	-1.99506
H	-5.9003	-1.98917	-0.40571
H	-5.26246	-0.61315	-1.33452
C	-1.69931	4.58503	0.22432
H	-2.76635	4.39215	0.38159
H	-1.42775	5.47863	0.79842
H	-1.54876	4.79245	-0.83816
C	1.05321	4.3352	-0.74178
H	0.84529	5.40189	-0.60604
H	2.12673	4.21764	-0.92715
H	0.51457	3.98362	-1.62801
C	1.42357	4.02047	1.72058
H	2.49571	4.07413	1.49975
H	1.085	5.02469	2.00129
H	1.28982	3.35492	2.57717
C	-1.2832	2.98086	2.10854
H	-2.34298	2.70779	2.11743
H	-0.71004	2.11168	2.44701
H	-1.13177	3.80233	2.81724
H	3.54211	-3.12655	3.10226
H	1.05701	-2.94148	3.38239
H	2.83781	0.26841	-2.54162
H	2.393	1.16114	-1.22662
H	5.12941	-0.17273	-1.80344

Thermal correction to Energy=0.574358

Thermal correction to Enthalpy=0.575508

Thermal correction to Gibbs Free Energy=0.46926

Sum of electronic and zero-point Energies= -1384.469598

Sum of electronic and thermal Energies= -1384.425163

Sum of electronic and thermal Enthalpies=-1384.424013

Sum of electronic and thermal Free Energies=-1384.551740

SCF Done: E(RM11L) = -1385.10349478

TS10

Number of Negative Frequencies = 1

Ir	0.2199	0.11514	-1.05272
H	1.43734	1.37807	-1.54461
C	-4.31669	1.17661	0.12547
C	-5.00506	2.39665	-0.11912
C	-2.89853	3.54389	0.1766
C	-2.30688	2.26076	0.39439
C	-0.90678	2.18956	0.64528
C	-0.1418	3.33423	0.69769
B	-0.76064	-1.61086	-0.3828
N	-3.02138	1.10009	0.37204
N	-0.29607	0.89555	0.79542
O	-1.20223	-2.69679	-1.13752
O	-1.01377	-1.84555	0.98225
C	-2.08826	4.70582	0.2213
C	-0.73928	4.59797	0.48582
H	-2.55538	5.68136	0.05487
H	-0.11616	5.4909	0.52687
C	-4.29555	3.57586	-0.0859
C	-1.88419	-3.0075	1.09717
C	-1.54902	-3.77939	-0.22373
C	3.77829	0.35507	1.16394
B	2.14739	0.23677	-0.47578
H	-4.86619	0.23921	0.11366
C	4.42793	-0.05984	-0.2078
O	3.26028	-0.44037	-0.98928
O	2.49352	0.89007	0.74207
C	5.09799	1.11787	-0.92644
H	6.02822	1.42792	-0.43413
H	5.33563	0.82263	-1.9522
H	4.42337	1.98694	-0.97186
C	5.38233	-1.24832	-0.13724
H	5.77678	-1.46338	-1.12977
H	6.22234	-1.03182	0.52886
H	4.87431	-2.14628	0.22674
C	3.49034	-0.84222	2.08022
H	4.41272	-1.25109	2.51014
H	2.8408	-0.52442	2.89638
H	2.97164	-1.64199	1.53578
C	4.5261	1.43781	1.93589
H	4.01158	1.6521	2.87019
H	5.54739	1.11316	2.17405
H	4.58172	2.3689	1.3575
C	-0.30198	-4.6721	-0.10437
H	-0.49173	-5.55226	0.53416
H	-0.01865	-5.02591	-1.10121
H	0.54312	-4.11717	0.32201
C	-2.70837	-4.57985	-0.82178

H	-2.37935	-5.07543	-1.73869
H	-3.04973	-5.34592	-0.12461
H	-3.5563	-3.9271	-1.06189
C	-3.32269	-2.48791	1.13508
H	-4.04403	-3.30639	1.30443
H	-3.42704	-1.7743	1.96339
H	-3.58578	-1.97036	0.21417
C	-1.54871	-3.75529	2.38448
H	-1.80909	-3.12925	3.25369
H	-2.12026	-4.68824	2.455
H	-0.48266	-3.9943	2.44624
H	-6.07449	2.38533	-0.31412
H	-4.78211	4.52761	-0.26675
H	0.92418	3.25979	0.88131
H	-0.9361	0.2327	1.25235
H	0.57289	0.95753	1.33637

Thermal correction to Energy=0.571160

Thermal correction to Enthalpy=0.572310

Thermal correction to Gibbs Free Energy=0.443545

Sum of electronic and zero-point Energies=-1384.405130

Sum of electronic and thermal Energies= -1384.360905

Sum of electronic and thermal Enthalpies=-1384.359755

Sum of electronic and thermal Free Energies=-1384.488520

SCF Done: E(RM11L) = -1385.04504706

2b

Number of Negative Frequencies = 0

Ir	-0.64772	-0.32544	-0.38174
B	0.80916	1.0778	-0.57534
O	1.64722	1.2093	-1.70302
O	1.16483	2.08917	0.3525
C	-4.52398	1.16517	0.48253
C	-3.04141	3.03875	0.70657
C	-1.95706	2.19813	0.41361
H	-0.94623	2.57873	0.39766
C	-4.83941	-1.59427	0.02654
N	-2.3831	-1.83627	-0.21503
N	-2.08643	0.8799	0.14301
C	-3.57286	-1.04362	0.00713
C	-3.38682	0.34441	0.21331
C	-5.96937	-0.78149	0.26154
C	-5.81212	0.56773	0.49288
H	-6.95929	-1.22812	0.26736
H	-6.67344	1.20111	0.68769
C	-4.32736	2.54766	0.72868
C	2.72455	2.12521	-1.39458
C	2.08479	3.01444	-0.2755
C	3.90689	1.28759	-0.88888
H	3.6381	0.74026	0.01953
H	4.17552	0.55554	-1.65773
H	4.78764	1.90636	-0.68302
C	3.12071	2.87343	-2.66448
H	3.86546	3.64766	-2.44463
H	3.56206	2.17589	-3.38559
H	2.25729	3.34533	-3.14076
C	1.25204	4.17616	-0.83577
H	0.68067	4.63298	-0.01989
H	1.88291	4.95141	-1.28479
H	0.54186	3.82344	-1.59089
C	3.06302	3.53669	0.77314
H	3.81833	4.18432	0.3119
H	2.52417	4.12734	1.52295
H	3.57279	2.72239	1.29234
C	0.54783	-3.31751	-0.81244
C	1.64022	-2.58807	-0.30849
C	0.50753	-3.70279	-2.15612
C	2.69701	-2.25845	-1.17697
C	1.56055	-3.36564	-3.00808
H	-0.33985	-4.27062	-2.53145
C	2.6569	-2.64618	-2.51226
H	1.53303	-3.66364	-4.05278
H	3.478	-2.38456	-3.17454
H	-0.25705	-3.60217	-0.14035
H	-4.95633	-2.66218	-0.13803
H	-2.49158	-2.42014	-1.04524
H	-2.23537	-2.47088	0.57212
H	-5.18105	3.18604	0.93544
H	-2.83304	4.08604	0.9027
C	3.88719	-1.4537	-0.62248
H	4.60198	-1.29123	-1.40195
N	4.51844	-2.20415	0.47262
H	1.63563	-2.28762	0.71845
C	5.95309	-1.88732	0.5205
C	6.14059	-0.35906	0.55005
H	7.09598	-0.12501	0.97116
H	6.08605	0.02631	-0.44665
H	5.37	0.08336	1.14617
C	6.57324	-2.50518	1.78749

H	6.42714	-3.56509	1.77564
H	7.62103	-2.28983	1.81317
H	6.10243	-2.08991	2.65397
C	6.64842	-2.4658	-0.72589
H	7.70731	-2.47352	-0.57226
H	6.30515	-3.46516	-0.89425
H	6.41593	-1.86065	-1.57715

Thermal correction to Energy=0.623325

Thermal correction to Enthalpy=0.624475

Thermal correction to Gibbs Free Energy=0.484974

Sum of electronic and zero-point Energies=-1455.437298

Sum of electronic and thermal Energies=-1455.388998

Sum of electronic and thermal Enthalpies= -1455.387848

Sum of electronic and thermal Free Energies=-1455.527349

SCF Done: E(RM11L) = -1456.1328824

TS3b

Number of Negative Frequencies = 1

B	-0.48289000	1.62276000	-0.34174000
C	-4.98402000	-1.15176000	1.20458000
C	-5.48115000	0.11191000	1.61108000
C	-4.74927000	1.24092000	1.32694000
C	-3.51099000	1.12189000	0.66746000
C	0.86719000	3.49721000	-0.05535000
C	-0.62018000	3.95220000	-0.24102000
N	-2.99728000	-0.04538000	0.26807000
O	0.71526000	2.08642000	0.22980000
O	-1.24223000	2.74388000	-0.74653000
C	0.82201000	-1.15215000	-1.00696000
C	0.91605000	-2.36298000	-1.75590000
C	2.07839000	-3.13916000	-1.69853000
H	2.12068000	-4.07524000	-2.25304000
C	3.18275000	-2.74185000	-0.95216000
H	4.06160000	-3.38105000	-0.92367000
C	3.16089000	-1.49779000	-0.25084000
C	1.96456000	-0.72055000	-0.31906000
C	-1.30994000	4.30152000	1.08464000
H	-2.38348000	4.43117000	0.90678000
H	-1.18041000	3.49965000	1.81904000
H	-0.92321000	5.23265000	1.51295000
C	-0.83100000	5.07725000	-1.25019000
H	-1.89771000	5.31911000	-1.31941000
H	-0.29780000	5.98388000	-0.94038000
H	-0.48638000	4.79307000	-2.24760000
C	1.60853000	4.16007000	1.10183000
H	2.63516000	3.77961000	1.15111000
H	1.65649000	5.24650000	0.96272000
H	1.12709000	3.95172000	2.06082000
C	1.69469000	3.60794000	-1.34343000
H	1.91083000	4.64997000	-1.60367000
H	2.64561000	3.08336000	-1.20072000
H	1.17395000	3.13734000	-2.18403000
H	0.08466000	-2.68503000	-2.37638000
H	-5.09429000	2.22912000	1.61278000
H	0.13004000	-0.19053000	-1.70334000
C	4.25791000	-0.98522000	0.48353000
H	4.13892000	-0.04795000	1.01466000
C	6.70074000	-0.89110000	1.02758000
Ir	-1.07191000	-0.31185000	-0.57072000
C	-3.73636000	-1.19378000	0.51031000
C	-3.23963000	-2.44429000	0.05880000
C	-5.67095000	-2.36510000	1.46999000
C	-5.14822000	-3.56923000	1.05310000
C	-3.93133000	-3.60611000	0.33445000
N	-2.00764000	-2.42461000	-0.69175000
H	-5.67249000	-4.49697000	1.26216000
H	-2.91894000	1.99755000	0.43800000
H	1.93831000	0.24264000	0.17870000
N	5.46961000	-1.61776000	0.63927000
C	6.48435000	-0.17404000	2.36987000
H	6.15608000	-0.88252000	3.13861000
H	7.42305000	0.28499000	2.69914000
H	5.73775000	0.62379000	2.29657000
C	7.80042000	-1.95119000	1.18502000
H	8.74526000	-1.48188000	1.47877000
H	7.52400000	-2.68582000	1.94989000
H	7.96972000	-2.48498000	0.24072000
C	7.09373000	0.12275000	-0.06476000
H	7.25581000	-0.38581000	-1.02295000
H	6.30027000	0.86565000	-0.20629000
H	8.01594000	0.65224000	0.20278000
H	-3.53392000	-4.55483000	-0.01608000
H	-6.61275000	-2.32278000	2.01001000
H	-6.42929000	0.16876000	2.13852000
H	-1.38032000	-3.17071000	-0.38947000
H	-2.19699000	-2.58352000	

Thermal correction to Energy= 0.629795

Thermal correction to Enthalpy= 0.630945

Thermal correction to Gibbs Free Energy= 0.478593

Sum of electronic and zero-point Energies= -1456.011280

Sum of electronic and thermal Energies= -1455.962860

Sum of electronic and thermal Enthalpies= -1455.961710

Sum of electronic and thermal Free Energies= -1456.101008

SCF Done: E(RM11L) = -1456.0787149

4b

Number of Negative Frequencies = 0

Ir	0.06967	-1.62392	-0.18977
B	-1.82894	-0.93326	-0.34887
C	3.40511	0.84365	-1.81427
C	1.3949	1.88611	-2.64818
C	0.65128	0.89105	-1.98124
H	-0.432	0.8953	-2.01233
C	4.56881	-1.33519	-0.48133
N	2.33122	-2.34391	-0.1167
N	1.20763	-0.0835	-1.2688
O	-2.56812	-1.03999	-1.54354
O	-2.6108	-0.30653	0.62578
C	3.1942	-1.28079	-0.59002
C	2.5822	-0.16359	-1.22291
C	5.38238	-0.30512	-1.00889
C	4.81456	0.75627	-1.67797
H	6.46085	-0.37187	-0.90157
H	5.43205	1.53547	-2.11603
C	2.76629	1.88296	-2.53795
C	-3.98097	-0.2438	0.16002
C	-3.80795	-0.29939	-1.3997
H	-0.66516	-2.90199	0.47763
C	-4.62577	1.03227	0.69316
H	-5.64205	1.1509	0.29972
H	-4.68817	0.98567	1.78612
H	-4.04472	1.91976	0.42995
C	-4.70343	-1.4723	0.72874
H	-4.25263	-2.39888	0.35849
H	-4.60994	-1.46485	1.81989
H	-5.76894	-1.47373	0.47412
C	-4.91596	-1.03903	-2.14417
H	-5.88502	-0.55201	-1.98334
H	-4.70919	-1.03303	-3.22043
H	-4.99174	-2.0806	-1.82187
C	-3.58141	1.07935	-2.031
H	-4.49112	1.68942	-2.019
H	-2.79099	1.62476	-1.50807
H	-3.27196	0.94806	-3.07376
C	0.49066	0.42701	2.07586
C	0.41722	-0.93709	1.66305
C	0.79614	-1.90293	2.63592
C	1.26049	-1.56273	3.90518
C	1.35689	-0.21806	4.27834
C	0.96356	0.75155	3.36637
H	0.72775	-2.95731	2.38225
H	1.53724	-2.34999	4.60404
H	1.70995	0.06417	5.26704
H	3.37042	2.65623	-3.00428
H	0.87004	2.65337	-3.20685
H	5.02783	-2.19187	0.00488
H	2.55215	-2.57413	0.8535
H	2.49292	-3.19291	-0.66153
C	1.01605	2.24275	3.74738
H	1.69837	2.75255	3.09973
N	1.46861	2.37716	5.13951
C	0.50989	3.20184	5.88896
C	-0.90063	2.59832	5.75554
H	-1.33729	2.91319	4.83082
H	-0.83486	1.5305	5.77359
H	-1.50978	2.93197	6.56949
C	0.51132	4.6337	5.32207
H	1.34024	4.75278	4.65603
H	-0.40099	4.80788	4.7908
H	0.59572	5.33531	6.12552
C	0.91461	3.23743	7.3744
H	1.92135	3.58926	7.46144
H	0.25967	3.89504	7.90685
H	0.844	2.2527	7.787
H	0.16564	1.24429	1.4665

Thermal correction to Energy=0.620406

Thermal correction to Enthalpy=0.621556

Thermal correction to Gibbs Free Energy=0.483927

Sum of electronic and zero-point Energies=-1455.479916

Sum of electronic and thermal Energies=-1455.432138

Sum of electronic and thermal Enthalpies=-1455.430988

Sum of electronic and thermal Free Energies=-1455.568618

SCF Done: E(RM11L) = -1456.16519379

TS5b

Number of Negative Frequencies = 1

Ir	0.18058	-0.80513	0.10581
B	-0.43067	1.26954	0.05565
C	4.5886	-0.92763	0.3118
C	4.05156	0.74895	1.95019
C	2.6863	0.56625	1.63809
H	1.93757	1.17954	2.11791
C	3.64946	-2.69665	-1.66621
N	1.31772	-1.97565	-1.20915
N	2.24219	-0.30888	0.74149
O	0.51739	2.23262	0.51808
O	-1.03403	1.7642	-1.1325
C	2.75224	-1.93136	-0.95486
C	3.19003	-1.04265	0.05488
C	5.03393	-2.59999	-1.39415
C	5.49451	-1.73009	-0.42901
H	5.73106	-3.21148	-1.95888
H	6.5577	-1.64349	-0.22223
C	5.00455	0.00074	1.3015
C	-0.19043	2.8167	-1.63729
C	0.4307	3.39863	-0.31901
H	-1.17135	-1.36608	-0.56583
C	-1.04988	3.79411	-2.43488
H	-0.46255	4.66377	-2.75278
H	-1.43578	3.29985	-3.33367
H	-1.90588	4.14411	-1.85198
C	0.86322	2.17654	-2.55552
H	1.49098	1.47606	-1.99553
H	0.34964	1.61373	-3.34273
H	1.50321	2.92825	-3.03118
C	1.82524	4.00045	-0.4782
H	1.81469	4.82883	-1.1962
H	2.17552	4.39102	0.48433
H	2.54603	3.25204	-0.81808
C	-0.50026	4.39903	0.38078
H	-0.56559	5.34946	-0.16074
H	-1.50819	3.98406	0.4837
H	-0.11325	4.60139	1.3856
C	-0.80432	0.32693	2.5024
C	-1.34997	0.52587	1.21292
C	-2.75958	0.29414	1.06589
C	-3.53477	-0.02689	2.17677
C	-2.94736	-0.25706	3.43113
C	-1.578	-0.10364	3.59269
H	-1.11159	-0.26813	4.56061
H	-3.57375	-0.53948	4.27377
H	0.23186	0.58017	2.68305
H	6.06217	0.11082	1.5246
H	4.32169	1.4813	2.704
H	3.2882	-3.36953	-2.43933
H	0.98454	-2.94358	-1.15904
H	1.11942	-1.66155	-2.16296
C	-5.06221	-0.14675	2.02136
H	-5.51098	-0.26108	2.98594
N	-5.3799	-1.31758	1.19122
C	-6.59389	-1.04768	0.40746
C	-6.50343	-1.77618	-0.94631
H	-7.41236	-2.3119	-1.1245
H	-6.35239	-1.06037	-1.72715
H	-5.68269	-2.46244	-0.92791
C	-6.72339	0.46793	0.16716
H	-6.60995	0.98726	1.09578
H	-5.96344	0.78709	-0.51513
H	-7.68674	0.6825	-0.24612
C	-7.82666	-1.55205	1.18045
H	-8.69601	-1.46227	0.56315
H	-7.68418	-2.578	1.44882
H	-7.9563	-0.96631	2.06645
H	-3.25755	0.48542	0.13835

Thermal correction to Energy=0.619022

Thermal correction to Enthalpy=0.620173

Thermal correction to Gibbs Free Energy=0.486147

Sum of electronic and zero-point Energies= -1455.446329

Sum of electronic and thermal Energies=-1455.399375

Sum of electronic and thermal Enthalpies=-1455.398225

Sum of electronic and thermal Free Energies=-1455.532250

SCF Done: E(RM11L) = -1456.13805901

3

Number of Negative Frequencies = 0

B	-0.29753	0.01209	1.32093
B	-1.55035	-1.38087	-0.72264
B	-1.56175	1.35225	-0.7201
C	1.79033	2.68045	-0.72271
H	0.80327	3.13117	-0.77065
C	2.95187	3.48101	-0.70104
C	4.22512	1.42535	-0.59824
C	3.00041	0.71468	-0.62227

C	2.99601	-0.72855	-0.56811
C	4.21508	-1.44453	-0.48593
N	1.79886	1.35151	-0.68775
N	1.79083	-1.35914	-0.58955
O	-1.24656	0.71576	2.07019
O	0.57601	-0.66952	2.1844
O	-2.18089	-1.76826	-1.92305
O	-2.07127	-2.15014	0.33236
O	-1.3358	2.73536	-0.92234
O	-2.94205	1.15015	-0.58046
C	5.44423	0.66928	-0.52876
C	5.4396	-0.69423	-0.47366
H	6.39211	1.19546	-0.51367
H	6.38388	-1.22389	-0.41648
C	4.19538	2.85048	-0.64318
C	0.00699	-0.64094	3.51539
C	-0.87166	0.65817	3.46481
C	-3.64732	2.3776	-0.8562
C	-2.54425	3.45851	-0.58907
C	-2.98993	-2.94054	-1.67246
C	-3.25771	-2.83277	-0.13032
Ir	-0.05406	-0.01903	-0.6519
C	-4.0952	2.32123	-2.32326
H	-4.69522	1.41731	-2.47434
H	-4.70254	3.18937	-2.60342
H	-3.23077	2.26584	-2.99329
C	-4.86604	2.46197	0.05925
H	-5.37549	3.42682	-0.05177
H	-5.57949	1.67134	-0.19972
H	-4.58678	2.33035	1.10758
C	-2.63249	4.70754	-1.4604
H	-3.57554	5.24001	-1.28817
H	-1.8107	5.39026	-1.21438
H	-2.5594	4.46433	-2.5237
C	-2.43459	3.84625	0.89226
H	-1.53373	4.45486	1.03235
H	-3.29795	4.43063	1.22963
H	-2.33613	2.94984	1.51102
C	-4.23828	-2.87492	-2.54829
H	-3.95659	-2.9486	-3.60514
H	-4.92105	-3.70239	-2.3212
H	-4.77222	-1.93156	-2.40843
C	-2.14622	-4.16717	-2.04729
H	-2.71034	-5.10115	-1.94694
H	-1.82165	-4.07289	-3.08948
H	-1.25098	-4.23204	-1.41923
C	-4.45304	-1.93236	0.21036
H	-5.40779	-2.39083	-0.07141
H	-4.46212	-1.75616	1.292
H	-4.3517	-0.96154	-0.28267
C	-3.37496	-4.16861	0.59873
H	-3.5605	-3.99526	1.66485
H	-4.20892	-4.76022	0.20268
H	-2.45696	-4.75536	0.5095
C	-2.14197	0.61408	4.30917
H	-1.90434	0.48292	5.37152
H	-2.69237	1.55537	4.19885
H	-2.80084	-0.19878	3.9938
C	-0.07511	1.93412	3.76961
H	-0.6903	2.80544	3.52074
H	0.20506	2.00028	4.82669
H	0.83462	1.97948	3.16124
C	1.14045	-0.61377	4.53603
H	0.74778	-0.50156	5.55363
H	1.70171	-1.55418	4.49255
H	1.8392	0.20364	4.33912
C	-0.82516	-1.92028	3.67512
H	-0.17181	-2.78721	3.52491
H	-1.27166	-1.99717	4.67292
H	-1.61285	-1.96269	2.91743
H	2.83643	4.54427	-0.73354
H	5.11189	3.4025	-0.62973
H	4.18447	-2.51268	-0.43104
H	1.85008	-2.20925	-0.06629
H	1.53991	-1.56652	-1.53508

Thermal correction to Energy= 0.763326

Thermal correction to Enthalpy=0.764476

Thermal correction to Gibbs Free Energy=0.604154

Sum of electronic and zero-point Energies=-1795.018708

Sum of electronic and thermal Energies= -1794.959284

Sum of electronic and thermal Enthalpies= -1794.958133

Sum of electronic and thermal Free Energies=-1795.118455

SCF Done: E(RM11L) = -1795.81323958

4c

Number of Negative Frequencies = 0

Ir	0.3177	0.08953	-0.15822
C	-3.74619	1.01192	1.58445

C	-2.4876	0.98324	0.93567	C	2.96105	2.52352	2.98764
C	-1.93938	2.18881	0.35938	H	3.43571	2.07273	2.11131
C	-2.6743	3.39908	0.40104	H	2.57757	3.50662	2.69105
C	-0.8315	4.47612	-0.73932	H	3.7091	2.67211	3.77453
C	-0.18327	3.22485	-0.71677	C	1.0884	2.31949	4.65152
H	0.80802	3.1215	-1.14557	H	1.73886	2.32474	5.53424
N	-1.74995	-0.15703	0.84678	H	0.8433	3.35922	4.40604
N	-0.70144	2.11924	-0.1987	H	0.1573	1.80689	4.90743
O	2.04668	-0.3797	2.33788	C	3.60451	-0.07947	4.15935
O	0.85151	1.5738	2.363	H	3.7698	0.38792	5.13747
O	2.54271	0.26602	-2.28499	H	3.78834	-1.15487	4.26335
O	3.17217	1.20493	-0.29868	H	4.33616	0.31901	3.45205
O	0.31648	-2.88186	0.58156	C	1.18376	-0.60212	4.56613
O	2.29485	-2.31134	-0.39837	H	1.4046	-1.67322	4.51734
C	-4.47268	2.25108	1.59622	H	1.24875	-0.2848	5.61285
C	-3.96595	3.38387	1.02883	H	0.15597	-0.45417	4.21745
H	-5.4469	2.28849	2.07064	C	3.74543	-4.1456	0.20103
H	-4.54856	4.29771	1.06175	H	3.79518	-5.21612	0.43357
C	-2.10356	4.57239	-0.17428	H	4.45039	-3.94324	-0.61334
C	1.78561	1.66048	3.46536	H	4.07313	-3.58059	1.07709
C	2.17718	0.15589	3.67496	C	1.9964	-4.3724	-1.5828
C	2.33588	-3.74261	-0.22499	H	2.70009	-3.99596	-2.3332
C	1.22443	-3.97675	0.85391	H	2.06906	-5.46557	-1.55929
C	3.83159	0.87668	-2.51965	H	0.98495	-4.09576	-1.8987
C	4.38701	1.05355	-1.06328	C	0.47438	-5.30062	0.73791
B	1.15879	0.42344	1.61777	H	1.1533	-6.14408	0.91192
B	2.1286	0.53022	-0.96431	H	-0.31823	-5.34371	1.49408
B	1.04388	-1.81368	-0.00077	H	0.00962	-5.42752	-0.24166
C	5.26468	2.28329	-0.84648	C	1.73667	-3.78936	2.28834
H	5.59604	2.32141	0.19753	H	2.25016	-2.83008	2.3873
H	6.15788	2.24778	-1.48181	H	0.87977	-3.78478	2.97157
H	4.72247	3.20869	-1.05862	H	2.40994	-4.59986	2.58951
C	3.58835	2.21391	-3.23296	C	-0.21992	1.40994	-3.68173
H	4.52662	2.72395	-3.47802	C	-1.25155	2.34325	-3.76924
H	3.05013	2.03032	-4.16911	C	-2.55829	1.97433	-3.41735
H	2.9792	2.88239	-2.61506	C	-2.82918	0.67757	-2.99337
C	4.65369	-0.04787	-3.4143	C	-1.79514	-0.2737	-2.91041
H	4.18647	-0.12063	-4.40328	C	-0.48664	0.10768	-3.24863
H	5.67203	0.33631	-3.54876	H	0.80093	1.688	-3.91805
H	4.71208	-1.05617	-2.99682	H	-1.04252	3.35915	-4.09459
C	5.09463	-0.20317	-0.53557	H	-3.36119	2.70539	-3.46886
H	6.0545	-0.37609	-1.03578	H	-3.83621	0.38045	-2.71761
H	5.28355	-0.07614	0.53621	C	-2.05152	-1.66178	-2.47628
H	4.45427	-1.08115	-0.65816	N	-3.23428	-2.12367	-2.36133

C	-3.48439	-3.51452	-1.9458
C	-4.52644	-3.42981	-0.81584
H	-4.82483	-4.43097	-0.48298
H	-4.1117	-2.88883	0.03902
H	-5.42024	-2.89371	-1.15459
C	-2.24986	-4.28815	-1.45539
H	-1.52567	-4.45317	-2.26233
H	-1.73605	-3.76108	-0.64486
H	-2.5544	-5.27303	-1.08386
C	-4.10151	-4.22467	-3.16599
H	-4.98072	-3.67995	-3.5281
H	-3.37543	-4.28626	-3.98534
H	-4.40861	-5.24367	-2.90178
H	-1.14863	-2.24943	-2.26981
H	0.33014	-0.60374	-3.16783
H	-1.05234	-0.35617	1.53502
H	-2.43081	-0.64038	1.39705
H	-4.11005	0.11861	2.04759
H	-2.6525	5.49081	-0.16614
H	-0.3307	5.30072	-1.20207

Thermal correction to Energy= 1.020422

Thermal correction to Enthalpy=1.021572

Thermal correction to Gibbs Free Energy=0.820858

Sum of electronic and zero-point Energies=-2277.787410

Sum of electronic and thermal Energies=-2277.708988

Sum of electronic and thermal Enthalpies=-2277.707838

Sum of electronic and thermal Free Energies=-2277.908552

SCF Done: E(RM11L) = -2278.80847733

TS5c

Number of Negative Frequencies = 1

B	-1.34498	0.25388	1.3179
B	-1.73797	-0.69287	-1.31641
B	-0.35507	1.76897	-0.41155
C	3.47136	-1.28259	2.34076
C	2.23245	-1.16003	1.74487
C	1.41159	-2.3135	1.58599
C	1.84736	-3.56342	2.12067
C	0.97688	-4.67626	1.98829
C	-0.22486	-4.52351	1.33802
C	-0.55279	-3.26777	0.77931
H	-1.46044	-3.11787	0.20519
C	-3.16573	0.57179	2.70388
C	-1.84608	0.62501	3.55085
C	-3.62665	-0.46464	-2.61562
C	-3.49706	-1.9577	-2.15683
C	0.15395	3.99378	-0.02994
C	-1.20186	3.87358	-0.80382
Ir	-0.0448	-0.26442	-0.26579
N	1.71432	0.08903	1.2658
N	0.23294	-2.20601	0.88855
O	-2.701	0.00725	1.44857
O	-0.83784	0.7854	2.51406
O	-2.29543	0.04413	-2.36073
O	-2.49273	-1.8584	-1.11633
O	0.70975	2.65998	-0.20445
O	-1.53241	2.4766	-0.61333
H	0.44792	0.13935	-1.77511
C	1.36924	-1.1956	-1.71488
C	0.93686	-2.41583	-2.27217
C	1.82602	-3.30411	-2.87824
H	1.4587	-4.24461	-3.28371
C	3.1859	-2.98255	-2.9655
H	3.88524	-3.66698	-3.43918
C	3.63019	-1.76508	-2.46203
C	2.73706	-0.86094	-1.85473
C	3.92317	-2.53211	2.82682
C	3.12041	-3.64789	2.74246
H	3.45015	-4.60559	3.13559
H	4.90459	-2.597	3.28737
C	-4.25831	-0.33034	3.26806
H	-4.57318	0.01235	4.26055
H	-5.13291	-0.30769	2.60851
H	-3.92392	-1.36813	3.34583
C	-3.72881	1.95999	2.385
H	-4.52547	1.8609	1.64045
H	-4.14316	2.44535	3.27524
H	-2.95338	2.5999	1.95659
C	-1.7444	1.79425	4.52328
H	-2.54324	1.74592	5.27223
H	-0.78395	1.75693	5.04968
H	-1.80846	2.75483	4.00653
C	-1.53561	-0.69449	4.26713
H	-0.51207	-0.65736	4.65591
H	-2.21702	-0.8704	5.10618
H	-1.60401	-1.54121	3.57642
C	-2.33612	4.73519	-0.26005
H	-3.24713	4.55837	-0.84256

H	-2.55661	4.50597	0.78476
H	-2.08409	5.79929	-0.33789
C	-1.04989	4.09363	-2.31478
H	-1.97331	3.78002	-2.81252
H	-0.86509	5.14535	-2.55818
H	-0.2292	3.49045	-2.71701
C	-0.02884	4.20354	1.47742
H	0.94294	4.09164	1.97137
H	-0.41539	5.20273	1.70579
H	-0.7038	3.45233	1.89751
C	1.11316	5.03542	-0.59671
H	0.6352	6.02207	-0.60579
H	2.01327	5.10378	0.02236
H	1.42081	4.78872	-1.61562
C	-2.93338	-2.87662	-3.24777
H	-2.66284	-3.8389	-2.79903
H	-3.66592	-3.0633	-4.04083
H	-2.03364	-2.44688	-3.69904
C	-4.76189	-2.5646	-1.55715
H	-5.57917	-2.56327	-2.28773
H	-4.57293	-3.60356	-1.26311
H	-5.08391	-2.0165	-0.66843
C	-3.96024	-0.26745	-4.09048
H	-4.93045	-0.71592	-4.33465
H	-4.01527	0.80339	-4.31661
H	-3.19881	-0.70839	-4.7392
C	-4.58797	0.34667	-1.73582
H	-4.48528	1.40752	-1.9867
H	-5.63202	0.05356	-1.89346
H	-4.33355	0.22621	-0.67798
H	-0.11109	-2.69096	-2.1951
H	1.27742	-5.63666	2.39879
H	-0.91596	-5.35165	1.21927
H	4.09986	-0.40332	2.44399
H	2.45954	0.72067	0.98068
H	1.16699	0.55638	1.99365
C	5.11291	-1.36443	-2.57435
H	5.66467	-2.16211	-3.0262
N	5.23247	-0.15555	-3.40212
C	6.20016	0.76503	-2.78809
C	6.22772	0.53979	-1.2649
H	5.24818	0.69565	-0.86353
H	6.54272	-0.46166	-1.05809
H	6.91141	1.22888	-0.81477
C	7.60083	0.50147	-3.37141
H	7.54522	0.48662	-4.43986
H	8.26872	1.27716	-3.05976
H	7.96174	-0.44251	-3.01989
C	5.78569	2.21825	-3.08469
H	6.64874	2.84971	-3.04869
H	5.34492	2.2718	-4.05822
H	5.07543	2.54293	-2.35325
H	3.10552	0.08633	-1.52034

Thermal correction to Energy=1.014856

Thermal correction to Enthalpy=1.016006

Thermal correction to Gibbs Free Energy=0.817029

Sum of electronic and zero-point Energies=-2277.742605

Sum of electronic and thermal Energies=-2277.664572

Sum of electronic and thermal Enthalpies=-2277.663422

Sum of electronic and thermal Free Energies=-2277.862399

SCF Done: E(RM11L) = -2278.75636911

6c

Number of Negative Frequencies = 0

B	0.96329	0.90005	-1.1662
B	1.10121	0.83242	1.76939
B	-0.87252	1.7832	-0.38162
C	-1.45891	-3.16189	-2.52596
C	-0.84	-2.28294	-1.66214
C	0.48951	-2.53364	-1.22432
C	1.19582	-3.6736	-1.71347
C	2.54776	-3.88925	-1.29049
C	3.11194	-2.97747	-0.40917
C	2.32477	-1.8913	0.04125
H	2.73637	-1.17599	0.74292
C	2.78795	1.75435	-2.29074
C	1.92963	0.86398	-3.26532
C	2.08881	2.38494	3.15609
C	2.8942	1.04151	3.22811
C	-2.31107	3.08117	-1.64755
C	-1.54146	3.9691	-0.60654
Ir	-0.16684	-0.01928	0.41816
N	-1.49298	-1.09346	-1.17629
N	1.07381	-1.66731	-0.33103
O	2.22888	1.42519	-0.98991
O	0.69326	0.68892	-2.5141
O	0.84474	1.95945	2.5481
O	2.36725	0.32402	2.08388

