Computational Mechanistic Analysis of a Cationic Suzuki-Miyaura Reaction Without Added Base

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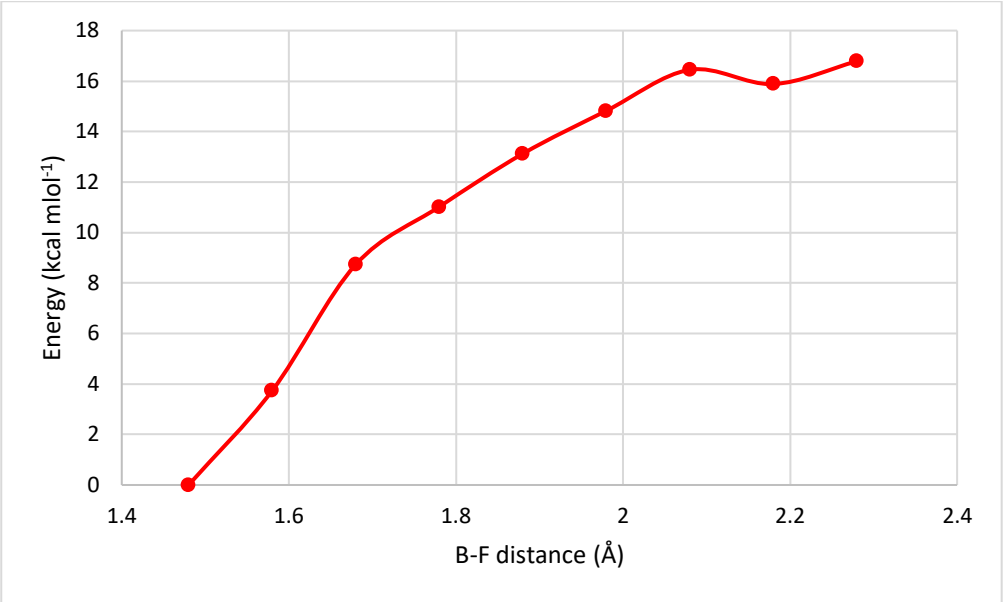
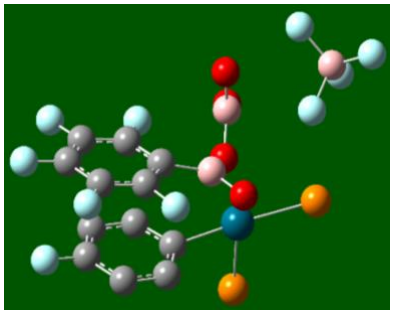
Content:

A. Scan Calculations

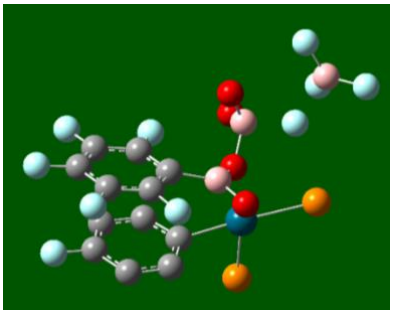
In the main text, we discuss conversion of the ion pair **11$^+$**●BF_4^- (ArPdL$^+$-O(B(OH)$_2$)-B(OH)Ar') to form B(OH)$_2$F, BF_3 and **3** (ArPdL-OB(OH)Ar'). This transformation is described in the text as occurring in two steps, with first fluoride transfer from BF_4^- to the B(OH)$_2$ moiety in **11'$^+$** to yield **12'** (ArPdL-O(B(OH)$_2$F)-B(OH)Ar') and BF_3, followed by loss of B(OH)$_2$F to yield **3**. Both of these steps are suggested to have no barrier (or possibly a very small barrier) above the endothermicity. We have studied the thermochemistry of this conversion using the full P(Ad)$_3$ model with **11$^+$** and BF_4^- as starting species, but were unable to locate any TSs. In order to check the feasibility of the process, as also mentioned in the text, we studied the same transformation but using a model species in which the bulky P(Ad)$_3$ ligand is replaced by two PH_3 ligands (with the corresponding starting species therefore being **11''$^+$**●BF_4^-). With this smaller model system, we carried out scan calculations mapping out the reaction profile from **11'$^+$**●BF_4^- to **12'** + BF_3 then from **12'** to **3'** + B(OH)$_2$F.