O	-2.05138	1.74233	-1.14267
O	-0.4571	3.09356	-0.20069
H	-1.18681	0.99199	1.14787
C	-0.79812	-1.4638	1.90251
C	0.16039	-2.18311	2.64939
C	-0.17656	-3.22693	3.51489
H	0.60409	-3.74018	4.0741
C	-1.51458	-3.60588	3.66882
H	-1.78906	-4.41697	4.33922
C	-2.4925	-2.91607	2.96013
H	-3.54137	-3.18229	3.06652
C	-2.15122	-1.85395	2.099
C	-0.77551	-4.30439	-2.99559
C	0.52384	-4.55007	-2.60795
H	1.03833	-5.42611	-2.98547
H	-1.27948	-4.98652	-3.67398
C	4.27815	1.42818	-2.26843
H	4.72848	1.58533	-3.2552
H	4.7871	2.08481	-1.55426
H	4.45846	0.39458	-1.96188
C	2.57823	3.25809	-2.49278
H	3.07075	3.7984	-1.67764
H	3.002	3.60289	-3.44189
H	1.51545	3.51327	-2.46462
C	1.60169	1.5091	-4.6078
H	2.51888	1.70151	-5.17617
H	0.97263	0.83382	-5.19833
H	1.0635	2.45166	-4.48742
C	2.51373	-0.53601	-3.48696
H	1.77783	-1.15062	-4.01537
H	3.42717	-0.49905	-4.08979
H	2.74537	-1.02612	-2.53802
C	-0.94843	5.2555	-1.16831
H	-0.40771	5.78895	-0.37886
H	-0.24649	5.05441	-1.98103
H	-1.73984	5.91422	-1.54368
C	-2.36566	4.26484	0.65238
H	-1.70934	4.70223	1.41172
H	-3.17877	4.96986	0.44913
H	-2.79389	3.34566	1.06632
C	-1.71938	3.15057	-3.05862
H	-2.17876	2.37005	-3.67491
H	-1.90885	4.11971	-3.53235
H	-0.64386	2.96528	-3.0368
C	-3.81695	3.31571	-1.69804
H	-4.03036	4.34414	-2.01193
H	-4.27483	2.6383	-2.42706
H	-4.29166	3.14189	-0.73036
C	2.57052	0.20763	4.47315
H	3.00862	-0.79001	4.35935
H	2.9815	0.66072	5.38186
H	1.48965	0.08824	4.59653
C	4.40398	1.18095	3.06261
H	4.8283	1.80032	3.86138
H	4.87655	0.1931	3.1149
H	4.66202	1.627	2.09888
C	1.78784	3.0279	4.50554
H	2.71503	3.28222	5.03242
H	1.21869	3.95243	4.35699
H	1.19459	2.36621	5.14217
C	2.71984	3.4073	2.20132
H	2.01371	4.23045	2.04914
H	3.65194	3.82143	2.60172
H	2.91699	2.95118	1.22578
H	1.20814	-1.90933	2.55896
C	-3.24491	-1.15212	1.38899
N	-4.33159	-1.73721	1.05482
C	-5.39879	-1.01365	0.33829
C	-6.68559	-1.22668	1.15708
H	-7.55222	-0.80139	0.63682
H	-6.86735	-2.29499	1.32003
H	-6.60311	-0.74273	2.13775
C	-5.53346	-1.70987	-1.03069
H	-6.38105	-1.30095	-1.59337
H	-4.6247	-1.56106	-1.62792
H	-5.68553	-2.78773	-0.90513
C	-5.16075	0.49024	0.12256
H	-6.00968	0.92291	-0.41893
H	-5.06588	1.02461	1.07604
H	-4.25644	0.68411	-0.46262
H	-3.04229	-0.10339	1.15095
H	-1.58377	-0.39398	-1.91436
H	-2.43572	-1.30755	-0.85336
H	-2.47769	-2.96166	-2.84654
H	4.11588	-3.05079	-0.04635
H	3.09062	-4.73428	-1.65945

Thermal correction to Energy=1.018235

Thermal correction to Enthalpy=1.019385

Thermal correction to Gibbs Free Energy=0.824097

Sum of electronic and zero-point Energies=-2277.765414

Sum of electronic and thermal Energies=-2277.687950

Sum of electronic and thermal Enthalpies=-2277.686800

Sum of electronic and thermal Free Energies=-2277.882088

SCF Done: E(RM11L) = -2278.78104258

7c

Number of Negative Frequencies = 0

Ir	0.27779	-0.08741	-0.68893
B	-1.55177	0.84709	-1.11307
B	0.15234	1.748	0.2969
O	-1.91211	1.22723	-2.40014
O	-2.60835	1.07931	-0.23217
C	1.30511	-3.16003	2.41082
C	2.73853	-3.74914	0.06733
N	1.77201	-1.7439	-0.92986
N	0.4634	-1.06349	1.39659
O	0.23143	1.79011	1.69626
O	-0.13201	3.01395	-0.20528
C	1.91767	-2.58446	0.14124
C	1.22278	-2.29003	1.34434
O	2.94474	0.37098	0.7135
O	2.82652	1.86745	-1.00582
C	2.80815	-4.61808	1.18707
C	2.0922	-4.33366	2.32884
H	3.42615	-5.50915	1.1221
H	2.13513	-5.00304	3.18284
C	3.44024	-3.98457	-1.14314
C	-0.05113	3.98077	0.87403
C	-0.24132	3.08386	2.1541
C	4.2447	1.76087	-0.6909
C	4.24489	1.01513	0.70247
C	-3.19344	1.90394	-2.35734
C	-3.80018	1.39105	-1.00071
H	0.42701	0.49957	-2.14593
C	3.29512	-3.10795	-2.19349
C	-2.90007	3.40739	-2.36063
H	-2.27105	3.67352	-1.50892
H	-2.35103	3.66061	-3.27426
H	-3.81911	4.00298	-2.33607
C	-3.98991	1.51616	-3.59985
H	-4.99752	1.94673	-3.56627
H	-3.48735	1.89963	-4.49466
H	-4.07567	0.43141	-3.70118
C	-4.59637	0.08866	-1.14493
H	-4.82608	-0.30389	-0.14869
H	-5.54015	0.25246	-1.67572
H	-4.01946	-0.67267	-1.67656
C	-4.62084	2.41939	-0.2287
H	-5.49656	2.73148	-0.80944
H	-4.97721	1.97961	0.70954
H	-4.0324	3.30658	0.01676
C	-1.12875	5.04297	0.68036
H	-1.11589	5.75571	1.5132
H	-0.9405	5.59927	-0.24426
H	-2.12668	4.60469	0.61531
C	1.33602	4.62382	0.77802
H	2.11816	3.8695	0.87948
H	1.44655	5.08165	-0.21035
H	1.48275	5.39867	1.53794
C	0.5926	3.50702	3.35918
H	0.31084	4.51268	3.69186
H	0.41811	2.81497	4.19074
H	1.6618	3.50029	3.13424
C	-1.70784	2.90227	2.55986
H	-2.1429	3.83431	2.93632
H	-2.29796	2.53976	1.71517
H	-1.76487	2.15419	3.3576
C	4.87881	0.94213	-1.82145
H	4.68996	1.44693	-2.77468
H	5.96185	0.84526	-1.69211
H	4.44348	-0.06011	-1.88041
C	4.84334	3.16425	-0.66886
H	4.77654	3.60831	-1.668
H	4.31381	3.82078	0.0251
H	5.9002	3.12917	-0.38128
C	4.29113	1.9521	1.91292
H	4.13502	1.36429	2.82397
H	5.2572	2.46136	1.99353
H	3.50164	2.7054	1.86316
C	5.31144	-0.06903	0.84952
H	6.31834	0.35891	0.78745
H	5.20749	-0.55207	1.82739
H	5.21204	-0.84179	0.08341
C	2.43444	-1.99767	-2.04786
H	2.28136	-1.30008	-2.86329
B	2.13337	0.92793	-0.2685

C	-2.02828	-2.35732	-0.5766
C	-1.09015	-1.64199	-1.36946
C	-0.9005	-2.12543	-2.68298
C	-1.55072	-3.25673	-3.17882
C	-2.44392	-3.96276	-2.36401
C	-2.67998	-3.50465	-1.07364
H	-0.21567	-1.59742	-3.34291
H	-1.36778	-3.58342	-4.20096
H	-3.39086	-4.01326	-0.42762
H	-2.96029	-4.84301	-2.73964
C	-2.40365	-1.87136	0.76949
N	-2.92696	-2.62495	1.66095
C	-3.34562	-2.07226	2.96244
C	-4.86154	-2.33136	3.06572
H	-5.4034	-1.75282	2.30753
H	-5.08347	-3.39223	2.90479
H	-5.23951	-2.0416	4.05353
C	-2.60514	-2.89352	4.03522
H	-1.52264	-2.72665	3.96729
H	-2.93218	-2.60827	5.04229
H	-2.79001	-3.96481	3.89845
C	-3.06902	-0.5734	3.18234
H	-3.44019	-0.26973	4.16771
H	-1.99706	-0.34486	3.15161
H	-3.56292	0.05	2.42974
H	-2.23597	-0.80625	0.92395
H	3.8152	-3.25515	-3.13404
H	4.08069	-4.85855	-1.22467
H	0.76587	-2.93213	3.32632
H	0.98605	-0.34683	1.9044
H	-0.40243	-1.20938	1.91189

Thermal correction to Energy=1.018992

Thermal correction to Enthalpy=1.020142

Thermal correction to Gibbs Free Energy=0.826566

Sum of electronic and zero-point Energies=-2277.759043

Sum of electronic and thermal Energies=-2277.681818

Sum of electronic and thermal Enthalpies=-2277.680668

Sum of electronic and thermal Free Energies=-2277.874244

SCF Done: E(RM11L) = -2278.77417125

TS8c

Number of Negative Frequencies = 1

Ir	0.118	0.47159	-0.8345
B	-1.8429	0.19907	-1.60174
B	-1.12913	1.72487	0.22213
O	-2.21015	0.57074	-2.89936
O	-2.99056	-0.12828	-0.8637
C	2.12673	-2.58384	1.70543
C	3.71501	-2.16475	-0.57643
N	2.15961	-0.40402	-1.23038
N	0.6981	-0.65388	1.08281
O	-1.25203	1.58961	1.61123
O	-1.89866	2.79093	-0.22829
C	2.56452	-1.35684	-0.33432
C	1.79529	-1.5593	0.84479
O	2.18789	1.77578	0.94997
O	1.42319	3.37411	-0.49022
C	4.03498	-3.20183	0.33816
C	3.24188	-3.41622	1.44328
H	4.90438	-3.82366	0.14365
H	3.47546	-4.21889	2.13642
C	4.47451	-1.893	-1.74346
C	-2.4063	3.52461	0.91332
C	-2.32595	2.45578	2.06621
C	2.66715	3.896	0.05782
C	2.89123	2.99046	1.32362
C	-3.65373	0.6112	-2.9933
C	-4.09645	-0.29198	-1.78469
H	0.03339	1.34826	-2.14728
C	4.07294	-0.8929	-2.59916
C	-4.0724	2.07711	-2.83579
H	-3.73435	2.46843	-1.87388
H	-3.59314	2.66735	-3.62479
H	-5.15711	2.20523	-2.92354
C	-4.06743	0.08608	-4.36597
H	-5.15905	0.02379	-4.44661
H	-3.70957	0.76775	-5.14582
H	-3.64491	-0.90241	-4.56369
C	-4.17938	-1.78302	-2.13883
H	-4.29419	-2.36252	-1.2163
H	-5.03641	-1.99484	-2.78711
H	-3.26919	-2.12595	-2.63768
C	-5.38063	0.14546	-1.08667
H	-6.23344	0.08742	-1.77293
H	-5.58434	-0.51746	-0.23824
H	-5.30778	1.16712	-0.70722
C	-3.81597	4.01822	0.59855
H	-4.25059	4.52571	1.46772

H	-3.7808	4.73537	-0.22894
H	-4.47781	3.19917	0.30841
C	-1.47097	4.72021	1.12145
H	-0.44806	4.38347	1.29872
H	-1.46165	5.32722	0.21009
H	-1.79208	5.35293	1.95589
C	-1.95142	3.01477	3.43534
H	-2.70028	3.73745	3.77982
H	-1.90716	2.20059	4.16776
H	-0.975	3.50526	3.41717
C	-3.58444	1.58856	2.17055
H	-4.45125	2.16776	2.50667
H	-3.80779	1.12558	1.20624
H	-3.4086	0.78962	2.89715
C	3.73603	3.69355	-1.02347
H	3.4163	4.20331	-1.9383
H	4.70449	4.1049	-0.72004
H	3.86368	2.6309	-1.25641
C	2.49161	5.38157	0.35314
H	2.32621	5.92863	-0.58148
H	1.63587	5.56647	1.00665
H	3.3906	5.78848	0.8304
C	2.21949	3.52608	2.59108
H	2.26302	2.75643	3.36927
H	2.71961	4.42508	2.96612
H	1.1673	3.75772	2.40943
C	4.34746	2.63773	1.61268
H	4.93628	3.54162	1.80644
H	4.40412	2.00039	2.50224
H	4.80337	2.09504	0.78088
C	2.88947	-0.17819	-2.31181
H	2.5191	0.58483	-2.9878
B	1.27206	2.06499	-0.06852
C	-0.89852	-2.61977	-1.04117
C	-0.55974	-1.45287	-1.77574
C	-0.1096	-1.64533	-3.09828
C	0.05978	-2.91179	-3.65641
C	-0.23922	-4.05111	-2.89826
C	-0.7251	-3.89863	-1.60435
H	0.11456	-0.76999	-3.7013
H	0.41531	-3.01306	-4.67973
H	-0.99837	-4.76612	-1.00987
H	-0.11614	-5.04429	-3.32342
C	-1.51349	-2.51151	0.29946
N	-1.5311	-3.48337	1.13074
C	-2.25051	-3.36006	2.41275
C	-3.3944	-4.39142	2.34834
H	-4.10082	-4.12963	1.55146
H	-3.00106	-5.39259	2.13904
H	-3.94184	-4.42455	3.29794
C	-1.25696	-3.7594	3.51958
H	-0.47357	-2.99979	3.63086
H	-1.76921	-3.85608	4.48425
H	-0.77619	-4.71491	3.28241
C	-2.82587	-1.96824	2.72374
H	-3.30769	-1.97858	3.70789
H	-2.04242	-1.20195	2.74422
H	-3.57623	-1.65983	1.98809
H	-1.98085	-1.5477	0.49851
H	1.52991	-2.74833	2.59695
H	-0.05022	-1.11434	1.5969
H	1.02158	0.13272	1.65123
H	5.3628	-2.48437	-1.94871
H	4.63007	-0.65754	-3.49984

Thermal correction to Energy=0.992975

Thermal correction to Enthalpy=0.993919

Thermal correction to Gibbs Free Energy= 0.857596

Sum of electronic and zero-point Energies=-2277.759108

Sum of electronic and thermal Energies=-2277.706361

Sum of electronic and thermal Enthalpies=-2277.705417

Sum of electronic and thermal Free Energies=-2277.841740

SCF Done: E(RM11L) = -2278.77461359

9c

Number of Negative Frequencies = 0

B	-0.92496	2.45436	0.37261
B	1.68561	1.61357	0.70723
C	-3.93839	-1.0692	-0.54947
C	-2.61892	-0.6048	-0.33558
C	-1.71698	-0.41933	-1.44254
C	-2.14742	-0.68818	-2.76145
C	0.05059	-0.04534	-3.533
C	0.37976	0.19643	-2.18452
H	1.36903	0.55288	-1.92095
N	-2.14767	-0.317	0.90695
N	-0.45547	0.02186	-1.16537
O	-1.53113	3.37126	1.2422
O	-1.06586	2.90064	-0.95212

O	1.94673	2.99731	0.76173	H	2.58621	4.38213	-1.35138
O	2.91343	0.94072	0.49685	H	4.24824	3.79542	-1.57006
C	-4.34983	-1.32331	-1.90097	C	5.15747	1.52053	-0.25736
C	-3.49726	-1.14091	-2.95117	H	5.9218	2.30676	-0.24235
H	-5.35938	-1.67018	-2.09172	H	5.62768	0.58905	0.0724
H	-3.84662	-1.34679	-3.95671	H	4.82189	1.38179	-1.28778
C	-1.22989	-0.5082	-3.83596	C	1.56666	-0.58402	3.82885
C	-1.54889	4.26288	-0.929	H	2.07322	-0.80302	4.77653
C	-2.28343	4.32421	0.45642	H	2.09921	0.22557	3.32523
C	3.3023	3.24473	0.33365	H	0.55467	-0.23835	4.03742
C	4.00056	1.88595	0.66873	C	3.02012	-2.15346	2.54301
Ir	-0.12017	0.7029	0.88096	H	3.39062	-1.32574	1.93258
C	1.58272	-1.82932	2.95933	H	3.66841	-2.2685	3.41777
C	0.80453	-3.04918	3.56071	H	3.07154	-3.07268	1.95042
B	0.30146	-2.82377	1.34412	C	1.66558	-4.01196	4.36813
O	0.33372	-3.73865	2.36129	H	2.11716	-3.49523	5.22206
O	0.84573	-1.60492	1.69629	H	1.04827	-4.83101	4.75229
H	-0.09356	1.25203	2.39582	H	2.4632	-4.44407	3.75901
C	-0.3212	5.17964	-0.99378	C	-0.4465	-2.64662	4.34659
H	0.34421	4.98626	-0.14797	H	-1.04664	-3.54222	4.53858
H	0.23375	4.96362	-1.9131	H	-0.18922	-2.19156	5.30806
H	-0.60162	6.23875	-1.00411	H	-1.05837	-1.93993	3.77695
C	-2.44299	4.49059	-2.14434	C	-0.29409	-3.21425	-0.04809
H	-2.89268	5.49025	-2.11765	C	-1.59769	-3.73963	-0.07411
H	-1.84851	4.41231	-3.06197	C	0.4267	-3.14151	-1.26321
H	-3.24421	3.74879	-2.19971	C	-2.19295	-4.15043	-1.26608
C	-3.72885	3.81113	0.389	H	-2.15671	-3.81606	0.85516
H	-4.10836	3.68217	1.40856	C	-0.17402	-3.5691	-2.45902
H	-4.38825	4.50975	-0.13795	C	-1.47477	-4.0626	-2.46348
H	-3.77481	2.83985	-0.11473	H	-3.20892	-4.53581	-1.26398
C	-2.23943	5.68213	1.15097	H	0.40092	-3.51501	-3.3779
H	-2.72527	6.45142	0.53901	H	-1.9302	-4.38319	-3.39697
H	-2.76939	5.62727	2.10887	C	1.8349	-2.68853	-1.25597
H	-1.21141	5.99347	1.3531	H	2.21752	-2.39084	-0.27693
C	4.45641	1.79298	2.131	N	2.55272	-2.67329	-2.3109
H	4.73486	0.75714	2.35213	C	3.98149	-2.31333	-2.25409
H	5.3249	2.43154	2.32738	C	4.16615	-1.0773	-3.15296
H	3.65014	2.08118	2.81284	H	3.63244	-0.21725	-2.73611
C	3.84986	4.45582	1.08422	H	5.22815	-0.81722	-3.23306
H	4.90952	4.61564	0.85152	H	3.77898	-1.26733	-4.15937
H	3.30006	5.35613	0.78701	C	4.73194	-3.51174	-2.86704
H	3.74331	4.34026	2.16592	H	4.59899	-4.40756	-2.24859
C	3.25999	3.53832	-1.17328	H	4.35218	-3.73299	-3.87097
H	2.87183	2.67793	-1.72864	H	5.80528	-3.29946	-2.93872

C	4.53284	-2.01517	-0.85063
H	4.01608	-1.16915	-0.38738
H	4.44186	-2.8854	-0.18987
H	5.59685	-1.76351	-0.92157
H	-1.53192	-0.73399	-4.8373
H	0.79853	0.12379	-4.27924
H	-4.57464	-1.22121	0.29727
H	-2.58928	-0.9133	1.57732
H	-2.34836	0.63769	1.1267

Thermal correction to Energy=1.018844

Thermal correction to Enthalpy=1.019994

Thermal correction to Gibbs Free Energy=0.822431

Sum of electronic and zero-point Energies=-2277.781573

Sum of electronic and thermal Energies=-2277.703919

Sum of electronic and thermal Enthalpies=-2277.702769

Sum of electronic and thermal Free Energies=-2277.900332

SCF Done: E(RM11L) = -2278.80804193

10

Number of Negative Frequencies = 0

B	1.90687	-1.41722	-0.87155
B	2.52659	1.11011	0.07034
C	-1.48293	-1.07298	-2.61545
H	-1.12489	-0.38566	-3.37626
C	-2.4051	-2.08524	-2.95666
C	-2.27854	-2.80807	-0.65018
C	-1.39122	-1.73408	-0.40963
C	-0.87416	-1.49672	0.91335
C	-1.23557	-2.34182	1.9874
N	-0.9837	-0.89394	-1.39934
N	-0.02362	-0.44265	1.07631
O	2.43188	-2.02617	-2.02072
O	2.06665	-2.27916	0.22607
O	3.86306	0.67377	-0.00323
O	2.46685	2.2001	0.97073
C	-2.6014	-3.67183	0.45149
C	-2.10365	-3.45157	1.70384
H	-3.26211	-4.51584	0.28675
H	-2.37967	-4.12478	2.50772
C	-2.80521	-2.98103	-1.96357
C	2.88868	-3.3979	-0.1707
C	2.67715	-3.42067	-1.72504
C	4.61861	1.28532	1.0667
C	3.81245	2.6028	1.3242
Ir	0.87529	0.2936	-0.77313
C	-0.05146	3.76227	-1.29768
C	-1.3445	4.2379	-2.03317
C	-4.25015	1.18729	2.19069
C	-4.75049	0.38914	0.93181
B	-1.85551	2.53108	-0.59136
B	-2.90349	1.61453	0.38189
O	-3.60985	0.49264	0.01986
O	-3.28873	2.11697	1.60274
O	-2.39692	3.61848	-1.23086
O	-0.48625	2.44664	-0.76698
H	1.4858	0.66645	-2.22084
C	4.33073	-3.0685	0.23392
H	4.66917	-2.15423	-0.26194
H	4.36354	-2.89757	1.31508
H	5.01993	-3.88628	-0.00475
C	2.40404	-4.64566	0.56359
H	2.93141	-5.53963	0.21043
H	2.59532	-4.54209	1.63792
H	1.3296	-4.79627	0.42892
C	1.4177	-4.1948	-2.14208
H	1.2103	-3.99359	-3.19862
H	1.53961	-5.2762	-2.01458
H	0.548	-3.86934	-1.56155
C	3.87918	-3.89747	-2.53425
H	4.14404	-4.92832	-2.27031
H	3.64148	-3.87272	-3.60392
H	4.7513	-3.25951	-2.36932
C	4.21726	3.74384	0.38206
H	3.48735	4.55578	0.46542
H	5.20592	4.14382	0.63316
H	4.23252	3.40559	-0.65863
C	6.06019	1.48423	0.60705
H	6.64177	2.0237	1.36406
H	6.53553	0.50975	0.44698
H	6.11107	2.03925	-0.33325
C	4.57945	0.3244	2.2634
H	3.55071	0.16107	2.6014
H	4.98624	-0.64395	1.95706
H	5.17183	0.69772	3.1062
C	3.81399	3.0952	2.76878
H	4.83292	3.32036	3.10518
H	3.22059	4.01325	2.8489
H	3.37958	2.35573	3.44678

C	1.1622	3.61746	-2.20008
H	1.39566	4.59341	-2.64283
H	2.02278	3.28458	-1.61828
H	0.99863	2.89609	-3.00126
C	0.29898	4.5987	-0.06414
H	1.04705	4.04907	0.51216
H	0.70752	5.57397	-0.34961
H	-0.58007	4.76101	0.56923
C	-1.55526	5.74707	-2.0351
H	-0.72658	6.24732	-2.54882
H	-2.48171	5.9931	-2.56537
H	-1.62942	6.1466	-1.02056
C	-1.48181	3.66967	-3.44931
H	-2.49956	3.85403	-3.80867
H	-0.78024	4.14427	-4.14267
H	-1.30538	2.58885	-3.45844
C	-5.0535	-1.08132	1.18447
H	-5.86257	-1.18158	1.91709
H	-5.37852	-1.55921	0.25416
H	-4.17834	-1.61797	1.55198
C	-5.92776	1.06046	0.21667
H	-6.09048	0.56306	-0.74519
H	-6.84955	0.9882	0.80299
H	-5.7206	2.11742	0.01878
C	-3.47141	0.32486	3.18489
H	-2.9947	0.97264	3.92783
H	-4.12608	-0.37913	3.70926
H	-2.68967	-0.23857	2.67405
C	-5.32534	1.99415	2.91013
H	-6.10619	1.33148	3.30045
H	-4.88073	2.52968	3.756
H	-5.78968	2.73086	2.2503
H	-2.75568	-2.13792	-3.96623
H	-3.48781	-3.78109	-2.16068
H	-0.86103	-2.12429	2.96582
H	0.57442	-0.61482	1.85907
H	-0.5525	0.39054	1.23781

Thermal correction to Energy=0.973017

Thermal correction to Enthalpy=0.974167

Thermal correction to Gibbs Free Energy=0.781272

Sum of electronic and zero-point Energies=-2206.715825

Sum of electronic and thermal Energies=-2206.641369

Sum of electronic and thermal Enthalpies=-2206.640219

Sum of electronic and thermal Free Energies=-2206.833114

SCF Done: E(RM11L) = -2207.70058107

TS11

Number of Negative Frequencies = 1

Ir	0.19725	0.31305	-0.41109
B	-0.01918	2.17425	-1.1044
H	1.21113	0.1626	-1.63473
C	-1.80073	-1.18293	-2.47542
C	-3.01121	-1.71314	-2.96969
C	-4.04345	-0.95214	-0.91556
C	-2.77861	-0.46205	-0.51434
C	-2.61239	0.17789	0.76588
C	-3.72101	0.34464	1.62882
B	0.68525	-2.27536	0.75563
N	-1.67803	-0.57571	-1.30284
N	-1.35942	0.59383	1.10705
O	1.42906	-2.61816	1.8587
O	-0.66098	-2.4898	0.94308
O	2.92903	1.72443	0.05886
O	1.97964	0.92407	1.97784
O	1.11563	-2.70332	-1.88547
O	2.89632	-1.82712	-0.73334
C	-5.14802	-0.7771	-0.01437
C	-4.99504	-0.15585	1.19181
H	-6.12829	-1.14235	-0.30029
H	-5.85656	-0.04189	1.84027
C	-4.15849	-1.59619	-2.18298
C	-0.84005	-3.19913	2.20554
C	0.52008	-2.92294	2.95509
C	3.47643	-2.48434	-1.88792
C	2.22755	-2.7382	-2.82421
C	3.7839	2.15587	1.1413
C	3.36347	1.18783	2.30062
C	-0.59758	3.85833	-2.56985
B	1.53123	-2.04337	-0.73924
H	-0.88661	-1.26721	-3.05222
B	1.81061	1.0586	0.58171
C	-0.38098	4.45965	-1.13702
O	-0.37678	3.27022	-0.3086
O	0.02668	2.55602	-2.45054
C	0.98549	5.13558	-0.97502
H	1.15275	5.35505	0.08416
H	1.78859	4.475	-1.31392

H	1.04045	6.07567	-1.53509
C	-1.48879	5.39009	-0.65245
H	-1.25183	5.75578	0.3532
H	-1.58699	6.25891	-1.31385
H	-2.45231	4.87595	-0.6045
C	-2.07761	3.61755	-2.8988
H	-2.61867	4.55614	-3.06222
H	-2.14616	3.01674	-3.81211
H	-2.57225	3.0646	-2.0928
C	0.07458	4.62805	-3.70263
H	-0.13006	4.13549	-4.65996
H	-0.31043	5.65297	-3.75983
H	1.15878	4.66884	-3.57094
C	5.23875	2.03237	0.6962
H	5.43892	2.7361	-0.12006
H	5.92321	2.26608	1.52053
H	5.45908	1.02556	0.33273
C	3.44693	3.62307	1.43574
H	3.57918	4.20981	0.52128
H	2.40528	3.72642	1.7552
H	4.09672	4.04358	2.21159
C	4.0975	-0.15982	2.25412
H	5.15242	-0.0599	2.53566
H	3.61288	-0.84814	2.95353
H	4.02679	-0.60645	1.25794
C	3.43726	1.78303	3.70383
H	3.11614	1.03656	4.43948
H	4.46297	2.08133	3.95136
H	2.78632	2.65575	3.80575
C	4.54456	-1.56742	-2.47842
H	5.35059	-1.42797	-1.7495
H	4.97914	-2.00309	-3.38564
H	4.13716	-0.58316	-2.72031
C	1.99603	-1.63003	-3.85693
H	2.79372	-1.61451	-4.60709
H	1.04828	-1.81416	-4.37488
H	1.93386	-0.6489	-3.38084
C	2.21305	-4.09821	-3.51937
H	1.29971	-4.1939	-4.11714
H	3.07166	-4.20094	-4.19252
H	2.2315	-4.92109	-2.80056
C	4.11983	-3.77402	-1.36316
H	4.86293	-3.51322	-0.60222
H	3.37333	-4.42222	-0.89293
H	4.62275	-4.33407	-2.15871
C	1.08463	-4.11598	3.72146
H	2.0409	-3.83702	4.17689
H	0.40334	-4.42284	4.52323
H	1.26215	-4.97208	3.06594
C	-1.04869	-4.67114	1.83507
H	-1.22664	-5.28897	2.72149
H	-1.92028	-4.75274	1.17696
H	-0.18174	-5.06937	1.29801
C	-2.08095	-2.64889	2.89936
H	-2.96594	-2.84986	2.28638
H	-2.22476	-3.13303	3.87203
H	-2.01268	-1.57097	3.05273
C	0.48639	-1.68639	3.85754
H	-0.17714	-1.83665	4.71603
H	1.49615	-1.49091	4.23124
H	0.16628	-0.80397	3.30156
H	-1.37526	1.57456	1.30177
H	-1.05313	0.0976	1.91942
H	-3.58675	0.77835	2.49019
H	-3.00614	-2.18799	-3.92853
H	-5.10777	-1.97139	-2.50389

Thermal correction to Energy= 0.970825

Thermal correction to Enthalpy= 0.971975

Thermal correction to Gibbs Free Energy=0.782367

Sum of electronic and zero-point Energies=-2206.714841

Sum of electronic and thermal Energies=-2206.640862

Sum of electronic and thermal Enthalpies=-2206.639712

Sum of electronic and thermal Free Energies=-2206.829319

SCF Done: E(RM11L) = -2207.69034999

12

Number of Negative Frequencies = 0

Ir	0.12303	0.26036	-0.44913
B	-0.99279	1.91774	-1.15877
H	0.84945	0.49195	-1.86655
C	-1.60347	-1.83907	-2.20734
C	-2.66218	-2.71764	-2.51617
C	-3.59894	-2.16226	-0.35456
C	-2.49776	-1.29665	-0.15163
C	-2.37322	-0.54093	1.06549
C	-3.35203	-0.65683	2.08145
B	1.00416	-1.34889	0.82176
N	-1.51481	-1.15179	-1.07687

N	-1.28427	0.26904	1.2044	H	4.92032	2.56038	-0.41283
O	2.10453	-1.32294	1.65588	C	2.284	4.70575	0.26932
O	0.14307	-2.38048	1.17439	H	2.20414	5.05125	-0.7668
O	2.29291	2.45194	-0.5584	H	1.27112	4.59832	0.66852
O	1.6865	1.93917	1.58333	H	2.81134	5.47359	0.84688
O	1.52754	-2.13937	-1.86266	C	4.03659	1.58224	1.86778
O	3.06712	-0.59552	-1.15697	H	5.02813	2.0338	1.98693
C	-4.57525	-2.26143	0.69411	H	3.81278	0.99393	2.76313
C	-4.4566	-1.54655	1.85072	H	4.04676	0.89542	1.01647
H	-5.42724	-2.91956	0.56502	C	2.8941	3.5728	2.89546
H	-5.21674	-1.65103	2.61685	H	2.8228	2.97866	3.81404
C	-3.6812	-2.89033	-1.57624	H	3.80129	4.18522	2.95976
C	0.76095	-3.18166	2.21504	H	2.02708	4.23797	2.8575
C	1.85585	-2.20387	2.78279	C	4.93376	-0.98612	-2.63568
C	3.82258	-1.63562	-1.81558	H	5.64644	-0.4928	-1.96506
C	2.71588	-2.36299	-2.66242	H	5.48013	-1.73729	-3.21822
C	3.0241	3.36315	0.29326	H	4.53926	-0.23054	-3.31974
C	2.94485	2.64556	1.68568	C	2.46888	-1.70074	-4.02373
C	-2.34597	3.17128	-2.55362	H	3.3033	-1.86306	-4.71445
B	1.72461	-0.97277	-1.10972	H	1.56597	-2.13089	-4.47121
H	-0.78034	-1.70353	-2.89955	H	2.31024	-0.62302	-3.91302
B	1.45749	1.65241	0.22636	C	2.91381	-3.86542	-2.83252
C	-2.205	3.89355	-1.16944	H	2.09335	-4.28363	-3.42663
O	-1.63403	2.84832	-0.34006	H	3.85387	-4.0788	-3.35439
O	-1.27417	2.193	-2.49873	H	2.9256	-4.37884	-1.8676
C	-1.19748	5.04888	-1.19355	C	4.42703	-2.52488	-0.72269
H	-1.0025	5.37382	-0.16617	H	5.03725	-1.90536	-0.05748
H	-0.24723	4.7296	-1.63155	H	3.64146	-2.98432	-0.11886
H	-1.57635	5.90739	-1.75895	H	5.06192	-3.31247	-1.14342
C	-3.51792	4.35235	-0.54207	C	3.17219	-2.86465	3.18009
H	-3.3192	4.82754	0.42532	H	3.87332	-2.10267	3.53813
H	-4.02209	5.0858	-1.18221	H	3.01748	-3.5899	3.98727
H	-4.19674	3.51304	-0.37063	H	3.63846	-3.37554	2.33439
C	-3.65625	2.38378	-2.691	C	1.34051	-4.42486	1.53187
H	-4.52167	3.0458	-2.80559	H	1.80087	-5.10858	2.25304
H	-3.59333	1.74279	-3.57695	H	0.53251	-4.95726	1.01858
H	-3.82085	1.73935	-1.82086	H	2.08767	-4.15022	0.78219
C	-2.14111	4.0642	-3.77345	C	-0.31685	-3.5932	3.21483
H	-2.25245	3.47337	-4.6897	H	-1.05299	-4.23474	2.7178
H	-2.88578	4.86857	-3.79707	H	0.11901	-4.1573	4.04758
H	-1.14398	4.51139	-3.78143	H	-0.84606	-2.72778	3.62019
C	4.43469	3.52848	-0.26656	C	1.34441	-1.31952	3.92605
H	4.3905	4.03274	-1.23874	H	1.18614	-1.89505	4.84453
H	5.05558	4.13708	0.40187	H	2.0846	-0.5384	4.12777

H	0.40651	-0.82687	3.6534
H	-2.64477	-3.22656	-3.45723
H	-4.50429	-3.55251	-1.74634
H	-3.23266	-0.09445	2.98388
H	-1.04529	0.34314	2.17259
H	-1.49595	1.17706	0.84287

Thermal correction to Energy=0.971624

Thermal correction to Enthalpy=0.972774

Thermal correction to Gibbs Free Energy=0.781631

Sum of electronic and zero-point Energies=-2206.727896

Sum of electronic and thermal Energies=-2206.653265

Sum of electronic and thermal Enthalpies=-2206.652115

Sum of electronic and thermal Free Energies=-2206.843258

SCF Done: E(RM11L) = -2207.69875113

TS13

Number of Negative Frequencies = 1

Ir	0.18502	0.16523	-0.40181
H	0.41689	0.60245	-1.95052
B	1.97063	-0.63032	-1.15043
C	-0.86003	-2.68226	-1.58274
C	-1.68743	-3.81605	-1.71164
C	-2.98449	-2.93326	0.12818
C	-2.09326	-1.8328	0.1688
C	-2.28587	-0.77403	1.12394
C	-3.3671	-0.82069	2.038
B	1.27401	-0.76173	1.22074
N	-1.04119	-1.72538	-0.68255
N	-1.40857	0.26924	1.10712
O	2.5804	-0.57574	1.66307
O	0.62172	-1.67842	2.04699
O	1.69695	2.80926	-0.9334
O	1.15156	2.52983	1.26743
O	2.15417	-2.00934	-1.31852
O	3.07275	0.05565	-1.643
C	-4.07108	-2.954	1.06712
C	-4.2512	-1.95148	1.97493
H	-4.76783	-3.78516	1.05333
H	-5.08625	-2.00655	2.66448
C	-2.76961	-3.95485	-0.84025
C	1.60423	-2.30983	2.90647
C	2.73397	-1.22584	2.95271
C	4.12474	-0.89179	-1.94625
C	3.32223	-2.22764	-2.14763
C	1.90532	4.09323	-0.30482
C	1.98574	3.70933	1.21367
C	-3.35181	1.43937	-2.60392
B	-1.33215	1.20305	-1.52686
H	0.00265	-2.55666	-2.22555
B	1.10914	1.94083	-0.00903
C	-2.84533	2.8423	-2.11773
O	-1.77718	2.47496	-1.20139
O	-2.14829	0.62885	-2.49452
C	-2.20922	3.67681	-3.23458
H	-2.95953	4.04633	-3.94206
H	-1.70079	4.53758	-2.78848
H	-1.46339	3.09462	-3.78561
C	-3.87297	3.67288	-1.35639
H	-3.42581	4.6257	-1.05171
H	-4.74136	3.89255	-1.98818
H	-4.21618	3.15854	-0.45502
C	-4.39044	0.81574	-1.6624
H	-5.35287	1.33545	-1.7194
H	-4.54643	-0.23068	-1.94536
H	-4.04261	0.83487	-0.62474
C	-3.84944	1.39225	-4.04411
H	-4.16641	0.37328	-4.29313
H	-4.71012	2.05754	-4.17966
H	-3.06819	1.684	-4.75035
C	2.8178	-2.42207	-3.58321
H	3.63571	-2.63845	-4.27878
H	2.1194	-3.26623	-3.60453
H	2.28489	-1.53219	-3.93448
C	4.87861	-0.40445	-3.18067
H	5.39832	0.53243	-2.95077
H	5.6286	-1.13944	-3.49598
H	4.20161	-0.21495	-4.01766
C	5.06092	-0.92727	-0.73281
H	5.44899	0.08213	-0.55696
H	4.51598	-1.23303	0.16294
H	5.91105	-1.5999	-0.89284
C	4.03145	-3.48922	-1.66487
H	3.38407	-4.35988	-1.81954
H	4.96092	-3.65355	-2.22243
H	4.26942	-3.43296	-0.59969
C	2.49455	-0.15371	4.02243
H	2.64521	-0.54762	5.03365
H	3.19838	0.66976	3.86337

H	1.48029	0.25155	3.94899				
C	4.15261	-1.77397	3.06743	Ir	0.05169	-0.23771	-0.01205
H	4.87224	-0.94779	3.05936	C	-3.84861	-1.16192	-2.0588
H	4.27865	-2.32503	4.0069	C	-2.60247	-1.14884	-1.46827
H	4.39761	-2.4426	2.2388	C	-2.07927	-2.34232	-0.89353
C	2.03903	-3.6003	2.20081	C	-2.82889	-3.55422	-0.9954
H	2.75828	-4.17252	2.79694	C	-1.04215	-4.65989	0.19227
H	1.15615	-4.22661	2.0319	C	-0.39108	-3.41063	0.28921
H	2.48085	-3.37377	1.22544	H	0.55719	-3.31668	0.80763
C	0.95338	-2.62671	4.24868	N	-1.80329	0.05364	-1.37565
H	0.16893	-3.37981	4.11188	N	-0.88099	-2.29213	-0.22522
H	1.68905	-3.02906	4.95502	O	2.41359	0.36262	-1.87874
H	0.49319	-1.73949	4.69158	O	1.38052	-1.64377	-2.27333
C	1.4255	4.75139	2.17789	O	1.52892	-0.31138	2.66004
H	1.97794	5.69535	2.10172	O	2.84364	-1.13147	0.97912
H	0.36832	4.95023	1.98129	O	0.09789	2.69672	-0.84291
H	1.51467	4.38971	3.20893	O	1.60434	2.32674	0.83719
C	3.39242	3.28222	1.65161	C	-4.60727	-2.35509	-2.127
H	4.08379	4.13154	1.69104	C	-4.10361	-3.53217	-1.61979
H	3.33307	2.83757	2.65075	H	-5.58753	-2.33466	-2.59397
H	3.79773	2.52625	0.97195	H	-4.67276	-4.45588	-1.68132
C	3.17163	4.72497	-0.87618	C	-2.26312	-4.72942	-0.43774
H	3.02631	4.94851	-1.93924	C	2.61488	-1.66958	-3.03071
H	3.4084	5.66425	-0.36215	C	2.9777	-0.1453	-3.10824
H	4.02911	4.05277	-0.78949	C	1.56164	3.75608	0.64635
C	0.68429	4.96132	-0.63887	C	0.93818	3.87843	-0.78515
H	0.59683	5.03983	-1.72773	C	2.71735	-0.83022	3.29573
H	-0.23301	4.49673	-0.26692	C	3.72742	-0.90668	2.09851
H	0.77469	5.97293	-0.22702	B	1.38822	-0.49316	-1.4625
H	-1.45565	-4.53246	-2.47187	B	1.58514	-0.57171	1.27419
H	-3.42958	-4.7959	-0.88452	B	0.64865	1.71091	0.01465
H	-3.49366	-0.01969	2.73606	C	4.73567	-2.0496	2.17497
H	-1.32603	0.65024	2.02801	H	5.39883	-2.02131	1.30275
H	-1.74246	0.97551	0.48287	H	5.35801	-1.96248	3.07353
Thermal correction to Energy=0.969581				H	4.2404	-3.02421	2.18768
Thermal correction to Enthalpy=0.970731				C	2.36934	-2.21048	3.87028
Thermal correction to Gibbs Free Energy=0.781817				H	3.21554	-2.65816	4.40333
Sum of electronic and zero-point Energies=-2206.724281				H	1.54039	-2.10798	4.57905
Sum of electronic and thermal Energies=-2206.650061				H	2.05491	-2.89614	3.07629
Sum of electronic and thermal Enthalpies=-2206.648911				C	3.12294	0.11606	4.42334
Sum of electronic and thermal Free Energies=-2206.837826				H	2.35648	0.10867	5.20711
SCF Done: E(RM11L) = -2207.69141802				H	4.07261	-0.19412	4.87553
4d				H	3.22456	1.14289	4.06316
Number of Negative Frequencies = 0				C	4.44899	0.4234	1.83764

H	5.17762	0.65696	2.62246
H	4.98209	0.35177	0.88308
H	3.72571	1.23986	1.75483
C	3.6268	-2.48271	-2.21219
H	3.78461	-2.02368	-1.23172
H	3.22256	-3.48879	-2.05119
H	4.58768	-2.57982	-2.73004
C	2.35583	-2.34225	-4.37517
H	3.24781	-2.30085	-5.01146
H	2.10063	-3.39674	-4.21988
H	1.52589	-1.87119	-4.90865
C	4.47177	0.16449	-3.12578
H	4.95587	-0.28249	-4.00236
H	4.62508	1.24878	-3.17076
H	4.96618	-0.20676	-2.22468
C	2.27565	0.57928	-4.26503
H	2.41053	1.65871	-4.14429
H	2.68359	0.28735	-5.23889
H	1.20011	0.37142	-4.26002
C	2.97547	4.31411	0.78641
H	2.99876	5.38727	0.56185
H	3.32889	4.17704	1.81482
H	3.674	3.80185	0.12004
C	0.65594	4.33	1.74493
H	1.03762	4.01149	2.72113
H	0.62779	5.42531	1.72748
H	-0.36667	3.9512	1.64189
C	0.09412	5.12865	-1.01587
H	0.71984	6.02759	-0.95939
H	-0.35522	5.09405	-2.01507
H	-0.71312	5.22749	-0.28811
C	1.98166	3.74531	-1.90226
H	2.5742	2.8377	-1.76665
H	1.46081	3.66515	-2.86303
H	2.64524	4.61636	-1.94523
C	-1.50567	-1.40883	3.20283
C	-2.43347	-2.43919	3.05206
C	-3.61031	-2.21947	2.32129
C	-3.85588	-0.97767	1.74502
C	-2.92659	0.06816	1.89312
C	-1.75121	-0.15852	2.6283
H	-0.57432	-1.56884	3.73424
H	-2.24246	-3.41441	3.49244
H	-4.33055	-3.02382	2.19735
H	-1.01556	0.63361	2.74039
H	-1.40428	0.29183	-2.28365
H	-2.3895	0.84061	-1.10041
H	-4.24851	-0.24082	-2.47259
H	-2.80698	-5.66753	-0.51045
H	-0.57853	-5.53677	0.63229
C	-5.13422	-0.72644	0.92384
H	-5.74497	-1.60491	0.93697
N	-5.87958	0.39734	1.50904
C	-7.10951	0.62471	0.73671
C	-7.75966	1.94704	1.18433
H	-7.83807	2.60757	0.34621
H	-8.73583	1.74998	1.57569
H	-7.15681	2.40232	1.94208
C	-6.76706	0.7028	-0.7627
H	-7.32278	-0.04089	-1.29467
H	-7.02068	1.67281	-1.13642
H	-5.71979	0.53075	-0.8988
C	-8.0903	-0.53751	0.97941
H	-8.13643	-0.7525	2.02658
H	-9.06302	-0.2625	0.62858
H	-7.7529	-1.40503	0.45172
H	-3.08156	1.02579	1.44164

Thermal correction to Energy=1.019746

Thermal correction to Enthalpy=1.020896

Thermal correction to Gibbs Free Energy=0.818436

Sum of electronic and zero-point Energies=-2277.788814

Sum of electronic and thermal Energies=-2277.710264

Sum of electronic and thermal Enthalpies=-2277.709114

Sum of electronic and thermal Free Energies=-2277.911573

SCF Done: E(RM11L) = -2278.8071403

TS5d

Number of Negative Frequencies = 1

B	-1.34498	0.25388	1.3179
B	-1.73797	-0.69287	-1.31641
B	-0.35507	1.76897	-0.41155
C	3.47136	-1.28259	2.34076
C	2.23245	-1.16003	1.74487
C	1.41159	-2.3135	1.58599
C	1.84736	-3.56342	2.12067
C	0.97688	-4.67626	1.98829
C	-0.22486	-4.52351	1.33802
C	-0.55279	-3.26777	0.77931

H	-1.46044	-3.11787	0.20519
C	-3.16573	0.57179	2.70388
C	-1.84608	0.62501	3.55085
C	-3.62665	-0.46464	-2.61562
C	-3.49706	-1.9577	-2.15683
C	0.15395	3.99378	-0.02994
C	-1.20186	3.87358	-0.80382
Ir	-0.0448	-0.26442	-0.26579
N	1.71432	0.08903	1.2658
N	0.23294	-2.20601	0.88855
O	-2.701	0.00725	1.44857
O	-0.83784	0.7854	2.51406
O	-2.29543	0.04413	-2.36073
O	-2.49273	-1.8584	-1.11633
O	0.70975	2.65998	-0.20445
O	-1.53241	2.4766	-0.61333
H	0.44792	0.13935	-1.77511
C	1.36924	-1.1956	-1.71488
C	0.93686	-2.41583	-2.27217
C	1.82602	-3.30411	-2.87824
H	1.4587	-4.24461	-3.28371
C	3.1859	-2.98255	-2.9655
H	3.88524	-3.66698	-3.43918
C	3.63019	-1.76508	-2.46203
C	2.73706	-0.86094	-1.85473
C	3.92317	-2.53211	2.82682
C	3.12041	-3.64789	2.74246
H	3.45015	-4.60559	3.13559
H	4.90459	-2.597	3.28737
C	-4.25831	-0.33034	3.26806
H	-4.57318	0.01235	4.26055
H	-5.13291	-0.30769	2.60851
H	-3.92392	-1.36813	3.34583
C	-3.72881	1.95999	2.385
H	-4.52547	1.8609	1.64045
H	-4.14316	2.44535	3.27524
H	-2.95338	2.5999	1.95659
C	-1.7444	1.79425	4.52328
H	-2.54324	1.74592	5.27223
H	-0.78395	1.75693	5.04968
H	-1.80846	2.75483	4.00653
C	-1.53561	-0.69449	4.26713
H	-0.51207	-0.65736	4.65591
H	-2.21702	-0.8704	5.10618
H	-1.60401	-1.54121	3.57642
C	-2.33612	4.73519	-0.26005
H	-3.24713	4.55837	-0.84256
H	-2.55661	4.50597	0.78476
H	-2.08409	5.79929	-0.33789
C	-1.04989	4.09363	-2.31478
H	-1.97331	3.78002	-2.81252
H	-0.86509	5.14535	-2.55818
H	-0.2292	3.49045	-2.71701
C	-0.02884	4.20354	1.47742
H	0.94294	4.09164	1.97137
H	-0.41539	5.20273	1.70579
H	-0.7038	3.45233	1.89751
C	1.11316	5.03542	-0.59671
H	0.6352	6.02207	-0.60579
H	2.01327	5.10378	0.02236
H	1.42081	4.78872	-1.61562
C	-2.93338	-2.87662	-3.24777
H	-2.66284	-3.8389	-2.79903
H	-3.66592	-3.0633	-4.04083
H	-2.03364	-2.44688	-3.69904
C	-4.76189	-2.5646	-1.55715
H	-5.57917	-2.56327	-2.28773
H	-4.57293	-3.60356	-1.26311
H	-5.08391	-2.0165	-0.66843
C	-3.96024	-0.26745	-4.09048
H	-4.93045	-0.71592	-4.33465
H	-4.01527	0.80339	-4.31661
H	-3.19881	-0.70839	-4.7392
C	-4.58797	0.34667	-1.73582
H	-4.48528	1.40752	-1.9867
H	-5.63202	0.05356	-1.89346
H	-4.33355	0.22621	-0.67798
H	-0.11109	-2.69096	-2.1951
H	1.27742	-5.63666	2.39879
H	-0.91596	-5.35165	1.21927
H	4.09986	-0.40332	2.44399
H	2.45954	0.72067	0.98068
H	1.16699	0.55638	1.99365
C	5.11291	-1.36443	-2.57435
H	5.66467	-2.16211	-3.0262
N	5.23247	-0.15555	-3.40212
C	6.20016	0.76503	-2.78809
C	6.22772	0.53979	-1.2649

H	5.24818	0.69565	-0.86353
H	6.54272	-0.46166	-1.05809
H	6.91141	1.22888	-0.81477
C	7.60083	0.50147	-3.37141
H	7.54522	0.48662	-4.43986
H	8.26872	1.27716	-3.05976
H	7.96174	-0.44251	-3.01989
C	5.78569	2.21825	-3.08469
H	6.64874	2.84971	-3.04869
H	5.34492	2.2718	-4.05822
H	5.07543	2.54293	-2.35325
H	3.10552	0.08633	-1.52034

Thermal correction to Energy=1.014855

Thermal correction to Enthalpy=1.016005

Thermal correction to Gibbs Free Energy=0.817016

Sum of electronic and zero-point Energies=-2277.742607

Sum of electronic and thermal Energies=-2277.664573

Sum of electronic and thermal Enthalpies=-2277.663423

Sum of electronic and thermal Free Energies=-2277.862411

SCF Done: E(RM11L) = -2278.7550052

6d

Number of Negative Frequencies = 0

B	1.85618	0.21129	1.03463
B	1.67566	-0.92244	-1.68544
B	0.9091	-1.72867	1.11274
C	-2.215	-0.14394	1.80843
H	-2.09494	-1.21992	1.81603
C	-3.22597	0.46424	2.58246
C	-3.32447	1.85562	2.57312
C	-2.40456	2.58785	1.76716
C	-1.44002	1.87443	1.01487
C	-0.51101	2.57782	0.16917
C	-0.53944	3.99164	0.09519
C	3.92957	0.9817	1.6852
C	2.81837	1.58526	2.61878
C	3.26831	-2.19706	-2.75663
C	3.13358	-0.818	-3.49054
C	0.70259	-3.06468	2.98794
C	1.81783	-3.62858	2.0381
Ir	0.26906	-0.33053	-0.32906
N	-1.35026	0.52105	1.05558
N	0.38644	1.84295	-0.54829
O	3.14829	0.43386	0.59067
O	1.66561	0.7572	2.29763
O	2.05977	-2.2341	-1.9611
O	2.3733	-0.04684	-2.5275
O	0.02667	-2.11787	2.1237
O	2.06282	-2.50268	1.15805
H	-0.07076	-1.90284	-0.37389
C	-1.183	-0.18846	-1.90551
C	-0.91847	0.39058	-3.16715
C	-1.91558	0.55245	-4.13653
H	-1.6694	0.99906	-5.09846
C	-3.22424	0.14362	-3.87531
H	-4.006	0.27479	-4.62137
C	-3.52918	-0.43581	-2.63407
C	-2.50584	-0.60156	-1.68266
C	-2.40826	4.02016	1.67322
C	-1.52017	4.68702	0.88054
H	-1.55881	5.76954	0.83806
H	-3.13583	4.58646	2.24367
C	4.91289	1.99851	1.11455
H	5.47189	2.49394	1.91683
H	5.6324	1.48945	0.46368
H	4.40334	2.76138	0.52001
C	4.68312	-0.19157	2.31843
H	5.3022	-0.6707	1.55287
H	5.33478	0.13606	3.13555
H	3.98421	-0.94242	2.69611
C	3.09882	1.47518	4.11361
H	4.00236	2.03497	4.3812
H	2.25964	1.8959	4.67873
H	3.22804	0.43659	4.42669
C	2.44156	3.02661	2.25823
H	1.53527	3.30696	2.80498
H	3.23788	3.72897	2.52718
H	2.23753	3.12623	1.18913
C	3.12431	-4.00888	2.72568
H	3.84824	-4.35201	1.9782
H	3.56532	-3.16143	3.25535
H	2.9627	-4.82302	3.44159
C	1.33075	-4.78316	1.15433
H	2.08509	-4.98228	0.38626
H	1.17363	-5.69972	1.73317
H	0.39616	-4.52354	0.64649
C	1.26294	-2.27275	4.17437

H	0.43838	-1.75668	4.67801
H	1.75765	-2.92582	4.90158
H	1.97027	-1.51209	3.83393
C	-0.31619	-4.09277	3.46964
H	0.17093	-4.87789	4.05954
H	-1.06217	-3.60356	4.10622
H	-0.8428	-4.55957	2.63331
C	2.29713	-0.8951	-4.77321
H	2.07834	0.12125	-5.1186
H	2.82957	-1.42101	-5.57332
H	1.34472	-1.40253	-4.59178
C	4.4489	-0.09398	-3.75996
H	5.09746	-0.68958	-4.4129
H	4.25135	0.86149	-4.26004
H	4.98521	0.11672	-2.83147
C	3.29533	-3.41597	-3.67303
H	4.1571	-3.37838	-4.34999
H	3.3767	-4.32852	-3.07169
H	2.38405	-3.48924	-4.27238
C	4.4491	-2.23822	-1.77612
H	4.37121	-3.14548	-1.16865
H	5.41197	-2.25262	-2.2992
H	4.41791	-1.37944	-1.09835
H	0.0928	0.71692	-3.39802
C	-4.9204	-0.82792	-2.33713
H	-5.6287	-0.67348	-3.16267
N	-5.26996	-1.29243	-1.20097
C	-6.66041	-1.66121	-0.89641
C	-7.05954	-0.81816	0.33112
H	-6.3423	-0.96489	1.14654
H	-7.0722	0.24906	0.07887
H	-8.05714	-1.10058	0.68824
C	-6.63094	-3.15266	-0.50925
H	-5.91134	-3.32682	0.29872
H	-7.62003	-3.48547	-0.17223
H	-6.33431	-3.76851	-1.36671
C	-7.67961	-1.4409	-2.02766
H	-8.67728	-1.74211	-1.68901
H	-7.73355	-0.38689	-2.32508
H	-7.43673	-2.03703	-2.91539
H	-2.78012	-1.05699	-0.73597
H	-4.06271	2.37705	3.14584
H	-3.87792	-0.16424	3.15242
H	0.14857	4.52533	-0.52668
H	1.22061	1.71847	-0.01101
H	0.60578	2.32197	-1.39825

Thermal correction to Energy=1.017394

Thermal correction to Enthalpy=1.018544

Thermal correction to Gibbs Free Energy=0.820168

Sum of electronic and zero-point Energies=-2277.756575

Sum of electronic and thermal Energies=-2277.678709

Sum of electronic and thermal Enthalpies=-2277.677559

Sum of electronic and thermal Free Energies=-2277.875935

SCF Done: E(RM11L) = -2278.77377452

7d

Number of Negative Frequencies = 0

Ir	0.27785	-0.08741	-0.68886
B	-1.55185	0.84677	-1.11304
B	0.1519	1.748	0.29693
O	-1.91228	1.22685	-2.40012
O	-2.60844	1.07871	-0.23215
C	1.30582	-3.16029	2.41067
C	2.73934	-3.7488	0.06712
N	1.77247	-1.74358	-0.9298
N	0.46384	-1.06367	1.39685
O	0.23078	1.79013	1.69631
O	-0.13253	3.01392	-0.20529
C	1.91832	-2.58423	0.14121
C	1.2234	-2.29009	1.34437
O	2.94466	0.3718	0.71363
O	2.82616	1.86791	-1.00598
C	2.80906	-4.61794	1.18669
C	2.09303	-4.33382	2.32849
H	3.4272	-5.5089	1.12153
H	2.13598	-5.00338	3.18235
C	3.44108	-3.98394	-1.14339
C	-0.05207	3.98075	0.87404
C	-0.24227	3.08381	2.15407
C	4.24434	1.76176	-0.69098
C	4.24472	1.01609	0.70245
C	-3.19373	1.90331	-2.35727
C	-3.80037	1.39029	-1.00065
H	0.427	0.49964	-2.14582
C	3.29583	-3.10719	-2.1936
C	-2.90068	3.40682	-2.36054
H	-2.27169	3.67306	-1.50884
H	-2.35171	3.66015	-3.27418

H	-3.81982	4.00224	-2.33596
C	-3.9902	1.51539	-3.59974
H	-4.99791	1.94574	-3.56609
H	-3.48779	1.89897	-4.49459
H	-4.07573	0.43063	-3.70106
C	-4.59636	0.08778	-1.14485
H	-4.82599	-0.3048	-0.14861
H	-5.54017	0.25144	-1.67564
H	-4.01933	-0.67347	-1.67648
C	-4.62114	2.4185	-0.22859
H	-5.49695	2.73043	-0.80928
H	-4.97739	1.97868	0.70968
H	-4.03284	3.3058	0.01683
C	-1.12994	5.04266	0.6802
H	-1.11744	5.75537	1.51306
H	-0.94166	5.59903	-0.24438
H	-2.12774	4.6041	0.61494
C	1.33493	4.62417	0.77833
H	2.11723	3.87005	0.87992
H	1.44553	5.08206	-0.21
H	1.48131	5.39902	1.53832
C	0.59137	3.50714	3.35929
H	0.30936	4.51276	3.69187
H	0.41684	2.81509	4.19084
H	1.66062	3.50059	3.13456
C	-1.70882	2.90202	2.5596
H	-2.14404	3.83397	2.9361
H	-2.29878	2.53953	1.7148
H	-1.76587	2.15385	3.35727
C	4.87877	0.94312	-1.82142
H	4.68982	1.44779	-2.77471
H	5.96183	0.84657	-1.69202
H	4.44372	-0.05923	-1.88033
C	4.84259	3.16532	-0.66902
H	4.77558	3.6093	-1.66818
H	4.3129	3.82173	0.02493
H	5.89948	3.13057	-0.3815
C	4.29101	1.95308	1.91288
H	4.13518	1.36523	2.82396
H	5.257	2.46252	1.99332
H	3.50137	2.70623	1.86327
C	5.31142	-0.06795	0.84943
H	6.31825	0.36012	0.78726
H	5.2076	-0.55097	1.82732
H	5.21206	-0.84075	0.08335
C	2.43493	-1.9971	-2.04784
H	2.28167	-1.29947	-2.8632
B	2.13319	0.9284	-0.26847
C	-2.02769	-2.35776	-0.57649
C	-1.0897	-1.6423	-1.36938
C	-0.90009	-2.12561	-2.68294
C	-1.55017	-3.25698	-3.17881
C	-2.44319	-3.9632	-2.36395
C	-2.67925	-3.50516	-1.07355
H	-0.21543	-1.59741	-3.3429
H	-1.36728	-3.58357	-4.20098
H	-2.95947	-4.84349	-2.73959
H	3.81597	-3.25419	-3.13416
H	4.0817	-4.85779	-1.22505
H	0.76653	-2.93267	3.32621
H	0.98638	-0.34697	1.90471
H	-0.40201	-1.20975	1.91206
C	-3.68635	-4.22596	-0.15824
H	-4.44649	-3.53774	0.14744
N	-2.98796	-4.74304	1.02741
C	-3.96007	-4.97934	2.10448
C	-3.28292	-4.74512	3.46764
H	-3.60116	-3.80488	3.86711
H	-3.55671	-5.52994	4.14143
H	-2.22041	-4.7378	3.34151
C	-4.46945	-6.43059	2.02694
H	-3.63571	-7.09842	1.96535
H	-5.04214	-6.65484	2.90252
H	-5.08442	-6.54685	1.15907
C	-5.14624	-4.00987	1.9472
H	-5.57756	-4.12872	0.97523
H	-5.88308	-4.22386	2.69298
H	-4.80224	-3.00345	2.06413
H	-2.29922	-2.00635	0.397

Thermal correction to Energy=1.018025

Thermal correction to Enthalpy=1.019175

Thermal correction to Gibbs Free Energy=0.821962

Sum of electronic and zero-point Energies=-2277.759608

Sum of electronic and thermal Energies=-2277.681903

Sum of electronic and thermal Enthalpies=-2277.680753

Sum of electronic and thermal Free Energies=-2277.877966

SCF Done: E(RM11L) = -2278.77529667

TS8d

Number of Negative Frequencies = 1

Ir	0.81943	-0.05901	-0.71136
B	0.61071	2.02925	-1.05701
B	2.41705	0.87277	0.23359
O	0.95315	2.68904	-2.24167
O	0.36215	2.9683	-0.03867
C	-2.1642	-1.64953	2.11945
C	-1.24737	0.25797	3.28879
C	-0.35257	0.40606	2.20955
H	0.37665	1.20459	2.20628
C	-2.12739	-3.31891	-0.21857
N	-0.38074	-1.89363	-1.10114
N	-0.33859	-0.38142	1.1408
O	2.59561	0.73473	1.618
O	3.44581	1.64968	-0.29388
C	-1.23933	-2.22395	-0.10272
C	-1.23414	-1.40492	1.08174
O	1.88105	-2.52804	0.71952
O	3.50997	-1.7649	-0.68704
C	-3.04424	-3.55582	0.86141
C	-3.06758	-2.75642	1.9672
H	-3.74341	-4.38144	0.79114
H	-3.7859	-2.96361	2.75244
C	-2.17258	-0.78643	3.25344
C	4.45504	1.85222	0.73094
C	3.63177	1.64796	2.05075
C	3.87571	-3.13351	-0.35822
C	3.01788	-3.40511	0.9263
C	1.00935	4.11249	-2.00474
C	0.20646	4.27283	-0.65501
H	1.58632	0.03681	-2.10809
C	2.48808	4.48981	-1.88213
H	2.9511	3.9326	-1.06806
H	3.00236	4.20911	-2.80815
H	2.62871	5.56503	-1.72443
C	0.38582	4.82581	-3.20382
H	0.34428	5.90888	-3.03852
H	0.99591	4.64392	-4.09576
H	-0.62448	4.46337	-3.40974
C	-1.29541	4.50464	-0.86761
H	-1.80863	4.41687	0.09637
H	-1.49482	5.50248	-1.27303
H	-1.72386	3.76033	-1.54295
C	0.75584	5.33589	0.29281
H	0.67681	6.33246	-0.15683
H	0.17629	5.33804	1.22315
H	1.80246	5.1562	0.54719
C	5.06985	3.23983	0.57494
H	5.81396	3.41675	1.36064
H	5.5752	3.31693	-0.39392
H	4.3204	4.032	0.62903
C	5.52906	0.77984	0.5165
H	5.09739	-0.22057	0.59285
H	5.93888	0.88564	-0.49383
H	6.35106	0.8794	1.23373
C	4.4043	1.01086	3.20126
H	5.22869	1.65897	3.52107
H	3.73623	0.86327	4.05726
H	4.81557	0.03779	2.92455
C	2.92237	2.91922	2.53097
H	3.62782	3.67237	2.8979
H	2.32006	3.347	1.72592
H	2.24709	2.65764	3.35374
C	3.45733	-3.99862	-1.55447
H	3.95034	-3.62023	-2.45619
H	3.7444	-5.04678	-1.41836
H	2.37508	-3.95003	-1.71654
C	5.38543	-3.21137	-0.15762
H	5.89718	-2.97344	-1.09668
H	5.73263	-2.50686	0.60167
H	5.68271	-4.22245	0.14402
C	3.703	-2.94771	2.21766
H	2.97606	-2.98294	3.03614
H	4.55136	-3.58854	2.48162
H	4.05083	-1.91523	2.12497
C	2.50926	-4.83581	1.073
H	3.34431	-5.54349	1.13346
H	1.9206	-4.92616	1.99289
H	1.86855	-5.12189	0.23473
B	2.24755	-1.51428	-0.16197
C	-2.12544	1.17225	-0.65942
C	-1.03551	0.94178	-1.51256
C	-1.33571	0.74353	-2.87368
C	-2.65733	0.70727	-3.33815
C	-3.72177	0.86476	-2.45219
C	-3.45647	1.10571	-1.09345
H	-0.51993	0.6069	-3.57823

H	-2.85387	0.54146	-4.39528
H	-4.75168	0.80917	-2.79277
C	-4.51656	1.23181	-0.08057
H	-4.14646	1.49841	0.92091
N	-5.75059	1.01203	-0.32003
C	-6.72693	1.11957	0.79382
C	-6.84029	2.58759	1.24659
H	-5.8966	2.94351	1.67647
H	-7.09277	3.23385	0.39774
H	-7.62258	2.69788	2.00688
C	-6.32048	0.222	1.98086
H	-7.1054	0.22282	2.74618
H	-6.16499	-0.81058	1.64613
H	-5.39538	0.56989	2.45325
C	-8.07586	0.64489	0.23065
H	-8.00725	-0.39508	-0.11072
H	-8.86452	0.70667	0.99004
H	-8.37214	1.26038	-0.62688
H	-1.94361	1.39232	0.3873
H	-2.09864	-3.86359	-1.02516
H	0.46255	-2.42227	-1.0041
H	-0.80241	-2.09789	-1.98458
H	-2.87957	-0.94676	4.04043
H	-1.18463	0.9571	4.09636

Thermal correction to Energy=1.016774

Thermal correction to Enthalpy=1.017924

Thermal correction to Gibbs Free Energy=0.821833

Sum of electronic and zero-point Energies=-2277.752951

Sum of electronic and thermal Energies=-2277.675923

Sum of electronic and thermal Enthalpies=-2277.674773

Sum of electronic and thermal Free Energies=-2277.870864

SCF Done: E(RM11L) = -2278.76872010

1'

Number of Negative Frequencies = 0

B	-2.32825	-0.60191	0.01045
C	-0.39578	2.01214	0.07563
H	-1.46462	1.85121	0.10201
C	0.12214	3.31521	0.03394
C	2.32625	2.35659	-0.03677
C	1.73317	1.07436	0.01513
C	2.551	-0.09832	0.01473
C	3.96048	-0.0136	-0.05818
C	4.02745	-2.43379	-0.008
C	2.61995	-2.40261	0.0729
H	2.06058	-3.33327	0.12929
N	0.35653	0.88963	0.06191
N	1.89431	-1.28806	0.0839
O	-3.03427	0.59319	-0.25071
O	-3.27735	-1.6384	0.17833
C	3.76233	2.41821	-0.10363
C	4.54109	1.29709	-0.11734
H	4.24043	3.39045	-0.14779
H	5.61912	1.4004	-0.1728
C	1.50374	3.5165	-0.02784
C	4.71857	-1.2199	-0.07096
C	-4.59267	-1.15468	-0.18429
C	-4.43994	0.39221	0.02247
Ir	-0.31852	-0.94764	0.09763
C	-4.8312	-1.543	-1.64935
H	-4.72262	-2.62831	-1.75108
H	-5.83506	-1.26589	-1.99037
H	-4.09436	-1.06603	-2.30375
C	-5.63356	-1.82411	0.71014
H	-6.63219	-1.41035	0.52551
H	-5.66881	-2.89917	0.49997
H	-5.39528	-1.69724	1.76941
C	-5.25803	1.25871	-0.93128
H	-6.33127	1.07539	-0.80227
H	-5.06889	2.31829	-0.72382
H	-4.99486	1.0693	-1.97508
C	-4.68782	0.8315	1.4722
H	-4.36631	1.87236	1.58939
H	-5.74705	0.76749	1.74475
H	-4.10815	0.21955	2.1709
C	-0.86641	4.45827	0.04853
H	-1.89346	4.0864	0.11273
H	-0.69734	5.12455	0.90277
H	-0.78748	5.06616	-0.86087
C	2.12045	4.89052	-0.08224
H	2.78805	5.05981	0.77234
H	2.72368	5.01939	-0.98989
H	1.36721	5.67977	-0.07359
C	6.22165	-1.15665	-0.16015
H	6.53638	-0.65065	-1.08148
H	6.64083	-0.58562	0.6774
H	6.68012	-2.14632	-0.1511
C	4.72141	-3.77486	-0.02071