The graph depicted below shows the electronic energy at the same B3LYP-D3BJ/6-31G(d), SDD level of theory used in the main study, for species lying along the scan calculation for the conversion of **11'$^+$**●BF_4^- to BF_3 + **12'**. Three-dimensional structure representations of key species along this scan are shown below. The scan starts with the complex of **11'$^+$**●BF_4^-. The x-axis coordinate is the distance between the boron of tetrafluoroborate and the fluoride that is migrating from boron to oxygen, which is the coordinate used in the relaxed scan calculations. Hydrogens are omitted for clarity. The final species in the plot corresponds to a complex between **12'** and BF_3; removal of BF_3 from this species is assumed to occur without a barrier but no scan has been performed. Separate calculations of **12'** and BF_3 show that their sum of electronic energies are considerably higher (14.2 kcal mol^{-1}) than the last species of the scan where they are separated. Here, it must be stated that while modeling the real system, we have modeled the Lewis acidic species BF_3 as its complex with an external molecule of solvent, BF_3-THF. Also, we treated **11$^+$** and **BF_4^-** separately in the real system. When electronic energy of the final species in the relaxed scan is compared with the sum of **12'** and BF_3-THF, the sum of the energies of the latter species in fact lie lower than the former (-11.2 kcal mol^{-1}). When the real system data (electronic energy) is analyzed between the cases of modeling the BF_3 as itself and as BF_3-THF, in the first case, the transformation of **11$^+$** + BF_4^- to BF_3 + **12** is uphill by 7.9 kcal mol^{-1}. On the other hand, electronic energy comparison of the same transformation using an externally solvated BF_3 would make the transformation downhill by 17.5 kcal mol^{-1}. Comparison of the electronic energies of the transformation including an externally solvated BF_3 using larger basis sets of Def2TZVP and Def2QZVP yields a result that is downhill by 5.9 kcal mol^{-1}. Comparing the Gibbs energies of the same transformation in the real system, using the described larger basis sets, **12** + BF_3-THF is shown to have a higher Gibbs free energy than **11$^+$** + BF_4^- by 4.2 kcal mol^{-1}.