H	5.30859	-3.91562	-0.93603
H	5.40849	-3.88254	0.82721
H	3.99325	-4.58986	0.03557

Thermal correction to Energy=.507836

Thermal correction to Enthalpy=0.508986

Thermal correction to Gibbs Free Energy=0.390162

Sum of electronic and zero-point Energies=-1244.178598

Sum of electronic and thermal Energies=-1244.138520

Sum of electronic and thermal Enthalpies=-1244.137369

Sum of electronic and thermal Free Energies=-1244.256193

SCF Done: E(RM11L) = -1244.76447873

2b'

Number of Negative Frequencies = 0

Ir	-0.20436	-0.32057	-0.4747
B	1.59795	0.55682	-0.90509
O	2.4545	0.08233	-1.92162
O	2.17516	1.73431	-0.36765
C	-3.45751	2.29355	0.2671
C	-1.51497	3.70845	0.20231
C	-0.74451	2.56425	-0.05031
H	0.32746	2.64371	-0.16585
C	-4.55465	-0.36111	0.07933
N	-2.27816	-1.14121	-0.28754
N	-1.24396	1.31186	-0.15364
C	-3.16586	-0.13265	-0.06441
C	-2.61723	1.18397	0.0164
C	-5.3902	0.77937	0.32459
C	-4.86521	2.03608	0.41524
H	-6.45939	0.64037	0.44084
H	-5.52919	2.87187	0.60503
C	-5.04358	-1.69484	-0.01903
C	-2.89906	3.59727	0.36212
C	3.68571	0.84251	-1.91744
C	3.23663	2.18386	-1.24464
C	-4.12056	-2.71766	-0.25859
C	4.7052	0.06522	-1.07534
H	4.3568	-0.04716	-0.044
H	4.82788	-0.93584	-1.50128
H	5.68461	0.55691	-1.06711
C	4.18473	0.97802	-3.35367
H	5.07052	1.62288	-3.40281
H	4.46342	-0.00745	-3.74402
H	3.41507	1.39275	-4.00997
C	2.60884	3.17449	-2.23578
H	2.14643	3.99527	-1.67614
H	3.35344	3.6038	-2.91514
H	1.82853	2.68985	-2.83168
C	4.31117	2.88652	-0.42051
H	5.15236	3.18522	-1.05742
H	3.89592	3.79187	0.03736
H	4.69105	2.24974	0.38055
C	-4.51878	-4.16891	-0.38098
H	-5.22288	-4.32674	-1.20677
H	-3.64367	-4.79974	-0.56633
H	-5.00303	-4.53297	0.53308
C	-6.51814	-1.96464	0.13563
H	-6.88262	-1.60883	1.10717
H	-7.09552	-1.43959	-0.63565
H	-6.75481	-3.02697	0.06225
C	-3.78366	4.78895	0.62508
H	-4.52797	4.91445	-0.172
H	-4.338	4.67344	1.56516
H	-3.21353	5.71697	0.69149
C	-0.78987	5.0318	0.28221
H	-1.15437	5.73629	-0.47511
H	-0.9252	5.50757	1.26115
H	0.2844	4.89831	0.12303
C	-2.7582	-2.379	-0.38298
H	-2.02423	-3.15763	-0.56679
C	0.78837	-3.3129	0.28763
C	1.99404	-2.73399	0.72245
C	0.76459	-4.15539	-0.82805
C	3.18214	-3.0429	0.03951
C	1.94907	-4.43972	-1.5111
H	-0.1743	-4.59481	-1.15504
C	3.1581	-3.88823	-1.06625
H	4.11128	-2.59944	0.38034
H	1.93501	-5.09355	-2.37907
H	4.0823	-4.11538	-1.5915
C	1.96381	-1.78998	1.85906
H	0.96681	-1.62733	2.2828
N	3.01192	-1.20225	2.28572
C	2.94276	-0.21973	3.38302
C	3.57816	1.07009	2.82886
H	2.99992	1.44648	1.97914
H	3.61449	1.84444	3.60497
H	4.60144	0.87588	2.48782

C	3.81286	-0.78213	4.52318
H	3.90148	-0.05252	5.33693
H	3.37415	-1.7009	4.93137
H	4.81911	-1.01854	4.15881
C	1.53053	0.0945	3.90562
H	0.88722	0.48267	3.1061
H	1.04706	-0.7888	4.34019
H	1.59046	0.85693	4.69041
H	-0.12769	-3.10644	0.83575

Thermal correction to Energy=0.764407

Thermal correction to Enthalpy=0.765557

Thermal correction to Gibbs Free Energy=0.604557

Sum of electronic and zero-point Energies=-1726.942068

Sum of electronic and thermal Energies=-1726.882794

Sum of electronic and thermal Enthalpies=-1726.881644

Sum of electronic and thermal Free Energies=-1727.042643

SCF Done: E(RM11L) = -1727.75804394

TS3b'

Number of Negative Frequencies = 1

Ir	-0.03311	-0.04061	0.13176
B	1.2587	-1.64948	0.09934
O	2.32854	-1.85463	0.9874
O	1.1282	-2.8094	-0.69972
C	-4.22957	-1.01361	-0.32788
C	-3.11115	-3.13273	-0.61847
C	-1.89486	-2.44807	-0.43887
H	-0.95276	-2.97472	-0.51289
C	-4.01767	1.82032	0.09297
N	-1.60794	1.51319	0.213
N	-1.79356	-1.13406	-0.20777
C	-2.86265	1.00439	0.0635
C	-2.96291	-0.41104	-0.15092
C	-5.29086	1.18032	-0.07769
C	-5.38917	-0.16652	-0.275
H	-6.19403	1.77983	-0.05403
H	-6.36948	-0.61077	-0.40449
C	-3.86273	3.22498	0.27882
C	-4.30727	-2.41709	-0.56011
C	2.9861	-3.11315	0.70685
C	1.89021	-3.89013	-0.10424
C	-2.56718	3.72937	0.41915
C	4.246	-2.81857	-0.11659
H	3.99634	-2.4027	-1.09694
H	4.86044	-2.08712	0.41903
H	4.84442	-3.72338	-0.27079
C	3.38576	-3.75342	2.03524
H	3.80915	-4.75273	1.87974
H	4.1471	-3.13642	2.52578
H	2.5336	-3.8355	2.71465
C	0.9316	-4.68301	0.79636
H	0.10776	-5.07898	0.19267
H	1.43348	-5.52934	1.27747
H	0.50413	-4.04318	1.57551
C	2.41805	-4.79394	-1.21527
H	3.04948	-5.59017	-0.80361
H	1.57801	-5.26572	-1.73764
H	2.99887	-4.23479	-1.95295
C	-2.27358	5.19732	0.61197
H	-2.74964	5.58696	1.51971
H	-1.19647	5.37048	0.6997
H	-2.63979	5.79485	-0.23133
C	-5.07751	4.11635	0.30672
H	-5.63347	4.04667	-0.63652
H	-5.76516	3.81925	1.10822
H	-4.81843	5.16442	0.46238
C	-5.6481	-3.07774	-0.74592
H	-6.29493	-2.90349	0.12253
H	-6.16787	-2.6677	-1.62088
H	-5.56128	-4.15601	-0.8854
C	-3.05698	-4.61914	-0.8779
H	-3.57088	-5.18416	-0.09078
H	-3.53273	-4.87867	-1.83094
H	-2.02115	-4.96845	-0.91679
C	-1.48472	2.8288	0.37456
H	-0.46935	3.1996	0.47932
C	1.61185	1.1446	0.91839
C	2.97507	1.19687	0.53317
C	1.25343	1.76212	2.13911
C	3.94224	1.69558	1.41191
C	2.22415	2.25966	3.00962
H	0.20821	1.81272	2.42793
C	3.57598	2.21072	2.65723
H	4.98742	1.68656	1.11461
H	1.92315	2.68328	3.9649
H	4.33586	2.59296	3.33375
H	0.97154	1.24659	-0.1986
C	3.38108	0.70859	-0.82223

H	3.44349	-0.378	-0.89765
N	3.67022	1.34643	-1.88789
C	3.63127	2.81773	-2.06345
C	2.47044	3.54654	-1.35581
H	2.59314	3.57829	-0.27136
H	2.41695	4.58065	-1.71736
H	1.51466	3.06021	-1.58327
C	3.48074	3.02732	-3.58331
H	3.50264	4.09417	-3.83627
H	4.29045	2.52451	-4.1241
H	2.52958	2.6105	-3.93672
C	4.9842	3.39273	-1.60448
H	5.09167	3.32228	-0.51786
H	5.8146	2.84866	-2.06949
H	5.06483	4.44886	-1.88868

Thermal correction to Energy= 0.760170

Thermal correction to Enthalpy=0.761320

Thermal correction to Gibbs Free Energy=0.604398

Sum of electronic and zero-point Energies=-1726.919476

Sum of electronic and thermal Energies=-1726.861304

Sum of electronic and thermal Enthalpies=-1726.860154

Sum of electronic and thermal Free Energies=-1727.017075

SCF Done: E(RM11L) = -1727.72956927

4b'

Number of Negative Frequencies = 0

Ir	0.02925	-1.39784	-0.63128
B	-2.0002	-1.38766	-0.64139
C	2.15443	2.46652	-1.05048
C	-0.11979	2.96592	-1.7067
C	-0.41622	1.61233	-1.45605
H	-1.42832	1.24536	-1.58696
C	4.11729	0.45786	-0.44924
N	2.34869	-1.19489	-0.65316
N	0.47295	0.71179	-1.03892
O	-2.73913	-1.35309	-1.83984
O	-2.88161	-1.39373	0.44365
C	2.76322	0.09925	-0.65039
C	1.77054	1.11313	-0.90304
C	4.46135	1.85061	-0.51558
C	3.53101	2.80331	-0.81484
H	5.4893	2.15125	-0.34629
H	3.84071	3.83995	-0.88358
C	5.07201	-0.57491	-0.2139
C	1.17479	3.42163	-1.44904
C	-4.22639	-1.62628	-0.04286
C	-4.13676	-1.12287	-1.527
H	-0.15881	-2.99489	-0.47744
C	4.62602	-1.89783	-0.21833
C	-5.20862	-0.86193	0.83948
H	-6.23214	-0.95806	0.45855
H	-5.18525	-1.26766	1.857
H	-4.95647	0.19977	0.89702
C	-4.48793	-3.13399	0.06281
H	-3.78899	-3.69779	-0.56366
H	-4.33933	-3.44888	1.10113
H	-5.51086	-3.39189	-0.23233
C	-5.00122	-1.89075	-2.523
H	-6.06268	-1.81049	-2.26047
H	-4.86961	-1.4742	-3.52816
H	-4.73074	-2.94898	-2.5591
C	-4.38842	0.38326	-1.66838
H	-5.44014	0.63931	-1.49987
H	-3.77733	0.95025	-0.96069
H	-4.11795	0.69735	-2.68262
C	5.54101	-3.07627	0.00932
H	6.02949	-3.02253	0.98946
H	4.98135	-4.01579	-0.03211
H	6.33259	-3.12426	-0.74793
C	6.51635	-0.21947	0.02578
H	6.94007	0.30306	-0.84085
H	6.61421	0.45314	0.88656
H	7.13201	-1.09878	0.21887
C	1.55375	4.87213	-1.59241
H	1.98266	5.25343	-0.65807
H	2.31205	5.00646	-2.37406
H	0.69822	5.49941	-1.84564
C	-1.22471	3.86792	-2.19989
H	-1.48049	4.63297	-1.45715
H	-0.93546	4.38677	-3.12077
H	-2.13144	3.29361	-2.41185
C	3.25523	-2.1418	-0.44759
H	2.88286	-3.16169	-0.4539
C	-0.16985	-0.23757	2.22619
C	0.20488	-1.3156	1.3712
C	0.91212	-2.38165	1.98841
C	1.25852	-2.38471	3.33757
C	0.90287	-1.30649	4.15544

C	0.19176	-0.25705	3.59202
H	1.20859	-3.23271	1.38424
H	1.80021	-3.23387	3.75034
H	-0.12056	0.58426	4.20403
H	1.15841	-1.2973	5.21218
C	-0.98824	0.91477	1.77989
N	-0.97672	2.0192	2.42546
C	-1.87718	3.13622	2.10625
C	-2.61615	3.46045	3.4205
H	-3.24921	2.61757	3.72307
H	-1.90055	3.65408	4.22748
H	-3.25414	4.34453	3.30047
C	-0.98142	4.32834	1.71577
H	-0.42517	4.10947	0.79818
H	-1.58394	5.23006	1.55219
H	-0.25407	4.53799	2.50835
C	-2.9134	2.87163	1.00187
H	-3.54307	3.75695	0.85755
H	-2.43824	2.64529	0.04485
H	-3.56768	2.03362	1.26697
H	-1.62507	0.73087	0.91359

Thermal correction to Energy=0.761379

Thermal correction to Enthalpy=0.762529

Thermal correction to Gibbs Free Energy=0.604600

Sum of electronic and zero-point Energies=-1726.977642

Sum of electronic and thermal Energies=-1726.918779

Sum of electronic and thermal Enthalpies=-1726.917629

Sum of electronic and thermal Free Energies=-1727.075558

SCF Done: E(RM11L) = -1727.78408100

5b'

Number of Negative Frequencies = 0

Ir	0.02925	-1.39784	-0.63128
B	-2.0002	-1.38766	-0.64139
C	2.15443	2.46652	-1.05048
C	-0.11979	2.96592	-1.7067
C	-0.41622	1.61233	-1.45605
H	-1.42832	1.24536	-1.58696
C	4.11729	0.45786	-0.44924
N	2.34869	-1.19489	-0.65316
N	0.47295	0.71179	-1.03892
O	-2.73913	-1.35309	-1.83984
O	-2.88161	-1.39373	0.44365
C	2.76322	0.09925	-0.65039
C	1.77054	1.11313	-0.90304
C	4.46135	1.85061	-0.51558
C	3.53101	2.80331	-0.81484
H	5.4893	2.15125	-0.34629
H	3.84071	3.83995	-0.88358
C	5.07201	-0.57491	-0.2139
C	1.17479	3.42163	-1.44904
C	-4.22639	-1.62628	-0.04286
C	-4.13676	-1.12287	-1.527
H	-0.15881	-2.99489	-0.47744
C	4.62602	-1.89783	-0.21833
C	-5.20862	-0.86193	0.83948
H	-6.23214	-0.95806	0.45855
H	-5.18525	-1.26766	1.857
H	-4.95647	0.19977	0.89702
C	-4.48793	-3.13399	0.06281
H	-3.78899	-3.69779	-0.56366
H	-4.33933	-3.44888	1.10113
H	-5.51086	-3.39189	-0.23233
C	-5.00122	-1.89075	-2.523
H	-6.06268	-1.81049	-2.26047
H	-4.86961	-1.4742	-3.52816
H	-4.73074	-2.94898	-2.5591
C	-4.38842	0.38326	-1.66838
H	-5.44014	0.63931	-1.49987
H	-3.77733	0.95025	-0.96069
H	-4.11795	0.69735	-2.68262
C	5.54101	-3.07627	0.00932
H	6.02949	-3.02253	0.98946
H	4.98135	-4.01579	-0.03211
H	6.33259	-3.12426	-0.74793
C	6.51635	-0.21947	0.02578
H	6.94007	0.30306	-0.84085
H	6.61421	0.45314	0.88656
H	7.13201	-1.09878	0.21887
C	1.55375	4.87213	-1.59241
H	1.98266	5.25343	-0.65807
H	2.31205	5.00646	-2.37406
H	0.69822	5.49941	-1.84564
C	-1.22471	3.86792	-2.19989
H	-1.48049	4.63297	-1.45715
H	-0.93546	4.38677	-3.12077
H	-2.13144	3.29361	-2.41185
C	3.25523	-2.1418	-0.44759

H	2.88286	-3.16169	-0.4539
C	-0.16985	-0.23757	2.22619
C	0.20488	-1.3156	1.3712
C	0.91212	-2.38165	1.98841
C	1.25852	-2.38471	3.33757
C	0.90287	-1.30649	4.15544
C	0.19176	-0.25705	3.59202
H	1.20859	-3.23271	1.38424
H	1.80021	-3.23387	3.75034
H	-0.12056	0.58426	4.20403
H	1.15841	-1.2973	5.21218
C	-0.98824	0.91477	1.77989
N	-0.97672	2.0192	2.42546
C	-1.87718	3.13622	2.10625
C	-2.61615	3.46045	3.4205
H	-3.24921	2.61757	3.72307
H	-1.90055	3.65408	4.22748
H	-3.25414	4.34453	3.30047
C	-0.98142	4.32834	1.71577
H	-0.42517	4.10947	0.79818
H	-1.58394	5.23006	1.55219
H	-0.25407	4.53799	2.50835
C	-2.9134	2.87163	1.00187
H	-3.54307	3.75695	0.85755
H	-2.43824	2.64529	0.04485
H	-3.56768	2.03362	1.26697
H	-1.62507	0.73087	0.91359

Thermal correction to Energy=0.761379

Thermal correction to Enthalpy=0.762529

Thermal correction to Gibbs Free Energy=0.604600

Sum of electronic and zero-point Energies=-1726.977642

Sum of electronic and thermal Energies=-1726.918779

Sum of electronic and thermal Enthalpies=-1726.917629

Sum of electronic and thermal Free Energies=-1727.075558

SCF Done: E(RM11L) = -1727.78408091

TS6b'

Number of Negative Frequencies = 1

Ir	0.24336	0.26635	0.55529
B	1.03778	-1.38066	-0.61011
C	-4.12675	-0.21922	0.66629
C	-3.39487	-2.44767	1.23161
C	-2.0732	-1.97583	1.10217
H	-1.25156	-2.66834	1.22105
C	-3.38383	2.43367	-0.16128
N	-1.05577	1.72264	0.01949
N	-1.73961	-0.72368	0.79618
O	0.20119	-2.52808	-0.72736
O	1.63164	-1.11684	-1.87055
C	-2.39992	1.46538	0.14063
C	-2.76455	0.14672	0.55575
C	-4.75937	2.04609	-0.00885
C	-5.11182	0.78692	0.38343
H	-5.53722	2.77101	-0.22053
H	-6.16319	0.53687	0.47329
C	-2.97822	3.72226	-0.60854
C	-4.45079	-1.55593	1.03229
C	0.8788	-1.83937	-2.8637
C	0.36053	-3.07715	-2.04684
H	1.50008	1.22511	0.28705
C	-1.60637	3.96462	-0.73409
C	1.80504	-2.17854	-4.02892
H	1.29258	-2.8078	-4.76614
H	2.12168	-1.25765	-4.53144
H	2.70375	-2.69955	-3.68822
C	-0.2582	-0.92443	-3.34233
H	-0.92486	-0.6703	-2.51258
H	0.17447	0.00834	-3.72012
H	-0.84326	-1.38513	-4.14596
C	-0.98141	-3.63985	-2.50978
H	-0.92491	-3.99048	-3.54705
H	-1.26402	-4.49147	-1.8798
H	-1.77418	-2.89097	-2.43504
C	1.40229	-4.20075	-1.95102
H	1.53358	-4.72501	-2.90424
H	2.3717	-3.80381	-1.63236
H	1.07086	-4.92841	-1.20192
C	-1.05059	5.28418	-1.21414
H	-1.35608	6.1109	-0.56186
H	0.04316	5.26234	-1.23535
H	-1.39973	5.51959	-2.22658
C	-4.01242	4.76648	-0.93812
H	-4.67416	4.42447	-1.744
H	-4.64859	4.97832	-0.06962
H	-3.56211	5.70774	-1.2559
C	-5.8924	-1.9729	1.16757
H	-6.42197	-1.32884	1.87986
H	-6.4167	-1.88885	0.20708

H	-5.99404	-3.00286	1.51252
C	-3.60448	-3.90268	1.57545
H	-4.14402	-4.0213	2.52283
H	-4.18621	-4.41795	0.80176
H	-2.64558	-4.42117	1.67203
C	-0.69683	2.94577	-0.40818
H	0.36757	3.11543	-0.50169
C	1.47655	-1.89745	1.95267
C	1.95294	-1.28029	0.77439
C	3.31397	-0.82497	0.78884
C	4.12279	-1.07554	1.89437
C	3.60148	-1.66017	3.0588
C	2.27014	-2.0503	3.10039
H	5.17241	-0.79799	1.85876
H	1.85451	-2.51047	3.99311
H	4.24812	-1.8138	3.91922
C	3.94122	-0.21518	-0.42384
H	3.91255	-0.88712	-1.28619
N	4.51427	0.90213	-0.63845
C	4.63584	2.08825	0.22881
C	6.14675	2.38388	0.30782
H	6.58154	2.46744	-0.69457
H	6.32643	3.32277	0.84513
H	6.67068	1.58039	0.84031
C	4.05033	2.06575	1.65496
H	3.00468	1.74783	1.65678
H	4.61485	1.41311	2.32491
H	4.09687	3.08066	2.07006
C	3.93535	3.21199	-0.56813
H	4.33127	3.26865	-1.58789
H	2.85829	3.01736	-0.62954
H	4.08653	4.18216	-0.07977
H	0.48377	-2.32801	1.95726

Thermal correction to Energy=0.759795

Thermal correction to Enthalpy=0.760945

Thermal correction to Gibbs Free Energy=0.603731

Sum of electronic and zero-point Energies=-1726.934326

Sum of electronic and thermal Energies=-1726.876159

Sum of electronic and thermal Enthalpies=-1726.875009

Sum of electronic and thermal Free Energies=-1727.032223

SCF Done: E(RM11L) = -1727.74340369

7'

Number of Negative Frequencies = 0

C	-3.70115	-1.24346	-1.89212
H	-3.59626	-2.2585	-2.25072
C	-4.37966	-0.2819	-2.65745
C	-3.91745	1.32471	-0.92348
C	-3.25843	0.30166	-0.21182
C	-2.64961	0.5566	1.04633
C	-2.67936	1.8381	1.63377
C	-1.37232	0.93186	3.45408
C	-1.40813	-0.30839	2.78734
H	-0.90854	-1.17198	3.21703
N	-3.13843	-0.99427	-0.68892
N	-2.0228	-0.51501	1.61959
C	-3.94102	2.62725	-0.31079
C	-3.35594	2.87274	0.90028
H	-4.43594	3.43986	-0.83135
H	-3.39471	3.87487	1.31319
C	-4.49956	1.03177	-2.18651
C	-2.02181	2.03172	2.8812
Ir	-2.16654	-2.25408	0.42433
O	1.13017	1.14268	0.06208
H	-2.34436	-3.56875	-0.57522
C	-0.61725	1.02394	4.75849
H	-1.27703	1.30417	5.58877
H	-0.15376	0.06537	5.01128
H	0.17917	1.77574	4.70695
C	-2.01144	3.39429	3.52381
H	-1.41047	4.0975	2.9318
H	-3.0232	3.81072	3.58977
H	-1.59577	3.37288	4.5323
C	-5.20318	2.11335	-2.96498
H	-6.04263	2.53039	-2.39404
H	-4.5226	2.9454	-3.18695
H	-5.5986	1.74906	-3.91435
C	-4.95871	-0.72158	-3.98213
H	-6.04515	-0.57515	-4.01121
H	-4.53054	-0.15247	-4.81583
H	-4.75991	-1.78174	-4.16492
B	2.17535	0.52025	-0.57442
O	2.85733	1.35003	-1.43138
C	0.95342	2.45007	-0.56788
C	2.37141	2.70789	-1.19885
C	3.35975	3.35976	-0.22591
H	3.38136	2.82706	0.73075

H	4.36492	3.32159	-0.65837
H	3.10678	4.40791	-0.03685
C	2.36075	3.45291	-2.52778
H	1.7861	2.91678	-3.28694
H	1.93134	4.45347	-2.40483
H	3.38584	3.56612	-2.89664
C	0.53744	3.45957	0.49604
H	0.52122	4.47156	0.07591
H	-0.46834	3.2239	0.85184
H	1.21505	3.44737	1.35342
C	-0.15978	2.28288	-1.60568
H	-1.06082	1.92016	-1.10266
H	-0.39792	3.23245	-2.09599
H	0.1185	1.55146	-2.37154
C	2.5009	-0.99295	-0.3546
C	1.40751	-1.87318	-0.25525
C	3.8083	-1.53287	-0.26471
C	1.58818	-3.24619	-0.08922
H	0.38903	-1.48813	-0.31396
C	3.98144	-2.91653	-0.08526
C	2.88383	-3.76867	-0.00246
H	0.71977	-3.89913	-0.03288
H	4.99172	-3.30722	-0.01118
H	3.03623	-4.83706	0.12939
C	4.98972	-0.64169	-0.32329
H	4.7639	0.41603	-0.46835
N	6.18162	-1.08407	-0.21298
C	7.33938	-0.17464	-0.26868
C	8.07679	-0.34412	1.074
H	9.01082	0.23017	1.07747
H	7.45289	0.00938	1.90377
H	8.31641	-1.39809	1.25349
C	8.22854	-0.69068	-1.41674
H	7.71672	-0.58169	-2.3804
H	9.16849	-0.12772	-1.4608
H	8.46384	-1.75138	-1.27495
C	7.01616	1.31326	-0.49566
H	7.94738	1.88913	-0.53371
H	6.48716	1.47295	-1.44271
H	6.40357	1.72561	0.31499

Thermal correction to Energy=0.761579

Thermal correction to Enthalpy=0.762729

Thermal correction to Gibbs Free Energy=0.596998

Sum of electronic and zero-point Energies=-1726.937878

Sum of electronic and thermal Energies=-1726.878222

Sum of electronic and thermal Enthalpies=-1726.877072

Sum of electronic and thermal Free Energies=-1727.042804

SCF Done: E(RM11L) = -1727.76233337

TS8'

Number of Negative Frequencies =1

Ir	0.31592	-0.98888	-0.1015
B	-1.95237	-0.307	-1.00216
B	-2.01438	-0.63414	0.81763
H	2.36675	-3.25946	-0.4186
C	4.38584	-2.47712	-0.33226
C	4.47175	-0.08552	0.01052
C	3.06105	-0.07856	0.02151
C	2.33159	1.13581	0.20133
C	3.00357	2.36233	0.38955
C	0.83967	3.41831	0.56108
C	0.26453	2.14695	0.36001
H	-0.81043	2.03235	0.34192
N	2.31833	-1.22543	-0.13534
N	0.96743	1.02578	0.18428
O	-2.53205	-1.16995	-1.90568
O	-2.17273	1.01715	-1.32089
C	5.13684	1.1756	0.19457
C	4.44005	2.33668	0.37681
H	6.2207	1.20422	0.19151
H	4.9852	3.26428	0.51352
C	5.15567	-1.32087	-0.17725
C	2.23101	3.54403	0.58044
C	-3.34968	-0.3709	-2.81542
C	-2.70527	1.05547	-2.67829
H	-0.00983	-2.57986	-0.31998
C	-3.22418	0.18359	2.58314
C	2.98278	-2.37746	-0.30218
O	-2.76802	-1.70433	1.241
O	-2.14587	0.46532	1.64158
C	-3.26367	-1.38782	2.57864
C	4.99536	-3.84366	-0.53511
H	5.65905	-4.11501	0.29407
H	4.21835	-4.61068	-0.6046
H	5.58863	-3.88476	-1.45663
C	6.66123	-1.34858	-0.19958
H	7.07269	-0.98854	0.75178
H	7.05552	-2.35045	-0.37402

H	7.05325	-0.69305	-0.9869
C	2.92055	4.86695	0.79118
H	3.52932	5.13594	-0.08154
H	2.21364	5.67956	0.96519
H	3.59836	4.82421	1.65264
C	-0.09022	4.59356	0.7469
H	0.06338	5.08147	1.71702
H	0.06115	5.35482	-0.02804
H	-1.1353	4.2724	0.69843
C	-4.78435	-0.44065	-2.28244
H	-5.48212	0.09196	-2.93697
H	-5.0932	-1.48939	-2.22715
C	-3.2701	-0.98079	-4.20963
H	-3.73755	-1.97125	-4.20791
H	-3.80405	-0.35427	-4.93321
H	-2.23541	-1.09514	-4.54082
C	-1.50938	1.27489	-3.6116
H	-1.82792	1.37246	-4.65473
H	-0.99583	2.1969	-3.31931
H	-0.79235	0.45118	-3.5357
C	-3.68384	2.21972	-2.77916
H	-3.14471	3.16697	-2.66892
H	-4.18004	2.22262	-3.75602
H	-4.44698	2.17255	-1.9984
C	-4.65234	-1.99577	2.73808
H	-4.5831	-3.08864	2.71642
H	-5.09066	-1.70163	3.69829
H	-5.3255	-1.68392	1.93569
C	-2.28275	-2.02092	3.57075
H	-2.61116	-1.87469	4.60514
H	-2.2245	-3.09662	3.3758
H	-1.27804	-1.6023	3.45442
C	-2.87749	0.81714	3.9254
H	-2.86907	1.90834	3.82865
H	-3.62321	0.54832	4.68199
H	-1.89247	0.50129	4.27723
C	-4.48694	0.82507	1.99805
H	-5.34217	0.71885	2.67339
H	-4.30253	1.89231	1.83717
H	-4.74527	0.37787	1.03297
H	-4.853	-0.01481	-1.27626

Thermal correction to Energy=0.713859

Thermal correction to Enthalpy=0.715009

Thermal correction to Gibbs Free Energy=0.567111

Sum of electronic and zero-point Energies=-1655.893615

Sum of electronic and thermal Energies=-1655.839028

Sum of electronic and thermal Enthalpies=-1655.837878

Sum of electronic and thermal Free Energies=-1655.985776

SCF Done: E(RM11L) = -1656.66241202

9'

Number of Negative Frequencies =0

Ir	0.22186	-0.35276	-1.16574
B	2.22096	0.01433	-1.03191
H	0.61014	-1.68269	-2.01958
C	-2.77679	-1.44163	-1.82613
C	-4.18432	-1.49777	-1.75873
C	-4.08036	0.53089	-0.44016
C	-2.67113	0.48917	-0.56363
C	-1.85095	1.48838	0.07232
C	-2.44756	2.52617	0.82707
C	-0.22865	3.33904	1.33556
C	0.26807	2.26992	0.56452
N	-2.03589	-0.49522	-1.25833
N	-0.49637	1.37418	-0.05752
O	-0.13023	-0.95222	1.73361
O	1.09161	-2.60119	0.70738
C	-4.65776	1.60718	0.31502
C	-3.88124	2.55515	0.91556
H	-5.73574	1.66543	0.41451
H	-4.35902	3.34781	1.48025
C	-4.85572	-0.4943	-1.05705
C	-1.61012	3.48283	1.47131
C	1.13788	-2.88516	2.12808
C	-0.07609	-2.05197	2.67095
C	4.31916	0.76543	-1.69141
B	0.44661	-1.37482	0.52538
H	1.33673	2.11362	0.4719
H	-2.22705	-2.20904	-2.36217
C	4.3198	0.51402	-0.1448
O	2.90491	0.40093	0.1408
O	3.12308	0.06676	-2.11096
C	-4.89469	-2.64056	-2.44279
H	-4.178	-3.30248	-2.93849
H	-5.46558	-3.24415	-1.72696
H	-5.59916	-2.28218	-3.20271
C	-6.35736	-0.47417	-0.93241
H	-6.66282	-0.50672	0.12065

H	-6.77341	0.44689	-1.35903
H	-6.8266	-1.31749	-1.44049
C	-2.22439	4.59886	2.27615
H	-2.8793	5.21835	1.65077
H	-2.84034	4.20099	3.09198
H	-1.47122	5.2532	2.71687
C	0.76438	4.27468	1.98207
H	0.64565	5.30326	1.62041
H	0.64656	4.29561	3.07182
H	1.79031	3.96191	1.7649
C	4.97527	-0.81687	0.24481
H	4.78922	-1.01097	1.3052
H	4.54915	-1.64475	-0.33061
H	6.05892	-0.7977	0.08411
C	4.90268	1.64724	0.69551
H	4.84276	1.38855	1.75887
H	5.95731	1.81648	0.44791
H	4.35769	2.5834	0.54705
C	4.13032	2.2448	-2.05592
H	5.02316	2.83958	-1.83352
H	3.92436	2.32314	-3.12891
H	3.28009	2.67576	-1.51607
C	5.51829	0.1922	-2.44107
H	5.43389	0.42081	-3.50962
H	6.45375	0.63062	-2.07382
H	5.57539	-0.89383	-2.33413
C	1.02723	-4.39247	2.33582
H	1.91348	-4.89078	1.92698
H	0.96568	-4.6344	3.40355
H	0.14846	-4.80485	1.83325
C	-1.41272	-2.79882	2.56212
H	-1.48517	-3.61909	3.28471
H	-2.2298	-2.09532	2.7565
H	-1.55057	-3.20649	1.55491
C	0.10148	-1.49355	4.07965
H	-0.78983	-0.9251	4.36923
H	0.23772	-2.30266	4.80686
H	0.96226	-0.82236	4.13892
C	2.48879	-2.37673	2.64586
H	3.29004	-2.87267	2.08883
H	2.58441	-1.29951	2.48273
H	2.62508	-2.59363	3.71131

Thermal correction to Energy=0.714457

Thermal correction to Enthalpy=0.715607

Thermal correction to Gibbs Free Energy=0.561717

Sum of electronic and zero-point Energies=-1655.968212

Sum of electronic and thermal Energies=-1655.912174

Sum of electronic and thermal Enthalpies=-1655.911024

Sum of electronic and thermal Free Energies=-1656.064914

SCF Done: E(RM11L) = -1656.72343530

TS10'

Number of Negative Frequencies =1

Ir	0.39229	0.82935	-0.38493
H	1.05302	0.03662	-1.62625
C	-0.13093	2.10803	-3.20959
C	-0.54504	3.07176	-4.14845
C	-1.25639	4.42889	-2.27978
C	-0.81804	3.3948	-1.42144
C	-0.95681	3.50215	-0.00017
C	-1.51774	4.66755	0.57177
N	-0.25686	2.24418	-1.88699
C	-1.81173	5.60472	-1.67155
C	-1.93179	5.71749	-0.31702
H	-2.14118	6.42224	-2.30265
H	-2.36127	6.62054	0.10157
C	-1.12536	4.25648	-3.68746
C	2.36545	-3.0306	-0.99889
B	1.05911	-1.13846	-0.6492
H	0.32552	1.18511	-3.54911
C	0.83991	-3.37777	-1.19575
O	0.17353	-2.2203	-0.62791
O	2.3522	-1.58677	-0.95426
C	0.41953	-3.4512	-2.66927
H	0.84197	-4.32738	-3.17313
H	-0.67243	-3.51629	-2.72392
H	0.73015	-2.55246	-3.21253
C	0.36405	-4.62334	-0.45366
H	-0.70503	-4.77878	-0.6369
H	0.90076	-5.5136	-0.8013
H	0.50972	-4.52704	0.62506
C	2.9421	-3.52645	0.33072
H	3.00984	-4.61917	0.36534
H	3.94695	-3.11181	0.46107
H	2.33409	-3.18021	1.16668
C	3.27367	-3.46761	-2.14765
H	4.30621	-3.17056	-1.93258

H	3.25399	-4.55667	-2.27113
H	2.98128	-3.00401	-3.09316
C	-0.72363	2.52079	2.07229
C	-1.65528	4.74813	1.98608
C	-1.26126	3.64035	2.73615
H	-0.43776	1.64702	2.64
N	-0.5437	2.43208	0.75121
C	-1.37002	3.59329	4.24123
H	-0.71473	4.33634	4.7124
H	-2.39219	3.7977	4.5794
H	-1.08228	2.60932	4.62197
C	-2.2247	5.98777	2.62455
H	-1.72563	6.88956	2.25256
H	-3.29285	6.09129	2.39221
H	-2.12177	5.97551	3.71051
C	-0.33044	2.78278	-5.61453
H	0.17819	1.82388	-5.75306
H	-1.28102	2.73783	-6.15982
H	0.28152	3.55885	-6.08884
C	-1.59751	5.33461	-4.62828
H	-2.62572	5.63725	-4.3989
H	-0.96995	6.23121	-4.54132
H	-1.57402	5.01134	-5.66994
C	2.16489	-0.52675	3.33011
C	0.68493	-1.01757	3.528
B	0.96101	-0.12268	1.38898
O	0.01606	-0.43406	2.38083
O	2.24413	-0.33273	1.89561
C	0.0067	-0.52045	4.80312
H	-1.03245	-0.86682	4.82656
H	0.5157	-0.91334	5.69097
H	-0.00252	0.56989	4.8673
C	2.44009	0.83782	3.97728
H	2.44594	0.7776	5.07108
H	3.42073	1.19641	3.64675
H	1.69467	1.5793	3.67104
C	0.51192	-2.53668	3.4227
H	0.97533	-3.05963	4.26609
H	-0.55775	-2.77212	3.41636
H	0.93793	-2.91912	2.49262
C	3.23692	-1.52589	3.75535
H	4.23015	-1.11131	3.55058
H	3.17061	-1.73158	4.8302
H	3.14972	-2.46996	3.21387

Thermal correction to Energy= 0.714496

Thermal correction to Enthalpy=0.715646

Thermal correction to Gibbs Free Energy=0.567206

Sum of electronic and zero-point Energies= -1655.933823

Sum of electronic and thermal Energies=-1655.878847

Sum of electronic and thermal Enthalpies=-1655.877697

Sum of electronic and thermal Free Energies= -1656.025693

SCF Done: E(RM11L) = -1656.68761988

2a'

Number of Negative Frequencies =0

Ir	-0.69921	-0.19664	-0.03912
B	0.7682	1.23353	-0.12337
O	1.70676	1.35906	-1.16779
O	0.98888	2.28582	0.79528
C	-4.66164	1.30695	0.05662
C	-3.25109	3.23788	0.30518
C	-2.14423	2.37941	0.25287
H	-1.1457	2.77522	0.36199
C	-4.86611	-1.55605	-0.15132
N	-2.4304	-1.61063	-0.09996
N	-2.21866	1.03878	0.08823
C	-3.60477	-0.918	-0.08414
C	-3.49859	0.50282	0.01735
C	-6.03255	-0.72111	-0.12547
C	-5.93159	0.63636	-0.02697
H	-7.01437	-1.1778	-0.18256
H	-6.8379	1.23134	-0.00542
C	-4.91447	-2.97606	-0.23856
C	-4.54322	2.71721	0.18739
C	2.69227	2.36221	-0.82329
C	1.92881	3.23354	0.23429
C	-3.70256	-3.67239	-0.25782
C	3.9067	1.6295	-0.24139
H	3.64199	1.067	0.65871
H	4.27437	0.91407	-0.98217
H	4.72082	2.32073	0.00225
C	3.10189	3.10394	-2.09424
H	3.78518	3.92992	-1.86342
H	3.62008	2.41698	-2.77313
H	2.2347	3.50681	-2.62378
C	1.11056	4.36916	-0.39661
H	0.47465	4.82039	0.37305
H	1.75285	5.15493	-0.80966

H	0.46231	3.994	-1.19544
C	2.79843	3.78965	1.35925
H	3.57597	4.45382	0.96314
H	2.18042	4.37026	2.05382
H	3.27954	2.98954	1.92724
C	-3.62259	-5.17706	-0.35235
H	-4.09999	-5.54893	-1.26687
H	-2.58042	-5.51122	-0.36185
H	-4.12032	-5.66329	0.49536
C	-6.2458	-3.67934	-0.30464
H	-6.85879	-3.44284	0.57405
H	-6.81456	-3.36089	-1.18732
H	-6.13901	-4.76397	-0.35191
C	-5.77321	3.58811	0.21291
H	-6.3914	3.42523	-0.6786
H	-6.40222	3.36379	1.0846
H	-5.52476	4.64994	0.25131
C	-2.98334	4.71368	0.48727
H	-3.35894	5.29781	-0.36158
H	-3.47002	5.10046	1.39058
H	-1.91055	4.90824	0.57527
C	-2.50226	-2.93785	-0.18848
H	-1.55521	-3.46739	-0.20462
C	1.94968	-2.20839	2.02245
C	3.22633	-1.89503	1.57132
C	0.97603	-2.67154	1.12309
C	3.55489	-2.03187	0.20908
C	1.28775	-2.79124	-0.2373
H	-0.0097	-2.94597	1.48615
C	2.57204	-2.46942	-0.68862
H	0.54659	-3.15493	-0.94298
H	2.81598	-2.56898	-1.74391
H	1.70495	-2.10523	3.07608
C	4.91048	-1.73393	-0.29501
H	5.03851	-1.88618	-1.37412
N	5.84539	-1.33276	0.47274
C	7.19896	-1.04426	-0.02979
C	8.14398	-1.98302	0.74579
H	8.01195	-1.85705	1.82616
H	7.93764	-3.0309	0.4973
H	9.18971	-1.76887	0.49572
C	7.49597	0.41829	0.35462
H	7.31706	0.58012	1.42327
H	8.54064	0.66795	0.13406
H	6.853	1.10485	-0.20701
C	7.40928	-1.2327	-1.54153
H	8.44424	-0.98488	-1.80198
H	7.22871	-2.26873	-1.85231
H	6.75425	-0.57784	-2.12861
H	3.99047	-1.54713	2.2594

Thermal correction to Energy=0.764554

Thermal correction to Enthalpy=0.765704

Thermal correction to Gibbs Free Energy=0.603837

Sum of electronic and zero-point Energies=-1726.937400

Sum of electronic and thermal Energies=-1726.878187

Sum of electronic and thermal Enthalpies=-1726.877037

Sum of electronic and thermal Free Energies=-1727.038904

SCF Done: E(RM11L) = -1727.75617711

TS3a'

Number of Negative Frequencies =1

B	0.17386	2.04673	-0.37942
C	-4.6426	-0.30185	0.73269
C	-5.1725	1.01697	0.82255
C	-4.33204	2.07654	0.48047
C	-3.00829	1.79997	0.09445
C	1.62366	3.78166	0.16475
C	0.22052	4.36868	-0.21646
N	-2.48343	0.5714	0.00409
O	1.3166	2.3797	0.36573
O	-0.41573	3.23173	-0.8575
C	1.37005	-0.70411	-1.16821
C	1.4653	-1.76399	-2.10157
C	2.61185	-2.56123	-2.1845
H	2.64472	-3.38171	-2.89786
C	3.71019	-2.30646	-1.36802
H	4.60721	-2.91545	-1.42389
C	3.67205	-1.21904	-0.47619
C	2.52388	-0.4181	-0.4039
C	-0.62822	4.73424	1.00805
H	-1.65095	4.95609	0.68418
H	-0.6697	3.90319	1.71983
H	-0.23643	5.61769	1.52338
C	0.25234	5.53453	-1.19978
H	-0.76949	5.86637	-1.41598
H	0.80248	6.38398	-0.77841
H	0.71999	5.25002	-2.14556
C	2.23459	4.34203	1.44532
H	3.20141	3.86217	1.63506

H	2.40507	5.42132	1.35657
H	1.59333	4.15984	2.31144
C	2.64067	3.85782	-0.98143
H	2.9749	4.88495	-1.16399
H	3.51584	3.25249	-0.72163
H	2.2188	3.45662	-1.90896
H	0.62183	-1.96775	-2.75673
H	0.70811	0.33546	-1.72885
C	-6.59531	1.23167	1.26769
H	-6.75213	0.84181	2.28118
H	-6.87134	2.28683	1.27115
H	-7.29623	0.70465	0.60868
C	4.8259	-0.87558	0.37621
H	4.67308	0.00955	1.0115
C	7.03445	-1.12675	1.24562
Ir	-0.50138	0.14246	-0.62528
C	-3.30544	-0.48427	0.3059
C	-2.7668	-1.80887	0.16571
C	-5.40963	-1.47145	1.06004
C	-4.88562	-2.72708	0.96072
C	-3.54179	-2.94325	0.50606
C	-2.95842	-4.23768	0.38036
C	-1.64119	-4.32101	-0.07277
C	-0.96388	-3.12631	-0.3927
N	-1.49263	-1.91125	-0.29993
H	-5.49951	-3.58019	1.22678
H	-2.34071	2.61133	-0.16433
C	-0.90788	-5.6299	-0.23871
H	0.1082	-5.46209	-0.60907
H	-0.83088	-6.17297	0.71077
H	-1.41838	-6.28938	-0.95088
C	-3.75865	-5.46065	0.74625
H	-4.67027	-5.52938	0.14004
H	-3.19333	-6.38234	0.6032
H	-4.07367	-5.42038	1.79631
H	0.06115	-3.17006	-0.74402
H	2.5121	0.44423	0.25481
N	5.91118	-1.54661	0.37113
C	6.60051	-1.06761	2.72269
H	6.17284	-2.02732	3.03606
H	7.46247	-0.85051	3.36453
H	5.85076	-0.2877	2.89631
C	8.1303	-2.19153	1.07501
H	9.01214	-1.95168	1.68102
H	7.76021	-3.1775	1.38062
H	8.4396	-2.25887	0.02533
C	7.56794	0.24316	0.78584
H	7.84453	0.21252	-0.27469
H	6.8152	1.02876	0.91777
H	8.45612	0.52449	1.36402
C	-4.77159	3.52082	0.51728
H	-5.62081	3.69929	-0.15282
H	-5.08073	3.82308	1.52503
H	-3.95719	4.18217	0.20634
H	-6.43187	-1.35093	1.40001

Thermal correction to Energy= 0.759422

Thermal correction to Enthalpy= 0.760572

Thermal correction to Gibbs Free Energy= 0.598654

Sum of electronic and zero-point Energies= -1726.938636

Sum of electronic and thermal Energies= -1726.879599

Sum of electronic and thermal Enthalpies= -1726.878449

Sum of electronic and thermal Free Energies= -1727.040366

SCF Done: E(RM11L) = -1727.74969915

4a'

Number of Negative Frequencies =0

Ir	-0.73884	-1.72224	-0.30824
B	1.15494	-2.4027	0.02782
C	-2.2609	1.505	2.35373
C	-0.16141	0.84753	3.35405
C	-0.06147	-0.12554	2.34149
H	0.79923	-0.78413	2.29475
C	-4.21618	1.12444	0.28701
N	-2.85392	-0.69437	-0.55916
N	-0.96426	-0.30975	1.37892
O	1.79904	-2.35609	1.28383
O	2.05603	-2.90082	-0.91886
C	-3.06657	0.29791	0.34465
C	-2.07263	0.49429	1.37691
C	-4.3689	2.14189	1.28705
C	-3.4408	2.31931	2.26983
H	-5.24094	2.78559	1.26078
H	-3.59502	3.10069	3.0051
C	-5.16657	0.91244	-0.75532
C	-1.27467	1.68646	3.36697
C	3.24977	-3.37206	-0.24833
C	3.22278	-2.55527	1.08888
H	-0.73027	-2.72831	-1.57526

C	-4.92265	-0.10851	-1.67499
C	4.45796	-3.10452	-1.14157
H	5.3898	-3.36733	-0.627
H	4.38996	-3.71312	-2.05026
H	4.50867	-2.05572	-1.44477
C	3.07939	-4.88107	-0.0307
H	2.22071	-5.08873	0.61644
H	2.89844	-5.36175	-0.99808
H	3.97179	-5.33331	0.4159
C	3.79349	-3.2738	2.30757
H	4.85496	-3.50552	2.16127
H	3.70719	-2.63015	3.19075
H	3.25908	-4.20399	2.51713
C	3.86085	-1.16621	0.9517
H	4.95114	-1.22886	0.86754
H	3.47265	-0.64066	0.0745
H	3.62061	-0.57026	1.83944
C	-5.85052	-0.42433	-2.82296
H	-5.95591	0.43121	-3.50079
H	-5.47095	-1.26749	-3.40834
H	-6.85476	-0.68768	-2.4703
C	-6.38831	1.78966	-0.84282
H	-6.97933	1.73268	0.07931
H	-6.10375	2.84036	-0.97935
H	-7.03898	1.51144	-1.67272
C	-1.45048	2.7639	4.40565
H	-1.47205	3.75652	3.93863
H	-2.39844	2.64102	4.94326
H	-0.64707	2.76015	5.14347
C	0.95648	0.94492	4.36389
H	1.42488	1.93624	4.35011
H	0.59658	0.76841	5.38462
H	1.7355	0.20551	4.15358
C	-3.75062	-0.8773	-1.52117
H	-3.53171	-1.67703	-2.22238
C	1.02422	0.63088	-0.91597
C	0.07835	-0.28165	-1.43247
C	-0.32195	-0.07226	-2.77062
C	0.18789	0.98721	-3.53444
C	1.1183	1.87347	-2.99949
C	1.54418	1.69252	-1.67268
H	-1.04058	-0.74853	-3.22573
H	-0.14752	1.1115	-4.5625
H	1.52202	2.69383	-3.58492
C	2.53171	2.5864	-1.03771
H	2.77547	2.32563	0.00117
N	3.05699	3.57656	-1.64658
C	4.03976	4.45886	-0.99589
C	4.41736	4.0968	0.45085
H	3.54983	4.13326	1.12074
H	4.85972	3.09544	0.51682
H	5.15676	4.81175	0.82861
C	5.29963	4.41734	-1.88285
H	5.73968	3.41296	-1.88185
H	5.05054	4.67793	-2.91756
H	6.05431	5.12421	-1.51784
C	3.42924	5.87373	-1.03314
H	2.52331	5.92089	-0.41669
H	4.14328	6.6141	-0.65315
H	3.15653	6.14766	-2.05845
H	1.37783	0.51317	0.10475

Thermal correction to Energy=0.760782

Thermal correction to Enthalpy=0.761932

Thermal correction to Gibbs Free Energy=0.599009

Sum of electronic and zero-point Energies=-1726.978530

Sum of electronic and thermal Energies=-1726.919083

Sum of electronic and thermal Enthalpies=-1726.917933

Sum of electronic and thermal Free Energies=-1727.080856

SCF Done: E(RM11L) = -1727.78521344

TS5a'

Number of Negative Frequencies =1

Ir	0.24336	0.26635	0.55529
B	1.03778	-1.38066	-0.61011
C	-4.12675	-0.21922	0.66629
C	-3.39487	-2.44767	1.23161
C	-2.0732	-1.97583	1.10217
H	-1.25156	-2.66834	1.22105
C	-3.38383	2.43367	-0.16128
N	-1.05577	1.72264	0.01949
N	-1.73961	-0.72368	0.79618
O	0.20119	-2.52808	-0.72736
O	1.63164	-1.11684	-1.87055
C	-2.39992	1.46538	0.14063
C	-2.76455	0.14672	0.55575
C	-4.75937	2.04609	-0.00885
C	-5.11182	0.78692	0.38343
H	-5.53722	2.77101	-0.22053

H	-6.16319	0.53687	0.47329
C	-2.97822	3.72226	-0.60854
C	-4.45079	-1.55593	1.03229
C	0.8788	-1.83937	-2.8637
C	0.36053	-3.07715	-2.04684
H	1.50008	1.22511	0.28705
C	-1.60637	3.96462	-0.73409
C	1.80504	-2.17854	-4.02892
H	1.29258	-2.8078	-4.76614
H	2.12168	-1.25765	-4.53144
H	2.70375	-2.69955	-3.68822
C	-0.2582	-0.92443	-3.34233
H	-0.92486	-0.6703	-2.51258
H	0.17447	0.00834	-3.72012
H	-0.84326	-1.38513	-4.14596
C	-0.98141	-3.63985	-2.50978
H	-0.92491	-3.99048	-3.54705
H	-1.26402	-4.49147	-1.8798
H	-1.77418	-2.89097	-2.43504
C	1.40229	-4.20075	-1.95102
H	1.53358	-4.72501	-2.90424
H	2.3717	-3.80381	-1.63236
H	1.07086	-4.92841	-1.20192
C	-1.05059	5.28418	-1.21414
H	-1.35608	6.1109	-0.56186
H	0.04316	5.26234	-1.23535
H	-1.39973	5.51959	-2.22658
C	-4.01242	4.76648	-0.93812
H	-4.67416	4.42447	-1.744
H	-4.64859	4.97832	-0.06962
H	-3.56211	5.70774	-1.2559
C	-5.8924	-1.9729	1.16757
H	-6.42197	-1.32884	1.87986
H	-6.4167	-1.88885	0.20708
H	-5.99404	-3.00286	1.51252
C	-3.60448	-3.90268	1.57545
H	-4.14402	-4.0213	2.52283
H	-4.18621	-4.41795	0.80176
H	-2.64558	-4.42117	1.67203
C	-0.69683	2.94577	-0.40818
H	0.36757	3.11543	-0.50169
C	1.47655	-1.89745	1.95267
C	1.95294	-1.28029	0.77439
C	3.31397	-0.82497	0.78884
C	4.12279	-1.07554	1.89437
C	3.60148	-1.66017	3.0588
C	2.27014	-2.0503	3.10039
H	1.85451	-2.51047	3.99311
H	4.24812	-1.8138	3.91922
H	0.48377	-2.32801	1.95726
C	5.61082	-0.68206	1.84389
H	6.1931	-1.42317	2.35046
N	5.79595	0.61988	2.50082
C	7.21683	0.99399	2.45545
C	7.9707	0.2862	3.59664
H	8.14448	-0.73527	3.32962
H	8.90752	0.77578	3.76272
H	7.3839	0.32633	4.49048
C	7.35157	2.51926	2.61971
H	7.55107	2.96431	1.66733
H	6.44061	2.91721	3.01556
H	8.15663	2.73603	3.29037
C	7.81675	0.56841	1.10246
H	7.21183	-0.20116	0.67033
H	7.84552	1.41139	0.44409
H	8.80974	0.1993	1.25289
H	3.76281	-0.38861	-0.07893

Thermal correction to Energy=0.759931

Thermal correction to Enthalpy=0.761081

Thermal correction to Gibbs Free Energy=0.602907

Sum of electronic and zero-point Energies=-1726.951996

Sum of electronic and thermal Energies=-1726.893746

Sum of electronic and thermal Enthalpies=-1726.892596

Sum of electronic and thermal Free Energies=-1727.050770

SCF Done: E(RM11L) = -1727.76592465

6a'

Number of Negative Frequencies =0

C	-1.06831	3.14216	0.91182
H	-0.02336	3.33373	1.11288
C	-2.0535	4.03854	1.35194
C	-3.70686	2.59202	0.36573
C	-2.66061	1.73881	-0.04267
C	-2.92439	0.53757	-0.75836
C	-4.24733	0.1536	-1.0892
C	-3.3004	-1.81107	-2.12901
C	-2.03288	-1.34152	-1.74915
H	-1.15487	-1.93135	-1.97146

N	-1.32761	2.00338	0.22932
N	-1.82119	-0.20279	-1.08391
C	-5.04361	2.18934	0.01889
C	-5.30068	1.03769	-0.66825
H	-5.87322	2.82211	0.31445
H	-6.32954	0.78849	-0.90068
C	-3.40367	3.7788	1.08547
C	-4.43921	-1.06341	-1.80063
Ir	-0.01538	0.70263	-0.37761
O	-0.24103	-3.10858	0.3057
H	1.28618	1.53247	0.19384
C	-3.40106	-3.12198	-2.86629
H	-3.89951	-3.00076	-3.83612
H	-2.41085	-3.55172	-3.04655
H	-3.98668	-3.85543	-2.29689
C	-5.79635	-1.57064	-2.21293
H	-5.96786	-2.58132	-1.82186
H	-6.61767	-0.93995	-1.87081
H	-5.86427	-1.64234	-3.30628
C	-4.51099	4.69964	1.52998
H	-5.09464	5.05997	0.67323
H	-5.2111	4.18351	2.19946
H	-4.1319	5.57424	2.0608
C	-1.59898	5.26365	2.11069
H	-1.89796	6.18656	1.5994
H	-2.03139	5.29367	3.11807
H	-0.51	5.27816	2.21528
B	0.85844	-2.37208	0.67703
O	1.0145	-2.26962	2.03833
C	-1.0253	-3.3461	1.5182
C	0.05806	-3.18446	2.65047
C	0.82011	-4.48071	2.94699
H	1.19659	-4.93897	2.02638
H	1.6787	-4.25223	3.58689
H	0.18764	-5.20871	3.46569
C	-0.44872	-2.5587	3.94475
H	-0.84181	-1.55323	3.77709
H	-1.23683	-3.17647	4.38956
H	0.37305	-2.48616	4.66545
C	-1.65137	-4.73255	1.41558
H	-2.18576	-4.98393	2.33864
H	-2.37299	-4.74762	0.59121
H	-0.90241	-5.50468	1.22316
C	-2.11923	-2.27522	1.58001
H	-2.75597	-2.35736	0.6951
H	-2.74604	-2.40804	2.46776
H	-1.68859	-1.26924	1.59141
C	1.88823	-1.76219	-0.32192
C	1.65888	-1.72667	-1.71136
C	3.0705	-1.16524	0.162
C	2.56893	-1.10522	-2.57842
H	0.77861	-2.20817	-2.12285
C	3.9921	-0.55286	-0.69246
C	3.72639	-0.52215	-2.07487
H	2.37107	-1.08577	-3.647
H	4.43809	-0.03559	-2.73481
C	5.19793	0.07936	-0.11998
H	5.27238	0.01066	0.97256
N	6.06476	0.66612	-0.84718
C	7.25054	1.32238	-0.27128
C	7.17551	2.79352	-0.72529
H	6.30486	3.29085	-0.28156
H	8.07652	3.33846	-0.41956
H	7.08418	2.85619	-1.81532
C	8.47146	0.64266	-0.92172
H	8.53863	-0.4082	-0.61579
H	8.39421	0.67489	-2.01426
H	9.3978	1.14761	-0.6236
C	7.37634	1.25966	1.25987
H	8.28605	1.78261	1.57521
H	6.52672	1.74179	1.75774
H	7.44604	0.22647	1.6205
H	3.26096	-1.17112	1.23269

Thermal correction to Energy= 0.762239

Thermal correction to Enthalpy=0.763389

Thermal correction to Gibbs Free Energy= 0.602959

Sum of electronic and zero-point Energies= -1726.948162

Sum of electronic and thermal Energies= -1726.889258

Sum of electronic and thermal Enthalpies= -1726.888108

Sum of electronic and thermal Free Energies= -1727.048538

SCF Done: E(RM11L) = -1727.77260169

3'

Number of Negative Frequencies =0

B	-0.29753	0.01209	1.32093
B	-1.55035	-1.38087	-0.72264
B	-1.56175	1.35225	-0.7201

C	1.79033	2.68045	-0.72271	H	-1.53373	4.45486	1.03235
H	0.80327	3.13117	-0.77065	H	-3.29795	4.43063	1.22963
C	2.95187	3.48101	-0.70104	H	-2.33613	2.94984	1.51102
C	4.22512	1.42535	-0.59824	C	-4.23828	-2.87492	-2.54829
C	3.00041	0.71468	-0.62227	H	-3.95659	-2.9486	-3.60514
C	2.99601	-0.72855	-0.56811	H	-4.92105	-3.70239	-2.3212
C	4.21508	-1.44453	-0.48593	H	-4.77222	-1.93156	-2.40843
C	2.926	-3.49288	-0.42411	C	-2.14622	-4.16717	-2.04729
C	1.77441	-2.6848	-0.5158	H	-2.71034	-5.10115	-1.94694
H	0.78982	-3.14229	-0.51885	H	-1.82165	-4.07289	-3.08948
N	1.79886	1.35151	-0.68775	H	-1.25098	-4.23204	-1.41923
N	1.79083	-1.35914	-0.58955	C	-4.45304	-1.93236	0.21036
O	-1.24656	0.71576	2.07019	H	-5.40779	-2.39083	-0.07141
O	0.57601	-0.66952	2.1844	H	-4.46212	-1.75616	1.292
O	-2.18089	-1.76826	-1.92305	H	-4.3517	-0.96154	-0.28267
O	-2.07127	-2.15014	0.33236	C	-3.37496	-4.16861	0.59873
O	-1.3358	2.73536	-0.92234	H	-3.5605	-3.99526	1.66485
O	-2.94205	1.15015	-0.58046	H	-4.20892	-4.76022	0.20268
C	5.44423	0.66928	-0.52876	H	-2.45696	-4.75536	0.5095
C	5.4396	-0.69423	-0.47366	C	-2.14197	0.61408	4.30917
H	6.39211	1.19546	-0.51367	H	-1.90434	0.48292	5.37152
H	6.38388	-1.22389	-0.41648	H	-2.69237	1.55537	4.19885
C	4.19538	2.85048	-0.64318	H	-2.80084	-0.19878	3.9938
C	4.17428	-2.86808	-0.41278	C	-0.07511	1.93412	3.76961
C	0.00699	-0.64094	3.51539	H	-0.6903	2.80544	3.52074
C	-0.87166	0.65817	3.46481	H	0.20506	2.00028	4.82669
C	-3.64732	2.3776	-0.8562	H	0.83462	1.97948	3.16124
C	-2.54425	3.45851	-0.58907	C	1.14045	-0.61377	4.53603
C	-2.98993	-2.94054	-1.67246	H	0.74778	-0.50156	5.55363
C	-3.25771	-2.83277	-0.13032	H	1.70171	-1.55418	4.49255
Ir	-0.05406	-0.01903	-0.6519	H	1.8392	0.20364	4.33912
C	-4.0952	2.32123	-2.32326	C	-0.82516	-1.92028	3.67512
H	-4.69522	1.41731	-2.47434	H	-0.17181	-2.78721	3.52491
H	-4.70254	3.18937	-2.60342	H	-1.27166	-1.99717	4.67292
H	-3.23077	2.26584	-2.99329	H	-1.61285	-1.96269	2.91743
C	-4.86604	2.46197	0.05925	C	2.78902	4.98097	-0.74688
H	-5.37549	3.42682	-0.05177	H	1.72975	5.25353	-0.78471
H	-5.57949	1.67134	-0.19972	H	3.22525	5.46263	0.13649
H	-4.58678	2.33035	1.10758	H	3.277	5.41381	-1.62855
C	-2.63249	4.70754	-1.4604	C	5.48637	3.62805	-0.62424
H	-3.57554	5.24001	-1.28817	H	6.06139	3.41212	0.2848
H	-1.8107	5.39026	-1.21438	H	6.12032	3.35642	-1.47757
H	-2.5594	4.46433	-2.5237	H	5.3203	4.70542	-0.66348
C	-2.43459	3.84625	0.89226	C	5.45856	-3.65147	-0.32216

H	6.10473	-3.44573	-1.18434
H	6.02395	-3.37461	0.57647
H	5.28474	-4.72772	-0.28665
C	2.75245	-4.98984	-0.34153
H	3.24637	-5.50131	-1.17644
H	3.1771	-5.39328	0.58553
H	1.69197	-5.25938	-0.36603

Thermal correction to Energy=0.904060

Thermal correction to Enthalpy=0.905210

Thermal correction to Gibbs Free Energy=0.720567

Sum of electronic and zero-point Energies=-2066.514712

Sum of electronic and thermal Energies=-2066.443896

Sum of electronic and thermal Enthalpies=-2066.442746

Sum of electronic and thermal Free Energies=-2066.627389

SCF Done: E(RM11L) = -2067.43065742

4c'

Number of Negative Frequencies =0

Ir	-0.11503	0.22534	-0.72
H	-0.30245	-3.22654	0.70258
C	-2.23535	-3.45738	1.65248
C	-3.41743	-1.36341	1.92439
C	-2.31737	-0.71223	1.3027
C	-2.30437	0.69779	1.11973
C	-3.38131	1.49642	1.58088
C	-2.18101	3.44859	0.81
C	-1.17719	2.59485	0.36381
H	-0.28803	2.99802	-0.10276
N	-1.22195	-1.40565	0.85995
N	-1.21982	1.24571	0.46325
O	2.35819	0.65627	1.22734
O	0.47114	1.85308	1.69319
O	1.774	0.44421	-3.12415
O	2.08874	2.17869	-1.67021
O	0.69376	-2.57345	0.37383
O	2.47347	-1.57939	-0.66982
C	-4.51385	-0.54069	2.35103
C	-4.49116	0.81546	2.19325
H	-5.37381	-1.00537	2.82126
H	-5.33561	1.40019	2.54166
C	-3.37984	-2.77035	2.09038
C	-3.3348	2.90284	1.41096
C	1.54233	2.54128	2.38848
C	2.66822	1.44689	2.41006
C	2.92578	-2.90701	-0.31034
C	1.85943	-3.35206	0.76005
C	2.63079	1.39291	-3.80824
C	3.18764	2.24246	-2.61588
B	1.04723	0.89952	0.85438
B	1.37341	0.99757	-1.90354
B	1.13355	-1.45497	-0.33796
C	3.47649	3.70468	-2.93592
H	3.84769	4.21412	-2.03953
H	4.24316	3.78887	-3.71476
H	2.57807	4.22863	-3.27337
C	1.74003	2.20449	-4.75748
H	2.32291	2.90858	-5.36141
H	1.22416	1.51791	-5.43728
H	0.9819	2.76531	-4.20082
C	3.68335	0.62285	-4.59922
H	3.20223	0.05754	-5.40549
H	4.41035	1.30715	-5.05244
H	4.21895	-0.08636	-3.9634
C	4.39749	1.58956	-1.93734
H	5.29224	1.6423	-2.56733
H	4.60619	2.11297	-0.9989
H	4.18702	0.54283	-1.69814
C	1.90274	3.76661	1.53765
H	2.23092	3.46415	0.53877
H	1.01025	4.39131	1.42256
H	2.68649	4.36953	2.00919
C	1.03233	2.98001	3.75685
H	1.83473	3.44311	4.34277
H	0.23493	3.72101	3.63151
H	0.62398	2.14031	4.3251
C	4.08983	1.98152	2.2656
H	4.3499	2.62816	3.11187
H	4.79855	1.1461	2.24559
H	4.21367	2.54999	1.34121
C	2.57869	0.51874	3.6254
H	3.30093	-0.29587	3.51482
H	2.81253	1.05142	4.55329
H	1.57985	0.07989	3.71504
C	4.35645	-2.80683	0.21229
H	4.71046	-3.78027	0.57102
H	5.02072	-2.48133	-0.59613
H	4.4367	-2.08094	1.02449
C	2.89279	-3.7507	-1.59004

H	3.52294	-3.2703	-2.34607
H	3.27101	-4.76448	-1.41923
H	1.87813	-3.81729	-1.99292
C	1.48352	-4.82922	0.72784
H	2.35592	-5.45636	0.94406
H	0.72283	-5.03312	1.49002
H	1.07458	-5.12089	-0.24264
C	2.22352	-2.91601	2.18099
H	2.46144	-1.85098	2.19377
H	1.36387	-3.08302	2.83926
H	3.0752	-3.47995	2.57622
C	-2.0002	4.93294	0.5979
H	-2.05922	5.48808	1.54207
H	-1.02474	5.14497	0.14803
H	-2.76978	5.34494	-0.0678
C	-4.4867	3.76217	1.86775
H	-5.41985	3.47582	1.36481
H	-4.66276	3.65998	2.94679
H	-4.31751	4.82097	1.66298
C	-4.54057	-3.48622	2.73536
H	-4.66349	-3.17621	3.78128
H	-5.48106	-3.25745	2.21991
H	-4.41551	-4.57011	2.72393
C	-2.06967	-4.95009	1.80812
H	-2.17329	-5.26171	2.85456
H	-2.81606	-5.50546	1.22648
H	-1.08027	-5.26773	1.46494
C	-1.20142	-2.72779	1.04586
C	-1.66275	1.84096	-2.77662
C	-2.91689	2.2017	-2.27222
C	-3.72269	1.23811	-1.65509
C	-3.28246	-0.07909	-1.54233
C	-2.02234	-0.44981	-2.04271
C	-1.2169	0.52463	-2.65823
H	-1.02807	2.58579	-3.24951
H	-3.26216	3.22891	-2.3533
H	-4.69125	1.51883	-1.24992
H	-3.8994	-0.83316	-1.06416
C	-1.52882	-1.83986	-1.95556
N	-2.24511	-2.7901	-1.49293
C	-1.75558	-4.1844	-1.49745
C	-2.39961	-4.87521	-0.28301
H	-2.18194	-5.94998	-0.28445
H	-2.01467	-4.4495	0.64874
H	-3.48687	-4.73875	-0.29519
C	-0.22645	-4.33399	-1.40694
H	0.28921	-3.92581	-2.28305
H	0.15676	-3.83423	-0.5121
H	0.03678	-5.39635	-1.34422
C	-2.2772	-4.82966	-2.7969
H	-3.3649	-4.71956	-2.87632
H	-1.82102	-4.35365	-3.67321
H	-2.03567	-5.89907	-2.81909
H	-0.51361	-1.98718	-2.34435
H	-0.25417	0.25417	-3.03889