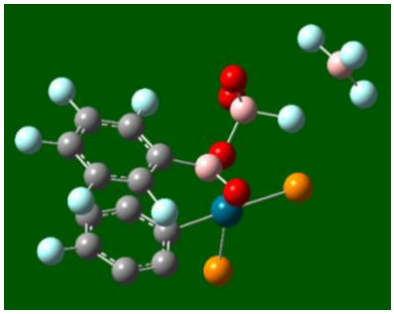




B-F distance: 1.48 Å

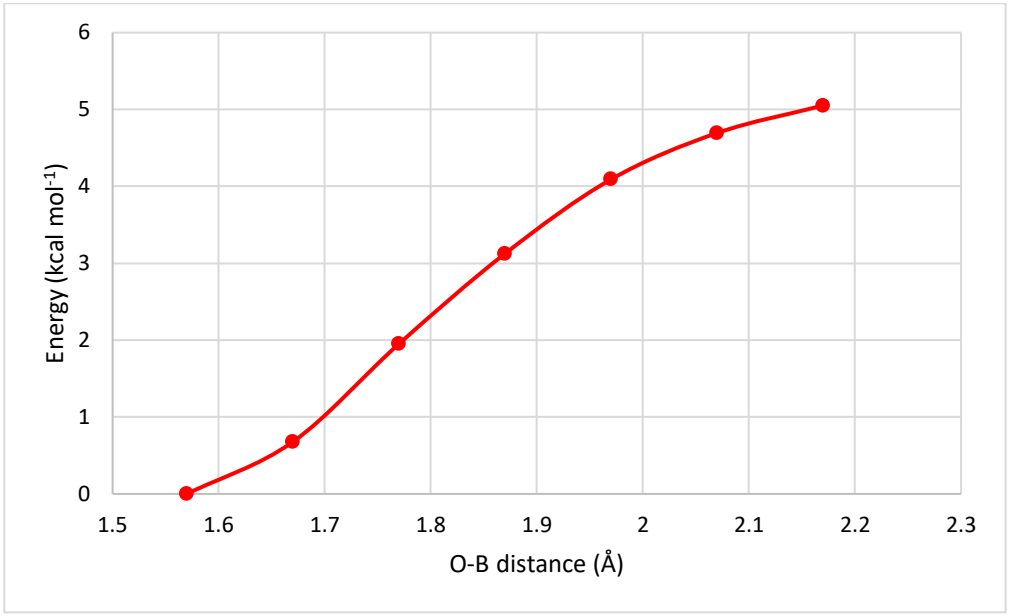


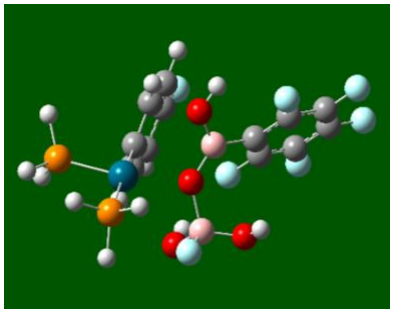
B-F distance: 1.88 Å



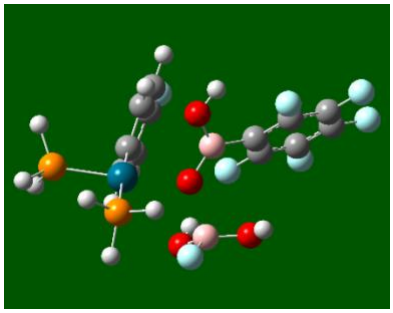
B-F distance: 2.28 Å

The graph depicted below shows the electronic energy at the same B3LYP-D3BJ/6-31G(d), SDD level of theory used in the main study, for species lying along the scan calculation for the conversion of **12'** to **3'**. Three-dimensional structure representations of key species along this scan are shown below. Scan starts with the complex of **12'** with PH_3 as the ligand. The values in x-axis are the distances between the boron of $B(OH)_2F$ and the oxygen of the arylboronic acid moiety that the $B(OH)_2F$ boron is coordinated. The selected species are shown below the graph. Hydrogens are omitted for clarity. Separate calculations of **3'** and $B(OH)_2F$ show that their sum of energies are considerably higher (15.1 kcal mol^{-1}) than the last species of the scan where they are separated. Comparing these calculations with the real system, similar results can be seen in terms of comparison of electronic energies between **12** and sum of **3** and $B(OH)_2F$. The dissociation-like reaction is uphill in terms of electronic energy by 18.9 kcal mol^{-1}. When the larger basis sets (Def2TZVP, Def2QZVP) are used for the calculations, the transformation is uphill in terms of electronic energy by 12.2 kcal mol^{-1}. The transformation is downhill in terms of Gibbs free energy (using larger basis sets) by 2.2 kcal mol^{-1}.

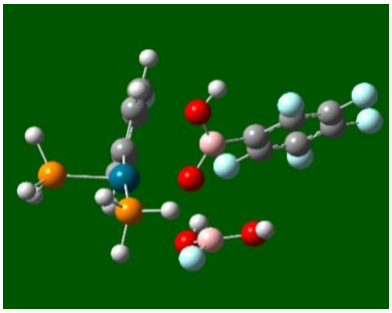




O-B distance: 1.57 Å



O-B distance: 1.87 Å



O-B distance: 2.17 Å

B. Optimized Cartesian Coordinates

For the Cartesian coordinates, E denotes the electronic energy of the species that is obtained after the optimization. G denotes the Gibbs free energy of the species that was found by the summation of E and the free energy correction using the quasi-harmonic approximation at 298 K. Esp is the energy obtained from the single point calculations that utilized larger basis sets, and ZPE denotes the zero-point energy of the species. All values are in atomic units.