Thermal correction to Energy=1.161165

Thermal correction to Enthalpy=1.162315

Thermal correction to Gibbs Free Energy=0.937800

Sum of electronic and zero-point Energies=-2549.286081

Sum of electronic and thermal Energies=-2549.196416

Sum of electronic and thermal Enthalpies=-2549.195266

Sum of electronic and thermal Free Energies=-2549.419781

SCF Done: E(RM11L) = -2550.42842331

TS5c'

Number of Negative Frequencies =1

B	1.21395	-0.28844	1.52724
B	2.2663	0.10293	-1.12144
B	0.49456	-1.97223	-0.22222
C	-2.40489	-0.68024	1.16754
H	-2.05339	-1.67298	0.92046
C	-3.5996	-0.49531	1.89213
C	-4.02446	0.80901	2.15211
C	-3.181	1.8826	1.73986
C	-1.97198	1.57703	1.0685
C	-1.02374	2.61673	0.76223
C	-1.32851	3.9685	1.05171
C	-0.35287	4.96875	0.76853
C	0.88111	4.55739	0.26283
C	1.09145	3.18383	0.02506
H	2.04153	2.82445	-0.35503
C	2.71115	-0.49488	3.27636
C	1.24899	-0.72067	3.8011
C	4.28694	-0.62661	-1.95396
C	4.33412	0.93081	-1.78869
C	-0.3054	-4.11694	0.12692
C	1.25044	-4.14769	-0.05642
Ir	0.36597	0.09104	-0.37861
N	-1.62944	0.306	0.74339

N	0.17801	2.24395	0.24189	H	2.91473	-2.47444	2.40157
O	2.47795	0.08613	1.96621	C	1.0542	-1.96048	4.66733
O	0.50564	-0.89372	2.56872	H	1.64625	-1.89378	5.58777
O	2.86485	-0.8855	-1.90759	H	-0.00066	-2.05176	4.95006
O	3.16255	1.17077	-0.96838	H	1.33882	-2.87167	4.13555
O	-0.63291	-2.79215	-0.37516	C	0.65972	0.51371	4.49685
O	1.59947	-2.75126	0.09664	H	-0.41385	0.35817	4.65
H	0.0838	-0.63112	-1.81661	H	1.12446	0.69724	5.4717
C	-0.55766	0.82314	-2.30763	H	0.78378	1.40678	3.87502
C	0.18143	1.82977	-2.96228	C	2.00847	-4.96013	0.98867
C	-0.38283	2.64208	-3.94534	H	3.0854	-4.89346	0.79832
H	0.2165	3.42011	-4.41388	H	1.82179	-4.59106	2.00011
C	-1.71671	2.45204	-4.32601	H	1.72011	-6.0168	0.94369
H	-2.16825	3.0796	-5.09052	C	1.6816	-4.5661	-1.46731
C	-2.44996	1.43067	-3.73597	H	2.75011	-4.36036	-1.58683
H	-3.47485	1.23909	-4.0405	H	1.51029	-5.63332	-1.64507
C	-1.88558	0.59905	-2.74602	H	1.14351	-3.99138	-2.22786
C	-3.47626	3.2651	1.99232	C	-0.73543	-4.15417	1.59814
C	-2.60171	4.25718	1.65242	H	-1.81176	-3.95833	1.66104
H	-2.86177	5.2876	1.8685	H	-0.54496	-5.13204	2.05335
H	-4.4116	3.52648	2.47446	H	-0.21755	-3.38076	2.1735
C	-4.36019	-1.72131	2.3388	C	-1.07114	-5.16047	-0.67901
H	-3.82676	-2.63204	2.04947	H	-0.76247	-6.1717	-0.3887
H	-4.48579	-1.74064	3.4279	H	-2.14538	-5.068	-0.488
H	-5.36026	-1.76794	1.89316	H	-0.90629	-5.04261	-1.75321
C	-5.32014	1.09771	2.86595	C	4.12811	1.68042	-3.11009
H	-5.14297	1.63479	3.80603	H	3.95427	2.74121	-2.89727
H	-5.97222	1.72975	2.25103	H	5.00464	1.60023	-3.7622
H	-5.87038	0.18575	3.10248	H	3.25711	1.29306	-3.64771
C	2.00825	5.51469	-0.04426	C	5.56083	1.47165	-1.06061
H	2.30059	6.09114	0.84127	H	6.47892	1.22602	-1.60734
H	2.89136	4.97247	-0.39647	H	5.49646	2.56338	-0.98189
H	1.72594	6.23295	-0.82361	H	5.63682	1.06665	-0.04863
C	-0.66703	6.4188	1.03135	C	4.84824	-1.15967	-3.26724
H	-1.57437	6.72398	0.49648	H	5.91349	-0.91896	-3.3639
H	-0.84852	6.59497	2.0992	H	4.74416	-2.25026	-3.29627
H	0.14116	7.08079	0.7175	H	4.31795	-0.74883	-4.13031
C	3.54942	0.47729	4.10023	C	4.91398	-1.36848	-0.7652
H	3.6735	0.11256	5.12662	H	4.66351	-2.43116	-0.84081
H	4.54515	0.57724	3.65415	H	6.00508	-1.26715	-0.74998
H	3.09669	1.47159	4.1344	H	4.50473	-0.99689	0.17882
C	3.48257	-1.80007	3.04794	H	1.21278	2.00548	-2.67323
H	4.42646	-1.57079	2.54209	C	-2.68742	-0.53986	-2.23545
H	3.71465	-2.30712	3.99096	N	-3.93062	-0.64887	-2.51218

C	-4.73379	-1.80926	-2.10426
C	-5.35514	-2.36458	-3.40179
H	-6.05779	-3.17599	-3.17736
H	-5.89308	-1.57642	-3.94053
H	-4.57506	-2.7579	-4.0648
C	-5.85038	-1.25715	-1.19637
H	-6.54332	-2.05447	-0.90139
H	-5.42144	-0.81327	-0.29179
H	-6.4199	-0.47844	-1.71643
C	-3.97427	-2.93761	-1.38805
H	-4.66042	-3.76677	-1.17896
H	-3.15887	-3.32421	-2.00752
H	-3.54883	-2.60947	-0.43754
H	-2.13106	-1.28028	-1.65246

Thermal correction to Energy=1.156265

Thermal correction to Enthalpy=1.157415

Thermal correction to Gibbs Free Energy=0.935589

Sum of electronic and zero-point Energies=-2549.240898

Sum of electronic and thermal Energies=-2549.151933

Sum of electronic and thermal Enthalpies=-2549.150783

Sum of electronic and thermal Free Energies=-2549.372609

SCF Done: E(RM11L) = -2550.37314743

6c'

Number of Negative Frequencies =o

B	1.28657	-0.19793	1.43493
B	1.37829	-1.52873	-1.24178
B	-0.41107	-1.56606	1.17926
C	-2.50271	1.32991	0.99621
H	-2.85879	0.3172	1.12982
C	-3.29478	2.42066	1.41291
C	-2.79329	3.71098	1.24371
C	-1.48583	3.85353	0.69548
C	-0.77229	2.68877	0.32088
C	0.56686	2.79334	-0.19626
C	1.19035	4.05869	-0.32038
C	2.53632	4.12689	-0.78191
C	3.18686	2.93017	-1.08408
C	2.47866	1.7218	-0.94411
H	2.94673	0.77559	-1.1843
C	3.1992	-0.27511	2.71796
C	2.23124	0.83282	3.26951
C	2.3208	-3.49303	-2.00251
C	3.14638	-2.27318	-2.5427
C	-1.67055	-2.44282	2.90777
C	-0.71363	-3.53899	2.32123
Ir	0.08518	-0.21899	-0.35576
N	-1.29571	1.44329	0.45903
N	1.21551	1.64189	-0.53
O	2.6177	-0.57528	1.42149
O	0.98499	0.51605	2.58762
O	1.09813	-2.85764	-1.55786
O	2.65094	-1.19247	-1.71278
O	-1.61343	-1.42206	1.87871
O	0.23025	-2.73959	1.56274
H	-0.84826	-1.52601	-0.46754
C	-0.64217	0.24802	-2.34991
C	0.26522	0.73658	-3.31754
C	-0.12346	1.15411	-4.59125
H	0.62428	1.51837	-5.29399
C	-1.4709	1.09263	-4.96483
H	-1.79	1.41685	-5.95271
C	-2.39257	0.58854	-4.05693
H	-3.44184	0.50282	-4.327
C	-1.99953	0.15951	-2.77042
C	-0.84148	5.12474	0.52481
C	0.43208	5.22161	0.04581
H	0.88684	6.2005	-0.05437
H	-1.37505	6.02898	0.7953
C	-4.64139	2.13708	2.03239
H	-4.81596	1.05949	2.1038
H	-4.71206	2.55394	3.04428
H	-5.45887	2.56984	1.44374
C	-3.58176	4.93326	1.63814
H	-3.08726	5.47347	2.45542
H	-3.66774	5.63047	0.79633
H	-4.59144	4.68298	1.96686
C	4.61993	2.86413	-1.55426
H	5.30493	3.30234	-0.8186
H	4.92599	1.8263	-1.71784
H	4.76099	3.40662	-2.4967
C	3.21842	5.46362	-0.91244
H	2.65623	6.1261	-1.58159
H	3.28018	5.96686	0.06058
H	4.23156	5.37468	-1.30639
C	4.64152	0.1746	2.5089
H	5.0937	0.48937	3.45643
H	5.23236	-0.6576	2.11041

H	4.70619	1.0028	1.79832
C	3.15751	-1.57405	3.52847
H	3.71094	-2.34835	2.98677
H	3.61103	-1.4529	4.51812
H	2.1284	-1.92348	3.64577
C	1.99242	0.7915	4.77517
H	2.92895	0.95721	5.31997
H	1.28937	1.58205	5.06039
H	1.57063	-0.16463	5.09312
C	2.62246	2.25125	2.83831
H	1.80499	2.93677	3.08478
H	3.52581	2.59347	3.35458
H	2.7958	2.30391	1.7603
C	0.05109	-4.35223	3.35905
H	0.71203	-5.06639	2.85566
H	0.66735	-3.71487	3.99705
H	-0.6407	-4.91827	3.9935
C	-1.41134	-4.47161	1.32342
H	-0.65308	-5.06297	0.80006
H	-2.10102	-5.15822	1.82607
H	-1.96884	-3.90063	0.57365
C	-1.14582	-1.81076	4.20117
H	-1.75898	-0.9359	4.44316
H	-1.19494	-2.51029	5.04251
H	-0.11614	-1.46792	4.07615
C	-3.12028	-2.88202	3.08549
H	-3.18633	-3.70973	3.80105
H	-3.71527	-2.04893	3.47639
H	-3.56616	-3.20108	2.14122
C	2.81424	-1.91503	-3.99587
H	3.27226	-0.95032	-4.23961
H	3.20003	-2.66357	-4.69637
H	1.73385	-1.81958	-4.13933
C	4.65681	-2.37805	-2.35625
H	5.05826	-3.2385	-2.90416
H	5.14189	-1.47453	-2.74379
H	4.9261	-2.47789	-1.30165
C	1.97504	-4.5503	-3.04609
H	2.88375	-4.99645	-3.46709
H	1.38923	-5.35127	-2.58115
H	1.38149	-4.13009	-3.86216
C	2.95955	-4.1468	-0.77064
H	2.24185	-4.84446	-0.32719
H	3.86763	-4.70285	-1.02904
H	3.20621	-3.39386	-0.016
H	1.3226	0.77662	-3.07347
C	-3.03812	-0.43085	-1.89389
N	-4.27641	-0.45497	-2.21048
C	-5.279	-1.11028	-1.35527
C	-6.05865	-2.06529	-2.28057
H	-6.89028	-2.5378	-1.74378
H	-6.46379	-1.52112	-3.14117
H	-5.40077	-2.85662	-2.65998
C	-6.21905	0.0037	-0.85548
H	-7.04863	-0.41753	-0.27461
H	-5.6737	0.70787	-0.21794
H	-6.63654	0.56426	-1.69954
C	-4.72884	-1.90345	-0.15619
H	-5.55582	-2.38576	0.37744
H	-4.03469	-2.68856	-0.47935
H	-4.20162	-1.26639	0.55985
H	-2.65902	-0.87197	-0.96988

Thermal correction to Energy=1.158943

Thermal correction to Enthalpy=1.160093

Thermal correction to Gibbs Free Energy=0.941530

Sum of electronic and zero-point Energies=-2549.260412

Sum of electronic and thermal Energies= -2549.171524

Sum of electronic and thermal Enthalpies=-2549.170374

Sum of electronic and thermal Free Energies=-2549.388937

SCF Done: E(RM11L) = -2550.39841894

7c'

Number of Negative Frequencies =0

Ir	-0.08865	-0.36403	-0.77302
B	1.94052	-0.75468	-1.12044
B	0.5292	-2.04442	0.3354
O	2.41777	-1.22287	-2.33626
O	2.99839	-0.48201	-0.25474
C	-1.87137	2.43153	2.19007
C	-0.01091	1.47312	3.39537
C	0.3081	0.77673	2.21321
H	1.16321	0.11661	2.18871
C	-3.4474	2.47659	-0.20903
N	-1.93478	0.82341	-1.12501
N	-0.3865	0.85489	1.08505
O	0.4594	-2.08127	1.73231
O	1.1498	-3.20533	-0.13132
C	-2.29699	1.65801	-0.11806

C	-1.48948	1.65274	1.07188	H	-0.39645	-4.03473	3.30141
O	-2.55332	-1.28653	0.81157	C	2.65663	-2.57174	2.54522
O	-2.04783	-2.90195	-0.71754	H	3.34352	-3.32223	2.9512
C	-3.78119	3.29223	0.92469	H	3.10145	-2.11483	1.65765
C	-3.03542	3.2642	2.06694	H	2.52957	-1.78642	3.29934
H	-4.65439	3.93305	0.87619	C	-4.27135	-2.57517	-1.54635
H	-3.33223	3.88198	2.90706	H	-3.97095	-3.09361	-2.46305
C	-4.23086	2.43271	-1.39835	H	-5.34397	-2.73609	-1.39484
C	-1.10259	2.34167	3.38509	H	-4.09509	-1.50512	-1.69184
C	1.30496	-4.13179	0.97728	C	-3.69023	-4.61489	-0.21521
C	1.28341	-3.16936	2.21585	H	-3.52544	-5.11987	-1.1734
C	-3.44584	-3.11757	-0.37371	H	-3.01906	-5.0629	0.52063
C	-3.60805	-2.27181	0.94439	H	-4.72428	-4.80519	0.09448
C	3.84809	-1.42502	-2.24931	C	-3.32026	-3.06437	2.22304
C	4.24278	-0.53896	-1.00778	H	-3.27422	-2.36966	3.06831
H	-0.12128	-1.21044	-2.1097	H	-4.10041	-3.80575	2.42604
C	-3.8314	1.56907	-2.42101	H	-2.35648	-3.57501	2.15932
C	4.07257	-2.92267	-2.02676	C	-4.9392	-1.53567	1.07599
H	3.56488	-3.24866	-1.11891	H	-5.77577	-2.24332	1.10084
H	3.63716	-3.47561	-2.86622	H	-4.95178	-0.96313	2.01011
H	5.13717	-3.17359	-1.96335	H	-5.09682	-0.83505	0.25207
C	4.47679	-0.99159	-3.57194	C	-4.58896	1.41924	-3.71782
H	5.57004	-1.05989	-3.52757	H	-4.62673	2.36386	-4.27302
H	4.12929	-1.65129	-4.37475	H	-4.11227	0.67346	-4.36138
H	4.19938	0.03203	-3.83522	H	-5.62335	1.09949	-3.54495
C	4.61242	0.89843	-1.39052	C	-5.45689	3.29978	-1.51872
H	4.71816	1.49946	-0.48258	H	-6.19048	3.04853	-0.74256
H	5.56133	0.93403	-1.93606	H	-5.20023	4.358	-1.38787
H	3.83559	1.35841	-2.00647	H	-5.94625	3.19217	-2.48748
C	5.32272	-1.1294	-0.10575	C	-1.47444	3.17113	4.58674
H	6.27303	-1.21837	-0.64464	H	-1.4924	4.23777	4.33284
H	5.48208	-0.47057	0.75527	H	-2.4751	2.90946	4.95263
H	5.04393	-2.11604	0.2716	H	-0.77278	3.03825	5.41135
C	2.59836	-4.92269	0.8109	C	0.86405	1.2664	4.6073
H	2.73132	-5.61218	1.65291	H	1.38482	2.18882	4.89114
H	2.55649	-5.51595	-0.10875	H	0.2786	0.93846	5.47406
H	3.47614	-4.27595	0.75777	H	1.62369	0.50347	4.4113
C	0.10623	-5.08523	0.92688	C	-2.67662	0.78692	-2.22507
H	-0.82897	-4.5301	1.0109	H	-2.34733	0.09708	-2.99338
H	0.09997	-5.59611	-0.04156	B	-1.6216	-1.72882	-0.11569
H	0.15226	-5.84119	1.71816	C	1.38298	2.48922	-1.44204
C	0.64277	-3.74633	3.47382	C	0.75576	1.30658	-1.91649
H	1.19793	-4.62418	3.82364	C	0.42998	1.29524	-3.29349
H	0.65545	-2.99578	4.27214	C	0.64767	2.37961	-4.14237

C	1.2288	3.54954	-3.64006
C	1.60051	3.588	-2.30355
H	-0.01567	0.39984	-3.71755
H	0.3727	2.30983	-5.19332
H	2.09031	4.46647	-1.89319
H	1.4111	4.40392	-4.28782
C	1.942	2.59657	-0.07067
N	2.23325	3.73316	0.43881
C	2.93616	3.87118	1.72374
C	4.11758	4.82175	1.44321
H	4.81927	4.36662	0.73363
H	3.75988	5.76187	1.00861
H	4.66319	5.04991	2.36698
C	1.95553	4.55324	2.69735
H	1.10025	3.90184	2.90277
H	2.45092	4.78888	3.64702
H	1.57401	5.48604	2.26652
C	3.47798	2.57045	2.34097
H	4.00307	2.79181	3.27729
H	2.68124	1.85979	2.56858
H	4.18756	2.07658	1.66766
H	2.14599	1.64447	0.42023

Thermal correction to Energy=1.159007

Thermal correction to Enthalpy=1.160157

Thermal correction to Gibbs Free Energy=0.941512

Sum of electronic and zero-point Energies=-2549.254152

Sum of electronic and thermal Energies=-2549.165256

Sum of electronic and thermal Enthalpies=-2549.164106

Sum of electronic and thermal Free Energies=-2549.382752

SCF Done: E(RM11L) = -2550.38817209

TS8c'

Number of Negative Frequencies =1

Ir	0.15681	0.44253	-0.69875
B	-1.82932	0.18699	-1.4045
B	-1.06443	1.80141	0.28538
O	-2.22556	0.55795	-2.69183
O	-2.95228	-0.18031	-0.65153
C	2.4065	-2.30335	2.00927
C	0.648	-1.479	3.44274
C	0.20161	-0.71899	2.34239
H	-0.65525	-0.06581	2.4395
C	3.83871	-2.02934	-0.46391
N	2.16039	-0.4241	-1.1501
N	0.77611	-0.71981	1.14606
O	-1.15706	1.83062	1.6834
O	-1.87217	2.80146	-0.25311
C	2.64123	-1.30845	-0.24103
C	1.91083	-1.45564	0.98974
O	2.3161	1.82592	0.96995
O	1.42856	3.35141	-0.47817
C	4.27519	-2.93616	0.56029
C	3.59406	-3.06418	1.7359
H	5.17482	-3.52009	0.40255
H	3.96904	-3.74412	2.49279
C	4.56031	-1.80518	-1.67198
C	1.7342	-2.3351	3.26536
C	-2.36481	3.64194	0.82156
C	-2.26005	2.68904	2.06269
C	2.69149	3.91672	-0.0318
C	2.99728	3.07399	1.2568
C	-3.668	0.53601	-2.78291
C	-4.07773	-0.35339	-1.54845
H	0.04923	1.29386	-2.02698
C	4.05551	-0.87102	-2.57945
C	-4.14383	1.98788	-2.67558
H	-3.80501	2.42769	-1.73701
H	-3.69891	2.56551	-3.49358
H	-5.23384	2.07021	-2.75127
C	-4.0593	-0.0438	-4.14131
H	-5.14771	-0.14767	-4.22303
H	-3.72332	0.62841	-4.93882
H	-3.6011	-1.02127	-4.31174
C	-4.17295	-1.84821	-1.8819
H	-4.27554	-2.41683	-0.95188
H	-5.04054	-2.06244	-2.51509
H	-3.27269	-2.20322	-2.3891
C	-5.34734	0.09088	-0.82673
H	-6.21683	0.01285	-1.48963
H	-5.52422	-0.55633	0.03969
H	-5.27437	1.12066	-0.46978
C	-3.78096	4.10669	0.49697
H	-4.18883	4.69639	1.3264
H	-3.77105	4.74062	-0.39627
H	-4.4524	3.26648	0.30774
C	-1.42293	4.8485	0.90545
H	-0.39856	4.52256	1.09616
H	-1.42741	5.37002	-0.05745

H	-1.73156	5.55513	1.68345
C	-1.91435	3.37571	3.3798
H	-2.68866	4.10148	3.65407
H	-1.84997	2.63036	4.18074
H	-0.95349	3.89304	3.32469
C	-3.48194	1.77897	2.23932
H	-4.36954	2.33835	2.55418
H	-3.6978	1.24444	1.31105
H	-3.25859	1.03297	3.01069
C	3.70301	3.6761	-1.16004
H	3.32566	4.13472	-2.0801
H	4.67959	4.11617	-0.93117
H	3.83651	2.60512	-1.34752
C	2.50979	5.41322	0.19864
H	2.26741	5.90633	-0.74923
H	1.69922	5.6214	0.90073
H	3.43233	5.85975	0.58736
C	2.36184	3.65048	2.52651
H	2.45513	2.91688	3.33455
H	2.85295	4.5772	2.84212
H	1.29669	3.84795	2.37658
C	4.47416	2.77592	1.49947
H	5.04402	3.70271	1.63307
H	4.58393	2.17595	2.40991
H	4.9119	2.21212	0.67178
C	4.73965	-0.53188	-3.88093
H	4.83011	-1.41152	-4.52926
H	4.17526	0.22898	-4.42876
H	5.751	-0.14227	-3.71494
C	5.83902	-2.55925	-1.93174
H	6.58399	-2.34306	-1.15595
H	5.66346	-3.64166	-1.91648
H	6.27956	-2.30675	-2.89704
C	2.21575	-3.25429	4.35796
H	2.28304	-4.28624	3.99408
H	3.2167	-2.9677	4.70508
H	1.54938	-3.25067	5.22177
C	-0.08646	-1.33954	4.7544
H	-0.60016	-2.26633	5.03598
H	0.59979	-1.08477	5.57019
H	-0.84041	-0.54863	4.69367
C	2.84995	-0.21425	-2.26483
H	2.42738	0.51017	-2.95238
B	1.33442	2.05361	0.00893
C	-0.87708	-2.66682	-1.05458
C	-0.5041	-1.45862	-1.69758
C	-0.07242	-1.56482	-3.0385
C	0.06524	-2.78586	-3.69329
C	-0.25526	-3.97256	-3.02015
C	-0.73673	-3.9031	-1.71989
H	0.16463	-0.65345	-3.5796
H	0.41407	-2.81539	-4.72361
H	-1.03776	-4.80417	-1.19361
H	-0.15376	-4.93459	-3.51699
C	-1.52354	-2.65965	0.27929
N	-1.87388	-3.74386	0.85841
C	-2.62259	-3.74161	2.12427
C	-3.88192	-4.59217	1.86491
H	-4.5306	-4.10422	1.12694
H	-3.608	-5.57915	1.47571
H	-4.45628	-4.72863	2.78928
C	-1.72678	-4.45169	3.15827
H	-0.8003	-3.88864	3.31363
H	-2.24358	-4.54948	4.12056
H	-1.45581	-5.45417	2.80756
C	-3.05162	-2.36118	2.65295
H	-3.63894	-2.4833	3.57007
H	-2.19286	-1.72977	2.89152
H	-3.66997	-1.82688	1.92307
H	-1.73209	-1.67168	0.68411

Thermal correction to Energy=1.157752

Thermal correction to Enthalpy=1.158902

Thermal correction to Gibbs Free Energy=0.944162

Sum of electronic and zero-point Energies=-2549.253056

Sum of electronic and thermal Energies=-2549.165347

Sum of electronic and thermal Enthalpies=-2549.164197

Sum of electronic and thermal Free Energies=-2549.378937

SCF Done: E(RM11L) = -2550.38809160

9c'

Number of Negative Frequencies =0

B	-0.92496	2.45436	0.37261
B	1.68561	1.61357	0.70723
C	-2.95402	-0.50575	1.94522
H	-2.53772	-0.24891	2.91436
C	-4.27466	-0.99122	1.8476
C	-3.93839	-1.0692	-0.54947
C	-2.61892	-0.6048	-0.33558

C	-1.71698	-0.41933	-1.44254	C	-0.3212	5.17964	-0.99378
C	-2.14742	-0.68818	-2.76145	H	0.34421	4.98626	-0.14797
C	0.05059	-0.04534	-3.533	H	0.23375	4.96362	-1.9131
C	0.37976	0.19643	-2.18452	H	-0.60162	6.23875	-1.00411
H	1.36903	0.55288	-1.92095	C	-2.44299	4.49059	-2.14434
N	-2.14767	-0.317	0.90695	H	-2.89268	5.49025	-2.11765
N	-0.45547	0.02186	-1.16537	H	-1.84851	4.41231	-3.06197
O	-1.53113	3.37126	1.2422	H	-3.24421	3.74879	-2.19971
O	-1.06586	2.90064	-0.95212	C	-3.72885	3.81113	0.389
O	1.94673	2.99731	0.76173	H	-4.10836	3.68217	1.40856
O	2.91343	0.94072	0.49685	H	-4.38825	4.50975	-0.13795
C	-4.34983	-1.32331	-1.90097	H	-3.77481	2.83985	-0.11473
C	-3.49726	-1.14091	-2.95117	C	-2.23943	5.68213	1.15097
H	-5.35938	-1.67018	-2.09172	H	-2.72527	6.45142	0.53901
H	-3.84662	-1.34679	-3.95671	H	-2.76939	5.62727	2.10887
C	-4.78589	-1.27168	0.57841	H	-1.21141	5.99347	1.3531
C	-1.22989	-0.5082	-3.83596	C	4.45641	1.79298	2.131
C	-1.54889	4.26288	-0.929	H	4.73486	0.75714	2.35213
C	-2.28343	4.32421	0.45642	H	5.3249	2.43154	2.32738
C	3.3023	3.24473	0.33365	H	3.65014	2.08118	2.81284
C	4.00056	1.88595	0.66873	C	3.84986	4.45582	1.08422
Ir	-0.12017	0.7029	0.88096	H	4.90952	4.61564	0.85152
C	1.58272	-1.82932	2.95933	H	3.30006	5.35613	0.78701
C	0.80453	-3.04918	3.56071	H	3.74331	4.34026	2.16592
B	0.30146	-2.82377	1.34412	C	3.25999	3.53832	-1.17328
O	0.33372	-3.73865	2.36129	H	2.87183	2.67793	-1.72864
O	0.84573	-1.60492	1.69629	H	2.58621	4.38213	-1.35138
H	-0.09356	1.25203	2.39582	H	4.24824	3.79542	-1.57006
C	1.10525	0.19315	-4.58527	C	5.15747	1.52053	-0.25736
H	0.72617	0.81355	-5.40473	H	5.9218	2.30676	-0.24235
H	1.97297	0.70111	-4.1572	H	5.62768	0.58905	0.0724
H	1.45357	-0.75266	-5.01781	H	4.82189	1.38179	-1.28778
C	-1.65524	-0.82619	-5.24615	C	1.56666	-0.58402	3.82885
H	-2.01729	-1.85893	-5.31867	H	2.07322	-0.80302	4.77653
H	-2.47659	-0.17372	-5.56848	H	2.09921	0.22557	3.32523
H	-0.83863	-0.7125	-5.96019	H	0.55467	-0.23835	4.03742
C	-6.18898	-1.78251	0.37551	C	3.02012	-2.15346	2.54301
H	-6.771	-1.0914	-0.24672	H	3.39062	-1.32574	1.93258
H	-6.18129	-2.75024	-0.14111	H	3.66841	-2.2685	3.41777
H	-6.72324	-1.91177	1.31767	H	3.07154	-3.07268	1.95042
C	-5.07261	-1.17224	3.11608	C	1.66558	-4.01196	4.36813
H	-5.97142	-0.54388	3.12182	H	2.11716	-3.49523	5.22206
H	-5.40063	-2.21099	3.24258	H	1.04827	-4.83101	4.75229
H	-4.47435	-0.90346	3.99231	H	2.4632	-4.44407	3.75901

C	-0.4465	-2.64662	4.34659
H	-1.04664	-3.54222	4.53858
H	-0.18922	-2.19156	5.30806
H	-1.05837	-1.93993	3.77695
C	-0.29409	-3.21425	-0.04809
C	-1.59769	-3.73963	-0.07411
C	0.4267	-3.14151	-1.26321
C	-2.19295	-4.15043	-1.26608
H	-2.15671	-3.81606	0.85516
C	-0.17402	-3.5691	-2.45902
C	-1.47477	-4.0626	-2.46348
H	-3.20892	-4.53581	-1.26398
H	0.40092	-3.51501	-3.3779
H	-1.9302	-4.38319	-3.39697
C	1.8349	-2.68853	-1.25597
H	2.21752	-2.39084	-0.27693
N	2.55272	-2.67329	-2.3109
C	3.98149	-2.31333	-2.25409
C	4.16615	-1.0773	-3.15296
H	3.63244	-0.21725	-2.73611
H	5.22815	-0.81722	-3.23306
H	3.77898	-1.26733	-4.15937
C	4.73194	-3.51174	-2.86704
H	4.59899	-4.40756	-2.24859
H	4.35218	-3.73299	-3.87097
H	5.80528	-3.29946	-2.93872
C	4.53284	-2.01517	-0.85063
H	4.01608	-1.16915	-0.38738
H	4.44186	-2.8854	-0.18987
H	5.59685	-1.76351	-0.92157

Thermal correction to Energy=1.159178

Thermal correction to Enthalpy=1.160329

Thermal correction to Gibbs Free Energy=0.939936

Sum of electronic and zero-point Energies=-2549.279848

Sum of electronic and thermal Energies=-2549.190895

Sum of electronic and thermal Enthalpies=-2549.189745

Sum of electronic and thermal Free Energies=-2549.410137

SCF Done: E(RM11L) = -2550.43103023

10'

Number of Negative Frequencies =0

B	1.90687	-1.41722	-0.87155
B	2.52659	1.11011	0.07034
C	-1.48293	-1.07298	-2.61545
H	-1.12489	-0.38566	-3.37626
C	-2.4051	-2.08524	-2.95666
C	-2.27854	-2.80807	-0.65018
C	-1.39122	-1.73408	-0.40963
C	-0.87416	-1.49672	0.91335
C	-1.23557	-2.34182	1.9874
C	0.07053	-0.92409	3.44728
C	0.39726	-0.16406	2.30667
H	1.05588	0.69411	2.39005
N	-0.9837	-0.89394	-1.39934
N	-0.02362	-0.44265	1.07631
O	2.43188	-2.02617	-2.02072
O	2.06665	-2.27916	0.22607
O	3.86306	0.67377	-0.00323
O	2.46685	2.2001	0.97073
C	-2.6014	-3.67183	0.45149
C	-2.10365	-3.45157	1.70384
H	-3.26211	-4.51584	0.28675
H	-2.37967	-4.12478	2.50772
C	-2.80521	-2.98103	-1.96357
C	-0.73665	-2.05205	3.29075
C	2.88868	-3.3979	-0.1707
C	2.67715	-3.42067	-1.72504
C	4.61861	1.28532	1.0667
C	3.81245	2.6028	1.3242
Ir	0.87529	0.2936	-0.77313
C	-0.05146	3.76227	-1.29768
C	-1.3445	4.2379	-2.03317
C	-4.25015	1.18729	2.19069
C	-4.75049	0.38914	0.93181
B	-1.85551	2.53108	-0.59136
B	-2.90349	1.61453	0.38189
O	-3.60985	0.49264	0.01986
O	-3.28873	2.11697	1.60274
O	-2.39692	3.61848	-1.23086
O	-0.48625	2.44664	-0.76698
H	1.4858	0.66645	-2.22084
C	0.62159	-0.48442	4.78202
H	1.28124	-1.24413	5.21822
H	1.20081	0.43814	4.67673
H	-0.18069	-0.29231	5.50447
C	-1.1157	-2.93371	4.45251
H	-2.20059	-2.91445	4.61876
H	-0.8384	-3.97737	4.26209

H	-0.63212	-2.6252	5.3804
C	-3.76662	-4.10787	-2.24119
H	-3.30561	-5.07897	-2.02208
H	-4.65911	-4.02512	-1.60846
H	-4.09691	-4.12393	-3.28065
C	-2.8997	-2.15956	-4.38098
H	-2.64362	-3.11764	-4.84883
H	-3.98939	-2.04996	-4.43564
H	-2.45461	-1.36483	-4.9876
C	4.33073	-3.0685	0.23392
H	4.66917	-2.15423	-0.26194
H	4.36354	-2.89757	1.31508
H	5.01993	-3.88628	-0.00475
C	2.40404	-4.64566	0.56359
H	2.93141	-5.53963	0.21043
H	2.59532	-4.54209	1.63792
H	1.3296	-4.79627	0.42892
C	1.4177	-4.1948	-2.14208
H	1.2103	-3.99359	-3.19862
H	1.53961	-5.2762	-2.01458
H	0.548	-3.86934	-1.56155
C	3.87918	-3.89747	-2.53425
H	4.14404	-4.92832	-2.27031
H	3.64148	-3.87272	-3.60392
H	4.7513	-3.25951	-2.36932
C	4.21726	3.74384	0.38206
H	3.48735	4.55578	0.46542
H	5.20592	4.14382	0.63316
H	4.23252	3.40559	-0.65863
C	6.06019	1.48423	0.60705
H	6.64177	2.0237	1.36406
H	6.53553	0.50975	0.44698
H	6.11107	2.03925	-0.33325
C	4.57945	0.3244	2.2634
H	3.55071	0.16107	2.6014
H	4.98624	-0.64395	1.95706
H	5.17183	0.69772	3.1062
C	3.81399	3.0952	2.76878
H	4.83292	3.32036	3.10518
H	3.22059	4.01325	2.8489
H	3.37958	2.35573	3.44678
C	1.1622	3.61746	-2.20008
H	1.39566	4.59341	-2.64283
H	2.02278	3.28458	-1.61828
H	0.99863	2.89609	-3.00126
C	0.29898	4.5987	-0.06414
H	1.04705	4.04907	0.51216
H	0.70752	5.57397	-0.34961
H	-0.58007	4.76101	0.56923
C	-1.55526	5.74707	-2.0351
H	-0.72658	6.24732	-2.54882
H	-2.48171	5.9931	-2.56537
H	-1.62942	6.1466	-1.02056
C	-1.48181	3.66967	-3.44931
H	-2.49956	3.85403	-3.80867
H	-0.78024	4.14427	-4.14267
H	-1.30538	2.58885	-3.45844
C	-5.0535	-1.08132	1.18447
H	-5.86257	-1.18158	1.91709
H	-5.37852	-1.55921	0.25416
H	-4.17834	-1.61797	1.55198
C	-5.92776	1.06046	0.21667
H	-6.09048	0.56306	-0.74519
H	-6.84955	0.9882	0.80299
H	-5.7206	2.11742	0.01878
C	-3.47141	0.32486	3.18489
H	-2.9947	0.97264	3.92783
H	-4.12608	-0.37913	3.70926
H	-2.68967	-0.23857	2.67405
C	-5.32534	1.99415	2.91013
H	-6.10619	1.33148	3.30045
H	-4.88073	2.52968	3.756
H	-5.78968	2.73086	2.2503