TS-0

E: -2874.60346
G: -2873.80373
Esp: -2875.63222
Gcorr: 0.79973
ZPE: 0.86507
Esp + Gcorr: -2874.83249

P	1.33719	-0.09083	0.10679
C	1.92511	1.59732	0.71175
H	1.40732	1.60373	1.67867
C	1.44634	2.89608	0.00651
C	3.44713	1.76392	1.01421
H	0.40987	2.79734	-0.28862
C	2.28388	3.28487	-1.22397
C	1.56144	4.03031	1.05013
H	3.86725	0.84226	1.42555
C	4.27432	2.16879	-0.22232
C	3.57166	2.89600	2.05956
H	1.87639	4.21533	-1.64174
H	2.20272	2.52831	-2.01335
C	3.75374	3.48340	-0.82133
H	0.93683	3.79645	1.92149
H	1.17469	4.96288	0.61813
C	3.03020	4.21486	1.47208
H	4.25828	1.38838	-0.98243
H	5.32189	2.28442	0.08698
H	3.01769	2.63125	2.97012
H	4.62530	3.01785	2.34463
H	4.35073	3.74705	-1.70366
C	3.85875	4.60064	0.23228
H	3.10254	5.00780	2.22736
H	4.90996	4.75328	0.51225
H	3.49194	5.54892	-0.18325
C	2.27012	-0.41711	-1.50147
H	2.40282	0.61698	-1.82974
C	1.46684	-1.10199	-2.63518
C	3.68643	-1.05020	-1.44799
H	0.44173	-0.71086	-2.63657
C	1.44212	-2.63213	-2.48642
C	2.16143	-0.73882	-3.96498
H	4.25791	-0.63641	-0.61146
C	3.64871	-2.58473	-1.32573
C	4.38696	-0.68881	-2.77896
H	0.85556	-3.06105	-3.31003
H	0.93557	-2.91261	-1.56136
C	2.87322	-3.19145	-2.50630
H	2.16564	0.35096	-4.10296
H	1.59979	-1.17076	-4.80403
C	3.60369	-1.28277	-3.96613
H	3.18889	-2.89406	-0.38435
H	4.68039	-2.96137	-1.31520
H	4.46059	0.40131	-2.88486
H	5.41172	-1.08340	-2.77194
H	2.84217	-4.28329	-2.40036
C	3.56433	-2.81593	-3.82879
H	4.10006	-1.00597	-4.90484
H	4.58484	-3.22201	-3.85155
H	3.02056	-3.25552	-4.67586
C	2.04751	-1.21169	1.45441
H	3.08690	-1.34409	1.13408
C	1.39727	-2.61933	1.54219
C	2.10433	-0.62669	2.89387
H	1.26637	-3.03697	0.54134
C	0.02698	-2.58003	2.24022
C	2.34090	-3.52031	2.36663
H	2.52031	0.37942	2.89034
C	0.71830	-0.59543	3.55854
C	3.04997	-1.52622	3.71840
H	-0.39192	-3.59419	2.25691
H	-0.67479	-1.96864	1.67149
C	0.15753	-2.02301	3.66214
H	3.32419	-3.58489	1.88137
H	1.93112	-4.53834	2.40562
C	2.49004	-2.95639	3.79288
H	0.03086	0.03115	2.97429
H	0.80573	-0.13956	4.55380
H	4.04962	-1.52814	3.26324
H	3.15535	-1.11019	4.72944
H	-0.83004	-1.99872	4.14041
C	1.11220	-2.91158	4.48044
H	3.17300	-3.59164	4.37118
H	1.21650	-2.52062	5.50195
H	0.69771	-3.92539	4.56175
Pd	-1.01310	-0.46774	-0.24707
C	-1.47867	1.46104	-0.09199
C	-1.69181	2.02224	1.17319
C	-1.68113	2.25351	-1.23024
C	-2.06570	3.36410	1.30793
H	-1.55650	1.42575	2.07071
C	-2.05709	3.59490	-1.11161
H	-1.52572	1.84011	-2.22087
C	-2.23374	4.12661	0.15978
H	-2.22101	3.81380	2.28383
H	-2.20421	4.22177	-1.98570
F	-2.58589	5.43265	0.28327
B	-1.83048	-2.25796	-1.47758
O	-1.07262	-2.76894	-0.60812
C	-3.12295	-0.74643	-0.44412
C	-3.76124	-1.10819	0.74133
C	-3.95562	-0.16434	-1.39398
C	-5.11446	-0.89480	0.98125
C	-5.31130	0.06459	-1.21622
C	-5.89424	-0.30049	-0.00541
F	-7.19889	-0.09201	0.20126
F	-3.05503	-1.65429	1.75802
F	-5.67475	-1.24090	2.15063
F	-3.44137	0.17846	-2.61620
F	-6.06158	0.62042	-2.17924
O	-2.31981	-2.33640	-2.72464
H	-2.76208	-1.52151	-3.01794