Thermal correction to Energy=1.113121

Thermal correction to Enthalpy=1.114271

Thermal correction to Gibbs Free Energy=0.896939

Sum of electronic and zero-point Energies=-2478.216262

Sum of electronic and thermal Energies=-2478.130139

Sum of electronic and thermal Enthalpies=-2478.128989

Sum of electronic and thermal Free Energies=-2478.346321

SCF Done: E(RM11L) = -2479.32152052

TS11'

Number of Negative Frequencies =1

Ir	0.24134	0.15435	-0.3536
B	-0.0017	2.00325	-1.06982
H	1.26364	-0.00939	-1.56828

C	-1.76716	-1.23743	-2.46224	H	-5.41229	-2.59419	-3.66168
C	-2.96897	-1.78553	-2.95816	C	-4.71972	1.14717	3.79735
C	-4.02424	-1.00457	-0.92338	H	-5.52775	1.70765	3.31163
C	-2.76676	-0.49826	-0.51897	H	-5.13477	0.17516	4.09216
C	-2.61539	0.15737	0.75522	H	-4.44662	1.68192	4.70825
C	-3.73043	0.31883	1.61087	C	-1.94094	2.10691	4.49449
C	-2.2668	1.41583	3.19238	H	-2.49971	3.04407	4.60478
C	-1.22101	1.20373	2.27055	H	-2.18548	1.47642	5.35771
B	0.65089	-2.11942	0.7427	H	-0.87444	2.34645	4.54837
N	-1.65955	-0.61146	-1.29815	C	0.95275	4.98273	-0.96988
N	-1.36979	0.59348	1.09834	H	1.11317	5.21601	0.08743
O	1.38468	-2.45226	1.85557	H	1.768	4.33237	-1.29954
O	-0.69629	-2.33892	0.91802	H	0.99374	5.91773	-1.53962
O	2.95022	1.61035	0.11441	C	-1.52644	5.19823	-0.65614
O	2.00035	0.81261	2.03474	H	-1.29923	5.57604	0.34726
O	1.15168	-2.54664	-1.94453	H	-1.63642	6.0598	-1.32517
O	2.90683	-1.62931	-0.78366	H	-2.48156	4.66874	-0.60734
C	-5.13492	-0.83655	-0.02839	C	-2.07932	3.3935	-2.88567
C	-4.99546	-0.20336	1.17322	H	-2.63527	4.32166	-3.05836
H	-6.10829	-1.21992	-0.31408	H	-2.13582	2.78399	-3.79407
H	-5.86098	-0.09665	1.81757	H	-2.56686	2.83943	-2.07608
C	-4.12503	-1.66113	-2.18565	C	0.05871	4.42982	-3.69435
C	-3.54839	0.97006	2.86601	H	-0.13707	3.92517	-4.64726
C	-0.88412	-3.04342	2.18212	H	-0.34071	5.44854	-3.76233
C	0.4657	-2.75422	2.94434	H	1.14195	4.48738	-3.56116
C	3.50716	-2.29269	-1.92456	C	5.25166	1.95452	0.76263
C	2.27251	-2.56434	-2.8733	H	5.44864	2.65732	-0.05522
C	3.79262	2.06246	1.19807	H	5.92834	2.1996	1.59007
C	3.37839	1.09913	2.36379	H	5.48592	0.94893	0.40446
C	-0.60438	3.66158	-2.55519	C	3.43399	3.52767	1.47688
B	1.54566	-1.87113	-0.79929	H	3.56188	4.10723	0.55718
H	-0.21199	1.52726	2.50008	H	2.38943	3.61959	1.79045
H	-0.84738	-1.3229	-3.02991	H	4.07429	3.96481	2.25147
B	1.83849	0.93313	0.6368	C	4.13177	-0.23809	2.33416
C	-0.40167	4.28194	-1.12835	H	5.18367	-0.12035	2.61997
O	-0.37937	3.10198	-0.28711	H	3.65381	-0.92664	3.03803
O	0.04059	2.37124	-2.42	H	4.07227	-0.69531	1.34206
C	-2.94398	-2.47985	-4.29846	C	3.43525	1.7088	3.76154
H	-1.92904	-2.49526	-4.70776	H	3.11881	0.96567	4.50254
H	-3.28804	-3.51808	-4.22173	H	4.45545	2.02254	4.01273
H	-3.58893	-1.9748	-5.02785	H	2.77275	2.57416	3.85075
C	-5.45501	-2.20151	-2.64476	C	4.57633	-1.37481	-2.51111
H	-5.79831	-3.01064	-1.98732	H	5.37588	-1.22716	-1.77663
H	-6.22468	-1.42091	-2.6208	H	5.02025	-1.81451	-3.41186

H	4.16697	-0.39382	-2.76288
C	2.03422	-1.45771	-3.90605
H	2.83395	-1.43425	-4.65383
H	1.08944	-1.65021	-4.42635
H	1.96092	-0.47769	-3.42923
C	2.28584	-3.92327	-3.57009
H	1.38022	-4.03245	-4.17729
H	3.15288	-4.01167	-4.23438
H	2.30979	-4.74686	-2.85222
C	4.15197	-3.57359	-1.3801
H	4.88066	-3.30166	-0.60923
H	3.40287	-4.22401	-0.91713
H	4.67157	-4.13521	-2.16375
C	1.02656	-3.93856	3.72649
H	1.97636	-3.65267	4.19108
H	0.33669	-4.24125	4.52246
H	1.21447	-4.79933	3.08007
C	-1.07844	-4.51848	1.81614
H	-1.2613	-5.13399	2.70312
H	-1.94247	-4.60898	1.14929
H	-0.20301	-4.91265	1.28988
C	-2.13557	-2.49886	2.86107
H	-3.0132	-2.70797	2.24031
H	-2.2854	-2.9799	3.83438
H	-2.07574	-1.41999	3.01088
C	0.4168	-1.50996	3.83565
H	-0.2564	-1.65419	4.68762
H	1.4216	-1.30841	4.2195
H	0.10069	-0.63334	3.2679

Thermal correction to Energy=1.111880

Thermal correction to Enthalpy=1.113030

Thermal correction to Gibbs Free Energy=0.900546

Sum of electronic and zero-point Energies=-2478.215129

Sum of electronic and thermal Energies=-2478.130053

Sum of electronic and thermal Enthalpies=-2478.128903

Sum of electronic and thermal Free Energies=-2478.341388

SCF Done: E(RM11L) = -2479.31240022

12'

Number of Negative Frequencies =0

Ir	0.12303	0.26036	-0.44913
B	-0.99279	1.91774	-1.15877
H	0.84945	0.49195	-1.86655
C	-1.60347	-1.83907	-2.20734
C	-2.66218	-2.71764	-2.51617
C	-3.59894	-2.16226	-0.35456
C	-2.49776	-1.29665	-0.15163
C	-2.37322	-0.54093	1.06549
C	-3.35203	-0.65683	2.08145
C	-2.07859	0.92521	3.39128
C	-1.16081	0.97594	2.32458
B	1.00416	-1.34889	0.82176
N	-1.51481	-1.15179	-1.07687
N	-1.28427	0.26904	1.2044
O	2.10453	-1.32294	1.65588
O	0.14307	-2.38048	1.17439
O	2.29291	2.45194	-0.5584
O	1.6865	1.93917	1.58333
O	1.52754	-2.13937	-1.86266
O	3.06712	-0.59552	-1.15697
C	-4.57525	-2.26143	0.69411
C	-4.4566	-1.54655	1.85072
H	-5.42724	-2.91956	0.56502
H	-5.21674	-1.65103	2.61685
C	-3.6812	-2.89033	-1.57624
C	-3.19314	0.09178	3.28273
C	0.76095	-3.18166	2.21504
C	1.85585	-2.20387	2.78279
C	3.82258	-1.63562	-1.81558
C	2.71588	-2.36299	-2.66242
C	3.0241	3.36315	0.29326
C	2.94485	2.64556	1.68568
C	-2.34597	3.17128	-2.55362
B	1.72461	-0.97277	-1.10972
H	-0.2736	1.59366	2.3884
H	-0.78034	-1.70353	-2.89955
B	1.45749	1.65241	0.22636
C	-2.205	3.89355	-1.16944
O	-1.63403	2.84832	-0.34006
O	-1.27417	2.193	-2.49873
C	-2.63763	-3.43553	-3.84364
H	-1.74506	-3.16369	-4.41593
H	-2.63078	-4.52429	-3.71293
H	-3.51372	-3.1857	-4.45431
C	-4.84102	-3.82341	-1.81592
H	-4.86231	-4.61912	-1.06084
H	-5.797	-3.29002	-1.74708

H	-4.79498	-4.29777	-2.79718
C	-4.20859	-0.03347	4.38915
H	-5.20831	0.25338	4.04023
H	-4.27675	-1.06973	4.7428
H	-3.96335	0.59496	5.24631
C	-1.78929	1.75917	4.61633
H	-2.59451	2.47537	4.81893
H	-1.67577	1.13379	5.51015
H	-0.86267	2.32673	4.48695
C	-1.19748	5.04888	-1.19355
H	-1.0025	5.37382	-0.16617
H	-0.24723	4.7296	-1.63155
H	-1.57635	5.90739	-1.75895
C	-3.51792	4.35235	-0.54207
H	-3.3192	4.82754	0.42532
H	-4.02209	5.0858	-1.18221
H	-4.19674	3.51304	-0.37063
C	-3.65625	2.38378	-2.691
H	-4.52167	3.0458	-2.80559
H	-3.59333	1.74279	-3.57695
H	-3.82085	1.73935	-1.82086
C	-2.14111	4.0642	-3.77345
H	-2.25245	3.47337	-4.6897
H	-2.88578	4.86857	-3.79707
H	-1.14398	4.51139	-3.78143
C	4.43469	3.52848	-0.26656
H	4.3905	4.03274	-1.23874
H	5.05558	4.13708	0.40187
H	4.92032	2.56038	-0.41283
C	2.284	4.70575	0.26932
H	2.20414	5.05125	-0.7668
H	1.27112	4.59832	0.66852
H	2.81134	5.47359	0.84688
C	4.03659	1.58224	1.86778
H	5.02813	2.0338	1.98693
H	3.81278	0.99393	2.76313
H	4.04676	0.89542	1.01647
C	2.8941	3.5728	2.89546
H	2.8228	2.97866	3.81404
H	3.80129	4.18522	2.95976
H	2.02708	4.23797	2.8575
C	4.93376	-0.98612	-2.63568
H	5.64644	-0.4928	-1.96506
H	5.48013	-1.73729	-3.21822
H	4.53926	-0.23054	-3.31974
C	2.46888	-1.70074	-4.02373
H	3.3033	-1.86306	-4.71445
H	1.56597	-2.13089	-4.47121
H	2.31024	-0.62302	-3.91302
C	2.91381	-3.86542	-2.83252
H	2.09335	-4.28363	-3.42663
H	3.85387	-4.0788	-3.35439
H	2.9256	-4.37884	-1.8676
C	4.42703	-2.52488	-0.72269
H	5.03725	-1.90536	-0.05748
H	3.64146	-2.98432	-0.11886
H	5.06192	-3.31247	-1.14342
C	3.17219	-2.86465	3.18009
H	3.87332	-2.10267	3.53813
H	3.01748	-3.5899	3.98727
H	3.63846	-3.37554	2.33439
C	1.34051	-4.42486	1.53187
H	1.80087	-5.10858	2.25304
H	0.53251	-4.95726	1.01858
H	2.08767	-4.15022	0.78219
C	-0.31685	-3.5932	3.21483
H	-1.05299	-4.23474	2.7178
H	0.11901	-4.1573	4.04758
H	-0.84606	-2.72778	3.62019
C	1.34441	-1.31952	3.92605
H	1.18614	-1.89505	4.84453
H	2.0846	-0.5384	4.12777
H	0.40651	-0.82687	3.6534

Thermal correction to Energy=1.111563

Thermal correction to Enthalpy=1.112713

Thermal correction to Gibbs Free Energy=0.898620

Sum of electronic and zero-point Energies=-2478.227301

Sum of electronic and thermal Energies=-2478.141197

Sum of electronic and thermal Enthalpies=-2478.140047

Sum of electronic and thermal Free Energies=-2478.354141

SCF Done: E(RM11L) = -2479.31752685

TS13'

Number of Negative Frequencies =1

Ir	0.18502	0.16523	-0.40181
H	0.41689	0.60245	-1.95052
B	1.97063	-0.63032	-1.15043
C	-0.86003	-2.68226	-1.58274

C	-1.68743	-3.81605	-1.71164	C	-3.69949	-5.13986	-0.90263
C	-2.98449	-2.93326	0.12818	H	-3.74993	-5.65159	0.06595
C	-2.09326	-1.8328	0.1688	H	-4.72065	-4.82526	-1.15297
C	-2.28587	-0.77403	1.12394	H	-3.38647	-5.87177	-1.64866
C	-3.3671	-0.82069	2.038	C	-1.36043	-4.82679	-2.7842
C	-2.62147	1.30005	2.92629	H	-1.15508	-5.8162	-2.35817
C	-1.58138	1.25868	1.97979	H	-2.18771	-4.94184	-3.49489
B	1.27401	-0.76173	1.22074	H	-0.47562	-4.51985	-3.35084
N	-1.04119	-1.72538	-0.68255	C	-2.20922	3.67681	-3.23458
N	-1.40857	0.26924	1.10712	H	-2.95953	4.04633	-3.94206
O	2.5804	-0.57574	1.66307	H	-1.70079	4.53758	-2.78848
O	0.62172	-1.67842	2.04699	H	-1.46339	3.09462	-3.78561
O	1.69695	2.80926	-0.9334	C	-3.87297	3.67288	-1.35639
O	1.15156	2.52983	1.26743	H	-3.42581	4.6257	-1.05171
O	2.15417	-2.00934	-1.31852	H	-4.74136	3.89255	-1.98818
O	3.07275	0.05565	-1.643	H	-4.21618	3.15854	-0.45502
C	-4.07108	-2.954	1.06712	C	-4.39044	0.81574	-1.6624
C	-4.2512	-1.95148	1.97493	H	-5.35287	1.33545	-1.7194
H	-4.76783	-3.78516	1.05333	H	-4.54643	-0.23068	-1.94536
H	-5.08625	-2.00655	2.66448	H	-4.04261	0.83487	-0.62474
C	-2.76961	-3.95485	-0.84025	C	-3.84944	1.39225	-4.04411
C	-3.53548	0.245	2.96674	H	-4.16641	0.37328	-4.29313
C	1.60423	-2.30983	2.90647	H	-4.71012	2.05754	-4.17966
C	2.73397	-1.22584	2.95271	H	-3.06819	1.684	-4.75035
C	4.12474	-0.89179	-1.94625	C	2.8178	-2.42207	-3.58321
C	3.32223	-2.22764	-2.14763	H	3.63571	-2.63845	-4.27878
C	1.90532	4.09323	-0.30482	H	2.1194	-3.26623	-3.60453
C	1.98574	3.70933	1.21367	H	2.28489	-1.53219	-3.93448
C	-3.35181	1.43937	-2.60392	C	4.87861	-0.40445	-3.18067
B	-1.33215	1.20305	-1.52686	H	5.39832	0.53243	-2.95077
H	-0.84599	2.05202	1.92928	H	5.6286	-1.13944	-3.49598
H	0.00265	-2.55666	-2.22555	H	4.20161	-0.21495	-4.01766
B	1.10914	1.94083	-0.00903	C	5.06092	-0.92727	-0.73281
C	-2.84533	2.8423	-2.11773	H	5.44899	0.08213	-0.55696
O	-1.77718	2.47496	-1.20139	H	4.51598	-1.23303	0.16294
O	-2.14829	0.62885	-2.49452	H	5.91105	-1.5999	-0.89284
C	-2.68849	2.48667	3.85819	C	4.03145	-3.48922	-1.66487
H	-2.61169	2.1792	4.90794	H	3.38407	-4.35988	-1.81954
H	-1.8701	3.18403	3.65436	H	4.96092	-3.65355	-2.22243
H	-3.63106	3.03602	3.74669	H	4.26942	-3.43296	-0.59969
C	-4.67892	0.21409	3.94738	C	2.49455	-0.15371	4.02243
H	-5.64273	0.18777	3.42368	H	2.64521	-0.54762	5.03365
H	-4.63161	-0.68151	4.57895	H	3.19838	0.66976	3.86337
H	-4.68256	1.08449	4.60491	H	1.48029	0.25155	3.94899

C	4.15261	-1.77397	3.06743
H	4.87224	-0.94779	3.05936
H	4.27865	-2.32503	4.0069
H	4.39761	-2.4426	2.2388
C	2.03903	-3.6003	2.20081
H	2.75828	-4.17252	2.79694
H	1.15615	-4.22661	2.0319
H	2.48085	-3.37377	1.22544
C	0.95338	-2.62671	4.24868
H	0.16893	-3.37981	4.11188
H	1.68905	-3.02906	4.95502
H	0.49319	-1.73949	4.69158
C	1.4255	4.75139	2.17789
H	1.97794	5.69535	2.10172
H	0.36832	4.95023	1.98129
H	1.51467	4.38971	3.20893
C	3.39242	3.28222	1.65161
H	4.08379	4.13154	1.69104
H	3.33307	2.83757	2.65075
H	3.79773	2.52625	0.97195
C	3.17163	4.72497	-0.87618
H	3.02631	4.94851	-1.93924
H	3.4084	5.66425	-0.36215
H	4.02911	4.05277	-0.78949
C	0.68429	4.96132	-0.63887
H	0.59683	5.03983	-1.72773
H	-0.23301	4.49673	-0.26692
H	0.77469	5.97293	-0.22702

Thermal correction to Energy=1.109659

Thermal correction to Enthalpy=1.110809

Thermal correction to Gibbs Free Energy=0.895619

Sum of electronic and zero-point Energies=-2478.223528

Sum of electronic and thermal Energies=-2478.137558

Sum of electronic and thermal Enthalpies=-2478.136407

Sum of electronic and thermal Free Energies=-2478.351597

SCF Done: E(RM11L) = -2479.30968299

4d'

Number of Negative Frequencies =0

Ir	0.3177	0.08953	-0.15822
H	-1.58188	-2.13224	1.3334
C	-3.43527	-1.32265	2.13692
C	-3.74619	1.01192	1.58445
C	-2.4876	0.98324	0.93567
C	-1.93938	2.18881	0.35938
C	-2.6743	3.39908	0.40104
C	-0.8315	4.47612	-0.73932
C	-0.18327	3.22485	-0.71677
H	0.80802	3.1215	-1.14557
N	-1.74995	-0.15703	0.84678
N	-0.70144	2.11924	-0.1987
O	2.04668	-0.3797	2.33788
O	0.85151	1.5738	2.363
O	2.54271	0.26602	-2.28499
O	3.17217	1.20493	-0.29868
O	0.31648	-2.88186	0.58156
O	2.29485	-2.31134	-0.39837
C	-4.47268	2.25108	1.59622
C	-3.96595	3.38387	1.02883
H	-5.4469	2.28849	2.07064
H	-4.54856	4.29771	1.06175
C	-4.23106	-0.1785	2.20163
C	-2.10356	4.57239	-0.17428
C	1.78561	1.66048	3.46536
C	2.17718	0.15589	3.67496
C	2.33588	-3.74261	-0.22499
C	1.22443	-3.97675	0.85391
C	3.83159	0.87668	-2.51965
C	4.38701	1.05355	-1.06328
B	1.15879	0.42344	1.61777
B	2.1286	0.53022	-0.96431
B	1.04388	-1.81368	-0.00077
C	5.26468	2.28329	-0.84648
H	5.59604	2.32141	0.19753
H	6.15788	2.24778	-1.48181
H	4.72247	3.20869	-1.05862
C	3.58835	2.21391	-3.23296
H	4.52662	2.72395	-3.47802
H	3.05013	2.03032	-4.16911
H	2.9792	2.88239	-2.61506
C	4.65369	-0.04787	-3.4143
H	4.18647	-0.12063	-4.40328
H	5.67203	0.33631	-3.54876
H	4.71208	-1.05617	-2.99682
C	5.09463	-0.20317	-0.53557
H	6.0545	-0.37609	-1.03578
H	5.28355	-0.07614	0.53621

H	4.45427	-1.08115	-0.65816
C	2.96105	2.52352	2.98764
H	3.43571	2.07273	2.11131
H	2.57757	3.50662	2.69105
H	3.7091	2.67211	3.77453
C	1.0884	2.31949	4.65152
H	1.73886	2.32474	5.53424
H	0.8433	3.35922	4.40604
H	0.1573	1.80689	4.90743
C	3.60451	-0.07947	4.15935
H	3.7698	0.38792	5.13747
H	3.78834	-1.15487	4.26335
H	4.33616	0.31901	3.45205
C	1.18376	-0.60212	4.56613
H	1.4046	-1.67322	4.51734
H	1.24875	-0.2848	5.61285
H	0.15597	-0.45417	4.21745
C	3.74543	-4.1456	0.20103
H	3.79518	-5.21612	0.43357
H	4.45039	-3.94324	-0.61334
H	4.07313	-3.58059	1.07709
C	1.9964	-4.3724	-1.5828
H	2.70009	-3.99596	-2.3332
H	2.06906	-5.46557	-1.55929
H	0.98495	-4.09576	-1.8987
C	0.47438	-5.30062	0.73791
H	1.1533	-6.14408	0.91192
H	-0.31823	-5.34371	1.49408
H	0.00962	-5.42752	-0.24166
C	1.73667	-3.78936	2.28834
H	2.25016	-2.83008	2.3873
H	0.87977	-3.78478	2.97157
H	2.40994	-4.59986	2.58951
C	-0.12495	5.63951	-1.3922
H	0.02364	6.47045	-0.69248
H	0.8597	5.33604	-1.76181
H	-0.69536	6.02785	-2.24474
C	-2.87679	5.86607	-0.16281
H	-3.84184	5.74962	-0.67109
H	-3.09122	6.18621	0.86432
H	-2.33619	6.67445	-0.65691
C	-5.5619	-0.16924	2.90921
H	-5.57984	0.58837	3.70203
H	-6.37361	0.07549	2.2127
H	-5.79416	-1.13252	3.3655
C	-3.82369	-2.6351	2.77485
H	-3.90634	-2.54139	3.86463
H	-4.78859	-3.00026	2.40451
H	-3.0743	-3.40396	2.56291
C	-2.21623	-1.2565	1.42926
C	-0.21992	1.40994	-3.68173
C	-1.25155	2.34325	-3.76924
C	-2.55829	1.97433	-3.41735
C	-2.82918	0.67757	-2.99337
C	-1.79514	-0.2737	-2.91041
C	-0.48664	0.10768	-3.24863
H	0.80093	1.688	-3.91805
H	-1.04252	3.35915	-4.09459
H	-3.36119	2.70539	-3.46886
H	0.33014	-0.60374	-3.16783
C	-4.25778	0.25607	-2.60217
H	-4.90688	1.10514	-2.6537
N	-4.73357	-0.78139	-3.52855
C	-6.10424	-1.17023	-3.16665
C	-6.23019	-1.23988	-1.63339
H	-6.44579	-2.2456	-1.33855
H	-5.31051	-0.92623	-1.18536
H	-7.02176	-0.59619	-1.31094
C	-7.09562	-0.12781	-3.71632
H	-6.82977	0.12145	-4.72235
H	-8.08564	-0.53335	-3.69907
H	-7.06025	0.75274	-3.10946
C	-6.42285	-2.55034	-3.7711
H	-5.60804	-2.86597	-4.38865
H	-6.56895	-3.2596	-2.98338
H	-7.31295	-2.48437	-4.36126
H	-1.98089	-1.27941	-2.59587

Thermal correction to Energy=1.160912

Thermal correction to Enthalpy=1.162062

Thermal correction to Gibbs Free Energy=0.938808

Sum of electronic and zero-point Energies=-2549.285404

Sum of electronic and thermal Energies=-2549.195883

Sum of electronic and thermal Enthalpies=-2549.194733

Sum of electronic and thermal Free Energies=-2549.417988

SCF Done: E(RM11L) = -2550.42810349

TS5d'

Number of Negative Frequencies =1

Ir	0.01845	-0.13626	-0.28289
O	-2.10361	-2.26452	0.58039
O	-0.7242	-1.71719	2.31591
O	2.72847	-1.20659	0.77188
O	1.85464	0.44256	2.07984
C	-2.72313	-2.82602	1.76536
C	-1.53859	-2.81796	2.79612
C	3.77302	-0.84338	1.70421
C	2.97258	-0.09621	2.82652
B	-0.98667	-1.52284	0.96508
B	1.63508	-0.35782	0.946
B	0.39836	-2.00597	-1.09615
O	0.15099	-2.27517	-2.45097
O	0.80398	-3.17175	-0.45718
C	0.08056	-3.71668	-2.61746
C	0.99856	-4.21046	-1.4485
C	-2.43324	1.6113	0.42806
C	-3.31959	2.46921	1.1249
N	-1.18821	1.32715	0.90465
C	-2.89183	3.05917	2.34977
C	-0.80657	1.8843	2.05017
C	-1.61038	2.75701	2.81019
H	0.18606	1.61104	2.38924
C	-2.84049	0.99507	-0.80954
C	-4.13419	1.23479	-1.33596
C	-2.31367	-0.39967	-2.56688
C	-4.50765	0.60142	-2.55701
C	-3.57337	-0.22803	-3.17763
H	-1.57061	-1.05203	-3.0116
N	-1.94936	0.18028	-1.43074
C	0.82338	3.24589	-3.17291
C	1.71911	4.06968	-2.48732
C	2.23152	3.6491	-1.25275
C	1.81014	2.428	-0.7075
C	0.90472	1.5848	-1.37678
C	0.43788	2.01482	-2.63438
H	0.43024	3.56218	-4.13702
H	2.0197	5.02538	-2.90688
H	1.15992	-0.0239	-1.4561
H	-0.24481	1.38231	-3.19609
C	3.19361	4.4906	-0.4741
H	2.74598	4.96548	0.41018
N	4.43084	4.74134	-0.64522
C	5.29395	4.20705	-1.72366
C	5.23029	5.19404	-2.90444
H	4.24353	5.17227	-3.37731
H	5.42993	6.21802	-2.56782
H	5.97858	4.92861	-3.66085
C	4.98316	2.77501	-2.20469
H	4.90288	2.08715	-1.35595
H	4.05956	2.71288	-2.78339
H	5.80247	2.42496	-2.84426
C	6.71607	4.22137	-1.12619
H	6.78405	3.53336	-0.27447
H	7.45723	3.91395	-1.8733
H	6.97469	5.22509	-0.77067
H	2.19745	2.13245	0.2635
C	4.74874	0.07062	0.95045
H	5.61434	0.34545	1.56346
H	5.11023	-0.45551	0.06053
H	4.2488	0.98589	0.61973
C	4.48729	-2.11258	2.1605
H	5.0153	-2.56602	1.31395
H	5.2248	-1.88788	2.93995
H	3.7802	-2.84986	2.54914
C	3.71417	1.05643	3.49622
H	3.06839	1.52528	4.24776
H	4.6172	0.69773	4.00362
H	4.00194	1.82493	2.77414
C	2.38974	-1.04178	3.88422
H	3.17026	-1.47166	4.52169
H	1.69754	-0.47926	4.52014
H	1.82172	-1.84849	3.41289
C	0.60111	-5.55202	-0.84048
H	0.64995	-6.34817	-1.59259
H	1.28892	-5.81104	-0.02801
H	-0.41116	-5.52286	-0.42963
C	2.48783	-4.21336	-1.81315
H	3.07636	-4.35737	-0.90128
H	2.73158	-5.01861	-2.51499
H	2.78386	-3.25745	-2.25711
C	-1.38979	-4.11596	-2.43146
H	-2.00033	-3.58993	-3.17402
H	-1.5386	-5.1922	-2.57103
H	-1.74633	-3.82878	-1.43728
C	0.55906	-4.07388	-4.0198
H	0.59795	-5.16141	-4.15172

H	-0.13712	-3.66877	-4.76336
H	1.54977	-3.66096	-4.22611
C	-3.2715	-4.20744	1.42261
H	-3.67753	-4.69931	2.31415
H	-4.07955	-4.11478	0.68801
H	-2.49891	-4.84983	0.99198
C	-0.66303	-4.07459	2.72097
H	0.22954	-3.92005	3.33707
H	-1.18735	-4.96242	3.09129
H	-0.33158	-4.2502	1.69391
C	-1.94007	-2.53581	4.24022
H	-2.61518	-3.31289	4.61745
H	-1.04757	-2.52461	4.87569
H	-2.43369	-1.56563	4.34015
C	-3.86796	-1.88025	2.15097
H	-4.54961	-1.78224	1.29908
H	-4.43789	-2.25538	3.00796
H	-3.48688	-0.88246	2.39277
C	-4.62133	2.69516	0.56251
C	-5.00975	2.10677	-0.6056
H	-6.00389	2.303	-0.99124
H	-5.31432	3.34769	1.08138
C	-1.0412	3.31243	4.09354
H	-1.00177	4.40818	4.07677
H	-1.64397	3.02029	4.96192
H	-0.02326	2.94467	4.25597
C	-3.81865	3.97501	3.10669
H	-4.11118	4.83337	2.48952
H	-4.7408	3.45205	3.38913
H	-3.36329	4.36153	4.01926
C	-3.84651	-0.95968	-4.4696
H	-4.68593	-1.6583	-4.36849
H	-4.09397	-0.26775	-5.28357
H	-2.96952	-1.53634	-4.78002
C	-5.87947	0.83547	-3.13612
H	-6.66057	0.51623	-2.43519
H	-6.04437	1.90116	-3.33708
H	-6.03043	0.29346	-4.07063

Thermal correction to Energy=1.155523

Thermal correction to Enthalpy=1.156673

Thermal correction to Gibbs Free Energy=0.932200

Sum of electronic and zero-point Energies=-2549.222787

Sum of electronic and thermal Energies=-2549.133405

Sum of electronic and thermal Enthalpies=-2549.132255

Sum of electronic and thermal Free Energies=-2549.356729

SCF Done: E(RM11L) = -2550.35424267

6d'

Number of Negative Frequencies =0

B	1.28657	-0.19793	1.43493
B	1.37829	-1.52873	-1.24178
B	-0.41107	-1.56606	1.17926
C	-2.50271	1.32991	0.99621
H	-2.85879	0.3172	1.12982
C	-3.29478	2.42066	1.41291
C	-2.79329	3.71098	1.24371
C	-1.48583	3.85353	0.69548
C	-0.77229	2.68877	0.32088
C	0.56686	2.79334	-0.19626
C	1.19035	4.05869	-0.32038
C	2.53632	4.12689	-0.78191
C	3.18686	2.93017	-1.08408
C	2.47866	1.7218	-0.94411
H	2.94673	0.77559	-1.1843
C	3.1992	-0.27511	2.71796
C	2.23124	0.83282	3.26951
C	2.3208	-3.49303	-2.00251
C	3.14638	-2.27318	-2.5427
C	-1.67055	-2.44282	2.90777
C	-0.71363	-3.53899	2.32123
Ir	0.08518	-0.21899	-0.35576
N	-1.29571	1.44329	0.45903
N	1.21551	1.64189	-0.53
O	2.6177	-0.57528	1.42149
O	0.98499	0.51605	2.58762
O	1.09813	-2.85764	-1.55786
O	2.65094	-1.19247	-1.71278
O	-1.61343	-1.42206	1.87871
O	0.23025	-2.73959	1.56274
H	-0.84826	-1.52601	-0.46754
C	-0.64217	0.24802	-2.34991
C	0.26522	0.73658	-3.31754
C	-0.12346	1.15411	-4.59125
H	0.62428	1.51837	-5.29399
C	-1.4709	1.09263	-4.96483
H	-1.79	1.41685	-5.95271
C	-2.39257	0.58854	-4.05693
C	-1.99953	0.15951	-2.77042

C	-0.84148	5.12474	0.52481	C	-1.14582	-1.81076	4.20117
C	0.43208	5.22161	0.04581	H	-1.75898	-0.9359	4.44316
H	0.88684	6.2005	-0.05437	H	-1.19494	-2.51029	5.04251
H	-1.37505	6.02898	0.7953	H	-0.11614	-1.46792	4.07615
C	-4.64139	2.13708	2.03239	C	-3.12028	-2.88202	3.08549
H	-4.81596	1.05949	2.1038	H	-3.18633	-3.70973	3.80105
H	-4.71206	2.55394	3.04428	H	-3.71527	-2.04893	3.47639
H	-5.45887	2.56984	1.44374	H	-3.56616	-3.20108	2.14122
C	-3.58176	4.93326	1.63814	C	2.81424	-1.91503	-3.99587
H	-3.08726	5.47347	2.45542	H	3.27226	-0.95032	-4.23961
H	-3.66774	5.63047	0.79633	H	3.20003	-2.66357	-4.69637
H	-4.59144	4.68298	1.96686	H	1.73385	-1.81958	-4.13933
C	4.61993	2.86413	-1.55426	C	4.65681	-2.37805	-2.35625
H	5.30493	3.30234	-0.8186	H	5.05826	-3.2385	-2.90416
H	4.92599	1.8263	-1.71784	H	5.14189	-1.47453	-2.74379
H	4.76099	3.40662	-2.4967	H	4.9261	-2.47789	-1.30165
C	3.21842	5.46362	-0.91244	C	1.97504	-4.5503	-3.04609
H	2.65623	6.1261	-1.58159	H	2.88375	-4.99645	-3.46709
H	3.28018	5.96686	0.06058	H	1.38923	-5.35127	-2.58115
H	4.23156	5.37468	-1.30639	H	1.38149	-4.13009	-3.86216
C	4.64152	0.1746	2.5089	C	2.95955	-4.1468	-0.77064
H	5.0937	0.48937	3.45643	H	2.24185	-4.84446	-0.32719
H	5.23236	-0.6576	2.11041	H	3.86763	-4.70285	-1.02904
H	4.70619	1.0028	1.79832	H	3.20621	-3.39386	-0.016
C	3.15751	-1.57405	3.52847	H	1.3226	0.77662	-3.07347
H	3.71094	-2.34835	2.98677	C	-3.87931	0.46707	-4.4396
H	3.61103	-1.4529	4.51812	H	-4.02964	0.87079	-5.41905
H	2.1284	-1.92348	3.64577	N	-4.27436	-0.9488	-4.42727
C	1.99242	0.7915	4.77517	C	-5.67307	-1.07106	-4.86265
H	2.92895	0.95721	5.31997	C	-6.25527	-2.40206	-4.35168
H	1.28937	1.58205	5.06039	H	-5.48632	-2.96376	-3.86372
H	1.57063	-0.16463	5.09312	H	-7.04584	-2.20288	-3.65869
C	2.62246	2.25125	2.83831	H	-6.63818	-2.96431	-5.1776
H	1.80499	2.93677	3.08478	C	-5.73642	-1.04	-6.40104
H	3.52581	2.59347	3.35458	H	-4.97538	-1.67619	-6.80226
H	2.7958	2.30391	1.7603	H	-6.69634	-1.38379	-6.72549
C	0.05109	-4.35223	3.35905	H	-5.58156	-0.03843	-6.74423
H	0.71203	-5.06639	2.85566	C	-6.49283	0.10078	-4.29136
H	0.66735	-3.71487	3.99705	H	-7.23601	-0.27729	-3.6208
H	-0.6407	-4.91827	3.9935	H	-5.84268	0.76728	-3.76413
C	-1.41134	-4.47161	1.32342	H	-6.96938	0.62656	-5.09221
H	-0.65308	-5.06297	0.80006	H	-2.74953	-0.26681	-2.13745
H	-2.10102	-5.15822	1.82607	Thermal correction to Energy=1.158587			
H	-1.96884	-3.90063	0.57365	Thermal correction to Enthalpy=1.159737			

Thermal correction to Gibbs Free Energy=0.938184

Sum of electronic and zero-point Energies=-2549.257931

Sum of electronic and thermal Energies=-2549.168769

Sum of electronic and thermal Enthalpies=-2549.167619

Sum of electronic and thermal Free Energies=-2549.389172

SCF Done: E(RM11L) = -2550.39621086

7d'

Number of Negative Frequencies =0

Ir	-0.08865	-0.36403	-0.77302
B	1.94052	-0.75468	-1.12044
B	0.5292	-2.04442	0.3354
O	2.41777	-1.22287	-2.33626
O	2.99839	-0.48201	-0.25474
C	-1.87137	2.43153	2.19007
C	-0.01091	1.47312	3.39537
C	0.3081	0.77673	2.21321
H	1.16321	0.11661	2.18871
C	-3.4474	2.47659	-0.20903
N	-1.93478	0.82341	-1.12501
N	-0.3865	0.85489	1.08505
O	0.4594	-2.08127	1.73231
O	1.1498	-3.20533	-0.13132
C	-2.29699	1.65801	-0.11806
C	-1.48948	1.65274	1.07188
O	-2.55332	-1.28653	0.81157
O	-2.04783	-2.90195	-0.71754
C	-3.78119	3.29223	0.92469
C	-3.03542	3.2642	2.06694
H	-4.65439	3.93305	0.87619
H	-3.33223	3.88198	2.90706
C	-4.23086	2.43271	-1.39835
C	-1.10259	2.34167	3.38509
C	1.30496	-4.13179	0.97728
C	1.28341	-3.16936	2.21585
C	-3.44584	-3.11757	-0.37371
C	-3.60805	-2.27181	0.94439
C	3.84809	-1.42502	-2.24931
C	4.24278	-0.53896	-1.00778
H	-0.12128	-1.21044	-2.1097
C	-3.8314	1.56907	-2.42101
C	4.07257	-2.92267	-2.02676
H	3.56488	-3.24866	-1.11891
H	3.63716	-3.47561	-2.86622
H	5.13717	-3.17359	-1.96335
C	4.47679	-0.99159	-3.57194
H	5.57004	-1.05989	-3.52757
H	4.12929	-1.65129	-4.37475
H	4.19938	0.03203	-3.83522
C	4.61242	0.89843	-1.39052
H	4.71816	1.49946	-0.48258
H	5.56133	0.93403	-1.93606
H	3.83559	1.35841	-2.00647
C	5.32272	-1.1294	-0.10575
H	6.27303	-1.21837	-0.64464
H	5.48208	-0.47057	0.75527
H	5.04393	-2.11604	0.2716
C	2.59836	-4.92269	0.8109
H	2.73132	-5.61218	1.65291
H	2.55649	-5.51595	-0.10875
H	3.47614	-4.27595	0.75777
C	0.10623	-5.08523	0.92688
H	-0.82897	-4.5301	1.0109
H	0.09997	-5.59611	-0.04156
H	0.15226	-5.84119	1.71816
C	0.64277	-3.74633	3.47382
H	1.19793	-4.62418	3.82364
H	0.65545	-2.99578	4.27214
H	-0.39645	-4.03473	3.30141
C	2.65663	-2.57174	2.54522
H	3.34352	-3.32223	2.9512
H	3.10145	-2.11483	1.65765
H	2.52957	-1.78642	3.29934
C	-4.27135	-2.57517	-1.54635
H	-3.97095	-3.09361	-2.46305
H	-5.34397	-2.73609	-1.39484
H	-4.09509	-1.50512	-1.69184
C	-3.69023	-4.61489	-0.21521
H	-3.52544	-5.11987	-1.1734
H	-3.01906	-5.0629	0.52063
H	-4.72428	-4.80519	0.09448
C	-3.32026	-3.06437	2.22304
H	-3.27422	-2.36966	3.06831
H	-4.10041	-3.80575	2.42604
H	-2.35648	-3.57501	2.15932
C	-4.9392	-1.53567	1.07599
H	-5.77577	-2.24332	1.10084
H	-4.95178	-0.96313	2.01011

H	-5.09682	-0.83505	0.25207
C	-4.58896	1.41924	-3.71782
H	-4.62673	2.36386	-4.27302
H	-4.11227	0.67346	-4.36138
H	-5.62335	1.09949	-3.54495
C	-5.45689	3.29978	-1.51872
H	-6.19048	3.04853	-0.74256
H	-5.20023	4.358	-1.38787
H	-5.94625	3.19217	-2.48748
C	-1.47444	3.17113	4.58674
H	-1.4924	4.23777	4.33284
H	-2.4751	2.90946	4.95263
H	-0.77278	3.03825	5.41135
C	0.86405	1.2664	4.6073
H	1.38482	2.18882	4.89114
H	0.2786	0.93846	5.47406
H	1.62369	0.50347	4.4113
C	-2.67662	0.78692	-2.22507
H	-2.34733	0.09708	-2.99338
B	-1.6216	-1.72882	-0.11569
C	1.38298	2.48922	-1.44204
C	0.75576	1.30658	-1.91649
C	0.42998	1.29524	-3.29349
C	0.64767	2.37961	-4.14237
C	1.2288	3.54954	-3.64006
C	1.60051	3.588	-2.30355
H	-0.01567	0.39984	-3.71755
H	0.3727	2.30983	-5.19332
H	1.4111	4.40392	-4.28782
C	2.29489	4.83339	-1.7218
H	2.32766	5.60305	-2.46439
N	1.54337	5.31219	-0.55267
C	1.59787	6.78033	-0.50279
C	0.76307	7.36453	-1.65754
H	0.50682	8.37919	-1.43461
H	1.33332	7.33121	-2.5623
H	-0.13094	6.78909	-1.77801
C	3.05975	7.24471	-0.6401
H	3.43029	7.54433	0.31794
H	3.65567	6.44002	-1.01726
H	3.10903	8.07244	-1.31637
C	1.02788	7.26981	0.8415
H	0.35499	6.53533	1.23221
H	1.8291	7.42365	1.5338
H	0.50352	8.19054	0.69251
H	1.78582	2.56658	-0.45379

Thermal correction to Energy=1.159234

Thermal correction to Enthalpy=1.160384

Thermal correction to Gibbs Free Energy=0.939254

Sum of electronic and zero-point Energies=-2549.258827

Sum of electronic and thermal Energies=-2549.169730

Sum of electronic and thermal Enthalpies=-2549.168580

Sum of electronic and thermal Free Energies=-2549.389710

SCF Done: E(RM11L) = -2550.39459666

TS8d'

Number of Negative Frequencies =1

Ir	0.15681	0.44253	-0.69875
B	-1.82932	0.18699	-1.4045
B	-1.06443	1.80141	0.28538
O	-2.22556	0.55795	-2.69183
O	-2.95228	-0.18031	-0.65153
C	2.4065	-2.30335	2.00927
C	0.648	-1.479	3.44274
C	0.20161	-0.71899	2.34239
H	-0.65525	-0.06581	2.4395
C	3.83871	-2.02934	-0.46391
N	2.16039	-0.4241	-1.1501
N	0.77611	-0.71981	1.14606
O	-1.15706	1.83062	1.6834
O	-1.87217	2.80146	-0.25311
C	2.64123	-1.30845	-0.24103
C	1.91083	-1.45564	0.98974
O	2.3161	1.82592	0.96995
O	1.42856	3.35141	-0.47817
C	4.27519	-2.93616	0.56029
C	3.59406	-3.06418	1.7359
H	5.17482	-3.52009	0.40255
H	3.96904	-3.74412	2.49279
C	4.56031	-1.80518	-1.67198
C	1.7342	-2.3351	3.26536
C	-2.36481	3.64194	0.82156
C	-2.26005	2.68904	2.06269
C	2.69149	3.91672	-0.0318
C	2.99728	3.07399	1.2568
C	-3.668	0.53601	-2.78291
C	-4.07773	-0.35339	-1.54845
H	0.04923	1.29386	-2.02698

C	4.05551	-0.87102	-2.57945	H	1.29669	3.84795	2.37658
C	-4.14383	1.98788	-2.67558	C	4.47416	2.77592	1.49947
H	-3.80501	2.42769	-1.73701	H	5.04402	3.70271	1.63307
H	-3.69891	2.56551	-3.49358	H	4.58393	2.17595	2.40991
H	-5.23384	2.07021	-2.75127	H	4.9119	2.21212	0.67178
C	-4.0593	-0.0438	-4.14131	C	4.73965	-0.53188	-3.88093
H	-5.14771	-0.14767	-4.22303	H	4.83011	-1.41152	-4.52926
H	-3.72332	0.62841	-4.93882	H	4.17526	0.22898	-4.42876
H	-3.6011	-1.02127	-4.31174	H	5.751	-0.14227	-3.71494
C	-4.17295	-1.84821	-1.8819	C	5.83902	-2.55925	-1.93174
H	-4.27554	-2.41683	-0.95188	H	6.58399	-2.34306	-1.15595
H	-5.04054	-2.06244	-2.51509	H	5.66346	-3.64166	-1.91648
H	-3.27269	-2.20322	-2.3891	H	6.27956	-2.30675	-2.89704
C	-5.34734	0.09088	-0.82673	C	2.21575	-3.25429	4.35796
H	-6.21683	0.01285	-1.48963	H	2.28304	-4.28624	3.99408
H	-5.52422	-0.55633	0.03969	H	3.2167	-2.9677	4.70508
H	-5.27437	1.12066	-0.46978	H	1.54938	-3.25067	5.22177
C	-3.78096	4.10669	0.49697	C	-0.08646	-1.33954	4.7544
H	-4.18883	4.69639	1.3264	H	-0.60016	-2.26633	5.03598
H	-3.77105	4.74062	-0.39627	H	0.59979	-1.08477	5.57019
H	-4.4524	3.26648	0.30774	H	-0.84041	-0.54863	4.69367
C	-1.42293	4.8485	0.90545	C	2.84995	-0.21425	-2.26483
H	-0.39856	4.52256	1.09616	H	2.42738	0.51017	-2.95238
H	-1.42741	5.37002	-0.05745	B	1.33442	2.05361	0.00893
H	-1.73156	5.55513	1.68345	C	-0.87708	-2.66682	-1.05458
C	-1.91435	3.37571	3.3798	C	-0.5041	-1.45862	-1.69758
H	-2.68866	4.10148	3.65407	C	-0.07242	-1.56482	-3.0385
H	-1.84997	2.63036	4.18074	C	0.06524	-2.78586	-3.69329
H	-0.95349	3.89304	3.32469	C	-0.25526	-3.97256	-3.02015
C	-3.48194	1.77897	2.23932	C	-0.73673	-3.9031	-1.71989
H	-4.36954	2.33835	2.55418	H	0.16463	-0.65345	-3.5796
H	-3.6978	1.24444	1.31105	H	0.41407	-2.81539	-4.72361
H	-3.25859	1.03297	3.01069	H	-0.15376	-4.93459	-3.51699
C	3.70301	3.6761	-1.16004	C	-1.16358	-5.18079	-0.97364
H	3.32566	4.13472	-2.0801	H	-2.21341	-5.14137	-0.7706
H	4.67959	4.11617	-0.93117	N	-0.86932	-6.35599	-1.80624
H	3.83651	2.60512	-1.34752	C	-2.11086	-7.10195	-2.05726
C	2.50979	5.41322	0.19864	C	-3.0941	-6.21319	-2.84144
H	2.26741	5.90633	-0.74923	H	-3.47958	-5.45196	-2.1958
H	1.69922	5.6214	0.90073	H	-2.58456	-5.75806	-3.66493
H	3.43233	5.85975	0.58736	H	-3.90132	-6.81202	-3.20844
C	2.36184	3.65048	2.52651	C	-2.74563	-7.50889	-0.71448
H	2.45513	2.91688	3.33455	H	-3.32306	-8.39971	-0.84836
H	2.85295	4.5772	2.84212	H	-1.97413	-7.68867	0.0048

H	-3.38076	-6.72104	-0.3669
C	-1.79352	-8.36524	-2.87883
H	-1.09745	-8.97473	-2.34133
H	-2.69475	-8.91688	-3.04726
H	-1.36786	-8.08185	-3.81872
H	-1.34374	-2.66164	-0.09172

Thermal correction to Energy=1.157137

Thermal correction to Enthalpy=1.158287

Thermal correction to Gibbs Free Energy=0.938176

Sum of electronic and zero-point Energies=-2549.252004

Sum of electronic and thermal Energies=-2549.163493

Sum of electronic and thermal Enthalpies=-2549.162343

Sum of electronic and thermal Free Energies=-2549.382454

SCF Done: E(RM11L) = -2550.38863846

TS2

Number of Negative Frequencies =1

Ir	-0.8444	-1.9253	-0.5702
B	0.9699	-1.4526	-1.4969
O	1.9994	-2.308	-1.887
O	1.3797	-0.1322	-1.7531
C	3.0491	-1.5728	-2.547
C	2.8032	-0.1126	-2.0286
O	0.7002	1.2657	0.9532
C	-0.0976	2.3771	0.4449
B	-0.0021	0.1009	0.8225
C	-1.2959	1.6852	-0.3326
B	0.4784	-1.4619	1.3995
O	-1.2096	0.3083	0.161
O	1.8365	-1.8495	1.3515
O	-0.0932	-1.9571	2.5923
C	2.2176	-2.2741	2.6775
C	0.8642	-2.8143	3.2548
C	4.3864	-2.1877	-2.1407
H	4.4489	-3.2112	-2.5231
H	5.2245	-1.6156	-2.5528
H	4.4847	-2.224	-1.0543
C	2.8294	-1.7282	-4.0555
H	2.7816	-2.7923	-4.2984
H	1.8781	-1.2826	-4.3524
H	3.6356	-1.2657	-4.6336
C	3.5171	0.1921	-0.7063
H	4.5998	0.2743	-0.8481
H	3.1383	1.1371	-0.3104
H	3.2978	-0.5793	0.0337
C	3.0923	0.9835	-3.052
H	4.1403	0.9482	-3.3688
H	2.4574	0.8862	-3.9347
H	2.9106	1.9665	-2.6081
C	-2.6834	2.2044	0.0392
H	-3.4387	1.6208	-0.4925
H	-2.886	2.1079	1.1044
H	-2.7891	3.2539	-0.2545
C	-0.5393	3.1693	1.6803
H	0.3511	3.4965	2.224
H	-1.1254	4.052	1.4083
H	-1.1344	2.5447	2.3506
C	0.8093	3.2254	-0.4419
H	1.6334	3.6242	0.1564
H	1.2276	2.6212	-1.2461
H	0.2583	4.0669	-0.874
C	-1.1575	1.6421	-1.8538
H	-0.2051	1.2087	-2.1496
H	-1.9567	1.0088	-2.2514
H	-1.2658	2.6439	-2.2809
C	3.3256	-3.3134	2.5679
H	3.011	-4.1506	1.9486
H	4.212	-2.8622	2.1114
H	3.6042	-3.6893	3.5584
C	2.7276	-1.0257	3.4147
H	3.0927	-1.264	4.4188
H	3.5486	-0.5892	2.8393
H	1.9381	-0.2732	3.493
C	0.6829	-2.6422	4.7616
H	1.4523	-3.1942	5.3121
H	0.7273	-1.5911	5.0542
H	-0.2952	-3.0349	5.0554
C	0.5724	-4.2613	2.849
H	-0.4557	-4.5063	3.1132
H	0.6833	-4.389	1.7743
H	1.24	-4.9627	3.3598
C	-2.47312	-4.03104	-1.44211
C	-2.94582	-5.10255	-2.24363
C	-3.39355	-3.26342	-0.656
C	-3.83413	-1.45203	0.90762
H	-3.47291	-0.62028	1.53074
C	-5.19122	-1.76426	0.87919
C	-5.66374	-2.81426	0.09533

C	-4.778	-3.5746	-0.67896
C	-5.22694	-4.66716	-1.50208
C	-4.35576	-5.39369	-2.24605
H	-4.70303	-6.22823	-2.87453
H	-6.30445	-4.89302	-1.50658
N	-2.92084	-2.19198	0.14553
N	-1.0887	-3.71994	-1.41906
H	-5.87844	-1.19115	1.46587
H	-6.70855	-3.04461	0.08156
H	-0.49299	-4.03533	-2.15775
H	-0.90763	-4.56322	-0.913
H	-2.26787	-5.68249	-2.83435

Thermal correction to Energy=0.762546

Thermal correction to Enthalpy=0.763696

Thermal correction to Gibbs Free Energy=0.609668

Sum of electronic and zero-point Energies=-1794.942030

Sum of electronic and thermal Energies=-1794.884111

Sum of electronic and thermal Enthalpies=-1794.882961

Sum of electronic and thermal Free Energies=-1795.036989

SCF Done: E(RM11L) = -1795.1140425488

TS2'

Number of Negative Frequencies =1

Ir	0.26294	0.08258	0.84806
B	-1.35585	-1.14569	0.76782
O	-1.18007	-2.54178	0.61708
O	-2.7308	-0.87286	0.83372
C	-2.4645	-3.20115	0.68957
C	-3.45629	-2.03001	0.35547
O	-2.35518	1.7642	-1.0024
C	-2.9599	2.83336	-0.22043
B	-1.05986	1.56975	-0.59192
C	-1.97988	2.99624	1.00693
B	0.06451	0.42885	-1.3044
O	-0.73826	2.38838	0.49682
O	-0.48526	-0.61102	-2.11839
O	1.2559	0.90644	-1.94494
C	0.26815	-0.69401	-3.33662
C	1.64824	-0.06834	-2.92643
C	-2.47801	-4.35785	-0.30651
H	-1.7515	-5.12004	-0.00111
H	-3.46632	-4.8309	-0.34814
H	-2.20907	-4.01979	-1.31051
C	-2.62199	-3.73257	2.12009
H	-1.78051	-4.39648	2.34877
H	-2.61277	-2.91126	2.84456
H	-3.54964	-4.30147	2.24812
C	-3.66645	-1.82622	-1.15133
H	-4.23352	-2.64922	-1.60138
H	-4.22678	-0.89767	-1.30171
H	-2.7056	-1.71532	-1.66243
C	-4.80156	-2.10277	1.07185
H	-5.34605	-3.0127	0.79235
H	-4.68375	-2.0883	2.15868
H	-5.41806	-1.24185	0.78917
C	-1.65453	4.4358	1.3935
H	-0.93444	4.43809	2.21926
H	-1.21753	4.99392	0.56197
H	-2.55693	4.95878	1.72971
C	-3.01548	4.06287	-1.13264
H	-3.59721	3.81541	-2.02696
H	-3.49336	4.91484	-0.6371
H	-2.01346	4.36174	-1.45718
C	-4.37004	2.38602	0.15761
H	-4.97426	2.28011	-0.75011
H	-4.34718	1.41917	0.6642
H	-4.85704	3.12334	0.80616
C	-2.39089	2.19852	2.24477
H	-2.59148	1.15616	1.99072
H	-1.57074	2.22328	2.97069
H	-3.2797	2.63434	2.71477
C	0.3312	-2.15392	-3.78181
H	0.71255	-2.79739	-2.9845
H	-0.67361	-2.50572	-4.04339
H	0.97117	-2.27122	-4.66489
C	-0.47051	0.14475	-4.39091
H	-0.00411	0.07376	-5.38029
H	-1.50175	-0.21631	-4.46987
H	-0.50446	1.19749	-4.09226
C	2.39411	0.63991	-4.05539
H	2.61669	-0.05357	-4.87524
H	1.81399	1.47637	-4.4539
H	3.3446	1.03844	-3.68124
C	2.58115	-1.08206	-2.24422
H	3.42187	-0.54417	-1.7938
H	2.05769	-1.61404	-1.44472
H	2.98343	-1.81434	-2.95399
C	2.83059	-1.3167	1.36676

C	3.74914	-2.33523	1.48215
C	3.25868	0.01377	1.11984
C	2.69453	2.22598	0.70333
H	1.89745	2.94945	0.56235
C	4.0549	2.59727	0.5991
C	5.02966	1.63652	0.74607
C	4.65134	0.29221	1.00873
C	5.57828	-0.77494	1.14041
C	5.13353	-2.06047	1.36445
H	5.84411	-2.87656	1.45454
H	6.64007	-0.56199	1.05152
N	2.30419	0.98589	0.9527
C	0.82866	-2.84368	1.72185
C	1.80862	-4.02361	1.8598
C	3.18203	-3.80613	1.75029
N	1.3143	-1.5573	1.48748
H	-0.22488	-3.01068	1.80579
C	4.41464	4.06589	0.30696
H	4.27202	4.26774	-0.73411
H	3.7843	4.70921	0.88463
H	5.43757	4.24112	0.56737
C	6.52347	1.98932	0.6209
H	6.97814	1.96461	1.58918
H	7.00545	1.27882	-0.01769
H	6.62473	2.96964	0.20423
C	1.2722	-5.44377	2.11868
H	1.57133	-6.08922	1.31942
H	1.66855	-5.81196	3.04184
H	0.204	-5.41685	2.17463
C	4.1579	-4.98943	1.88843
H	4.73374	-5.08342	0.9915
H	4.81314	-4.81657	2.71648
H	3.60485	-5.89046	2.05328

Thermal correction to Energy=0.903127

Thermal correction to Enthalpy=0.904278

Thermal correction to Gibbs Free Energy=0.726600

Sum of electronic and zero-point Energies=-2066.447527

Sum of electronic and thermal Energies=-2066.378172

Sum of electronic and thermal Enthalpies=-2066.377022

Sum of electronic and thermal Free Energies=-2066.554699

SCF Done: E(RM11L) = -2067.37494436

B_2Pin_2

Number of Negative Frequencies =0

6	-2.97843	0.65355	0.42156
6	-2.97768	-0.65371	-0.42175
6	2.97823	0.65369	-0.42155
6	2.97791	-0.65373	0.42158
5	-0.84902	0.00079	0.00057
5	0.84904	0.00074	0.00039
8	1.61113	-0.72276	0.88179
8	1.61132	0.72374	-0.88121
8	-1.61068	-0.72264	-0.88131
8	-1.61174	0.72355	0.88195
6	-3.22433	-1.90433	0.4106
1	-4.26846	-1.9739	0.73812
1	-2.9946	-2.78377	-0.20039
1	-2.57748	-1.93062	1.29482
6	-3.89752	-0.64376	-1.62457
1	-3.81523	-1.59807	-2.15608
1	-4.94266	-0.51781	-1.31338
1	-3.64052	0.15541	-2.32522
6	-3.22553	1.90404	-0.41085
1	-4.26955	1.97294	-0.73886
1	-2.9967	2.78358	0.20033
1	-2.57826	1.93086	-1.29474
6	-3.89893	0.64284	1.62387
1	-3.81761	1.59712	2.15556
1	-4.9438	0.51618	1.31205
1	-3.64177	-0.15627	2.32454
6	3.89832	-0.64398	1.62397
1	3.81626	-1.59837	2.15539
1	4.94332	-0.51803	1.31229
1	3.64171	0.15509	2.32488
6	3.22571	1.90406	0.41091
1	4.26991	1.973	0.73829
1	2.99641	2.78371	-0.19996
1	2.57895	1.93063	1.29518
6	3.89812	0.64317	-1.62434
1	3.81643	1.59752	-2.15588
1	4.94317	0.51659	-1.31309
1	3.64067	-0.15586	-2.32497
6	3.22411	-1.90427	-0.41102
1	4.26802	-1.97373	-0.73924
1	2.99487	-2.78377	0.20008
1	2.57667	-1.93062	-1.2948

Thermal correction to Energy=0.393992

Thermal correction to Enthalpy=0.395142

Thermal correction to Gibbs Free Energy=0.304019

Sum of electronic and zero-point Energies=-822.226944

Sum of electronic and thermal Energies=-822.198739

Sum of electronic and thermal Enthalpies=-822.197589

Sum of electronic and thermal Free Energies=-822.288712

SCF Done: E(RB3LYP) = -822.594662061

HBPin

Number of Negative Frequencies =0

C	-0.05146	3.76227	-1.29768
C	-1.3445	4.2379	-2.03317
B	-1.85551	2.53108	-0.59136
O	-2.39692	3.61848	-1.23086
O	-0.48625	2.44664	-0.76698
C	1.1622	3.61746	-2.20008
H	1.39566	4.59341	-2.64283
H	2.02278	3.28458	-1.61828
H	0.99863	2.89609	-3.00126
C	0.29898	4.5987	-0.06414
H	1.04705	4.04907	0.51216
H	0.70752	5.57397	-0.34961
H	-0.58007	4.76101	0.56923
C	-1.55526	5.74707	-2.0351
H	-0.72658	6.24732	-2.54882
H	-2.48171	5.9931	-2.56537
H	-1.62942	6.1466	-1.02056
C	-1.48181	3.66967	-3.44931
H	-2.49956	3.85403	-3.80867
H	-0.78024	4.14427	-4.14267
H	-1.30538	2.58885	-3.45844
H	-2.58349	1.8944	0.08472

Thermal correction to Energy=0.205041

Thermal correction to Enthalpy=0.206191

Thermal correction to Gibbs Free Energy=0.148281

Sum of electronic and zero-point Energies=-411.701648

Sum of electronic and thermal Energies=-411.687883

Sum of electronic and thermal Enthalpies=-411.686733

Sum of electronic and thermal Free Energies= -411.744643

SCF Done: E(RM11L) = -411.897595782

TS5a-1

Number of Negative Frequencies=1

Ir	0.15652	-0.28158	-0.23437
H	1.19475	0.41848	-1.54887
C	-3.77151	2.40492	0.90023
C	-4.32806	3.4789	0.16134
C	-2.09505	4.01621	-0.58662
C	-1.64251	2.90147	0.18573
C	-0.25142	2.59535	0.18648
C	0.64524	3.37025	-0.5172
N	-2.48242	2.11899	0.92068
N	0.19084	1.4341	0.91917
C	-1.15458	4.79386	-1.31225
C	0.18679	4.47696	-1.26872
H	-1.50843	5.63947	-1.8959
H	0.90763	5.0749	-1.81853
C	-3.48916	4.28354	-0.57518
C	4.186	0.40792	0.7015
B	2.16248	-0.18152	-0.25933
H	-4.41837	1.7614	1.49366
C	4.41853	-0.65815	-0.42585
O	3.07614	-1.1635	-0.65072
O	2.85004	0.87732	0.39033
C	4.8979	-0.0371	-1.74328
H	5.93449	0.31047	-1.67493
H	4.84069	-0.79258	-2.53399
H	4.26404	0.80695	-2.03392
C	5.31974	-1.82346	-0.03093
H	5.41898	-2.51699	-0.87318
H	6.3218	-1.46683	0.23432
H	4.90973	-2.37859	0.81644
C	4.13877	-0.2076	2.10586
H	5.13116	-0.52371	2.44441
H	3.75862	0.5407	2.81002
H	3.46806	-1.07261	2.13479
C	5.14206	1.59566	0.67754
H	4.89895	2.28378	1.49513
H	6.17762	1.26282	0.81236
H	5.07069	2.14935	-0.26196
H	-5.39887	3.65381	0.18941
H	-3.87468	5.12135	-1.15068
H	1.69895	3.10798	-0.50399
H	-0.41558	1.28614	1.73115
H	1.15874	1.55596	1.23784
C	-0.98334	-1.17872	1.24233
C	-2.28927	-1.62728	0.919
C	-0.56419	-1.38609	2.5736

C	-3.11944	-2.23486	1.869
C	-1.37855	-2.01489	3.5234
H	0.43019	-1.05652	2.87358
C	-2.66148	-2.44317	3.17337
H	-4.12378	-2.54687	1.58826
H	-1.01314	-2.16564	4.53746
H	-3.3023	-2.92709	3.90632
C	-2.82376	-1.30608	-0.44744
H	-3.35586	-0.3463	-0.48743
N	-2.74916	-1.91603	-1.5669
C	-2.10431	-3.23708	-1.77157
C	-0.63568	-3.26919	-1.30972
H	-0.09607	-2.39274	-1.7072
H	-0.54179	-3.28541	-0.22361
H	-0.12967	-4.15709	-1.70762
C	-2.15075	-3.48052	-3.29122
H	-1.57235	-2.71463	-3.82238
H	-1.7337	-4.46256	-3.54368
H	-3.18309	-3.43779	-3.65691
C	-2.91635	-4.33335	-1.05582
H	-2.86374	-4.22088	0.03055
H	-3.96939	-4.29045	-1.35839
H	-2.52645	-5.32401	-1.31801

Thermal correction to Energy=0.619178

Thermal correction to Enthalpy=0.620328

Thermal correction to Gibbs Free Energy=0.486164

Sum of electronic and zero-point Energies=-1455.428653

Sum of electronic and thermal Energies= -1455.382069

Sum of electronic and thermal Enthalpies=-1455.380919

Sum of electronic and thermal Free Energies=-1455.515083

SCF Done: E(RM11L) = -1456.001247

TS5b'-1

Number of Negative Frequencies=1

Ir	0.26909	0.35502	-0.80971
C	-0.71618	3.22357	0.03861
C	-1.66791	4.17463	0.45378
C	-3.34624	2.44832	0.23182
C	-2.31675	1.57132	-0.17356
C	-2.5837	0.20994	-0.49547
C	-3.89637	-0.30488	-0.42875
N	-1.00818	1.95732	-0.27026
C	-4.6763	1.90911	0.29296
C	-4.93436	0.6045	-0.02137
H	-5.49491	2.5524	0.59674
H	-5.9538	0.23963	0.03811
C	-3.01124	3.79412	0.55366
C	3.28671	1.46455	1.15032
B	2.61634	1.59853	-1.04174
H	0.33215	3.4928	-0.03517
C	4.53421	1.56052	0.18393
O	3.94553	1.35947	-1.15013
O	2.16512	1.7901	0.23905
C	5.18653	2.94445	0.1535
H	5.69166	3.16808	1.0984
H	5.93064	2.96832	-0.6489
H	4.45008	3.72991	-0.0452
C	5.58445	0.4776	0.40047
H	6.39671	0.60531	-0.32259
H	6.00934	0.55236	1.40743
H	5.16582	-0.52257	0.26837
C	3.02341	0.06358	1.69596
H	3.78708	-0.21499	2.42925
H	2.04707	0.05019	2.18897
H	3.00488	-0.68287	0.9008
C	3.26173	2.48698	2.28014
H	2.34896	2.35415	2.87019
H	4.12076	2.34074	2.94368
H	3.27999	3.51305	1.90545
C	-1.7491	-1.84549	-1.17894
C	-4.12806	-1.67206	-0.74546
C	-3.02126	-2.43725	-1.12667
N	-1.49323	-0.56224	-0.85842
H	-0.89226	-2.43557	-1.47052
C	-3.12372	-3.90463	-1.4705
H	-3.5166	-4.48389	-0.62637
H	-3.79263	-4.07512	-2.32256
H	-2.14271	-4.3153	-1.72736
C	-5.51893	-2.24482	-0.66063
H	-5.93233	-2.13173	0.34956
H	-6.2024	-1.72733	-1.34603
H	-5.54305	-3.30677	-0.90942
C	-1.18915	5.57157	0.77042
H	-0.10669	5.65331	0.63066
H	-1.66523	6.31756	0.12268
H	-1.41368	5.84984	1.80712
C	-4.09019	4.75205	0.98913
H	-4.86961	4.84151	0.22222

H	-4.58169	4.39882	1.90442
H	-3.7023	5.75257	1.18571
H	1.82289	1.65048	-1.94404
C	1.396	-1.31174	-1.27073
C	2.14983	-1.36998	-2.4746
C	1.48801	-2.47887	-0.44686
C	2.9187	-2.47438	-2.84264
H	2.13285	-0.51421	-3.1471
C	2.26876	-3.59202	-0.818
C	2.98376	-3.60013	-2.00869
H	3.47111	-2.46031	-3.78085
H	3.58488	-4.46251	-2.28716
C	2.31235	-4.80395	0.13117
H	2.66425	-4.49181	1.09224
N	3.22018	-5.82246	-0.41597
C	2.54287	-7.12707	-0.42771
C	1.19244	-6.99783	-1.15656
H	0.40848	-6.88355	-0.43737
H	1.21439	-6.14257	-1.79917
H	1.01617	-7.87757	-1.73956
C	2.30222	-7.59356	1.02008
H	2.84433	-6.96245	1.69292
H	1.25723	-7.53875	1.24342
H	2.6379	-8.6036	1.12981
C	3.42439	-8.15656	-1.15892
H	4.39774	-8.17209	-0.7148
H	2.98045	-9.12685	-1.0792
H	3.50747	-7.88603	-2.19082
H	0.93879	-2.50841	0.47096

Thermal correction to Energy=0.760929

Thermal correction to Enthalpy=0.762079

Thermal correction to Gibbs Free Energy=0.601551

Sum of electronic and zero-point Energies=-1726.918153

Sum of electronic and thermal Energies= -1726.859490

Sum of electronic and thermal Enthalpies= -1726.858340

Sum of electronic and thermal Free Energies=-1727.018869

SCF Done: E(RM11L) = -1727.73962871692

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