0

E: -2874.60754
G: -2873.80885
Esp: -2875.63699
Gcorr: 0.79869
ZPE: 0.86495
Esp + Gcorr: -2874.83830

P	1.33577	-0.12426	0.11080
C	2.00158	1.60175	0.47914
H	1.44606	1.78276	1.40781

C	1.60897	2.78812	-0.44433
C	3.51369	1.75631	0.82596
H	0.58119	2.67799	-0.77208
C	2.51654	2.94943	-1.67650
C	1.73003	4.06873	0.41377
H	3.87200	0.89513	1.39724
C	4.41006	1.93009	-0.41658
C	3.64381	3.03380	1.68678
H	2.17005	3.81861	-2.25180
H	2.43701	2.08395	-2.34451
C	3.97514	3.15339	-1.23683
H	1.06033	3.99864	1.27900
H	1.40431	4.93634	-0.17541
C	3.18606	4.26242	0.87464
H	4.38953	1.04247	-1.04777
H	5.44835	2.05240	-0.07945
H	3.04017	2.93588	2.59911
H	4.68849	3.16158	2.00116
H	4.62057	3.25235	-2.11898
C	4.08480	4.41772	-0.36604
H	3.25939	5.16125	1.50019
H	5.12863	4.57262	-0.06064
H	3.77975	5.30204	-0.94173
C	2.31934	-0.74001	-1.37918
H	2.49720	0.22321	-1.86505
C	1.53991	-1.57670	-2.42345
C	3.71473	-1.38952	-1.17317
H	0.52626	-1.16819	-2.52557
C	1.47667	-3.06687	-2.04528
C	2.28754	-1.43546	-3.76672
H	4.26491	-0.86817	-0.38428
C	3.63561	-2.88743	-0.82444
C	4.47275	-1.24710	-2.51430
H	0.90125	-3.60860	-2.80894
H	0.95272	-3.19404	-1.09721
C	2.89312	-3.65096	-1.93254
H	2.31914	-0.38003	-4.06897
H	1.74710	-1.98235	-4.55095
C	3.71734	-1.99624	-3.63016
H	3.12982	-3.04394	0.13157
H	4.65663	-3.27633	-0.71296
H	4.57972	-0.18726	-2.77870
H	5.48566	-1.65812	-2.40904
H	2.83054	-4.71372	-1.66659
C	3.63799	-3.49048	-3.26851
H	4.25249	-1.87108	-4.57988
H	4.64862	-3.91383	-3.19096
H	3.11409	-4.04225	-4.06071
C	1.93827	-1.06792	1.63558
H	2.98154	-1.29694	1.39247
C	1.20495	-2.41318	1.88854
C	1.96259	-0.28348	2.97750
H	1.10457	-2.96841	0.95279
C	-0.19492	-2.20158	2.49171
C	2.04992	-3.23127	2.88787
H	2.43798	0.68843	2.85132
C	0.55048	-0.08291	3.55111
C	2.81008	-1.10040	3.97633
H	-0.67575	-3.17840	2.63038
H	-0.83072	-1.63750	1.80400
C	-0.10178	-1.44799	3.82375
H	3.05048	-3.41652	2.47433
H	1.57910	-4.21022	3.04908
C	2.16096	-2.47239	4.22402
H	-0.06702	0.48725	2.84587
H	0.61528	0.50613	4.47572
H	3.82889	-1.22342	3.58470
H	2.89089	-0.54631	4.92125
H	-1.10897	-1.30137	4.23377
C	0.75498	-2.25610	4.81551
H	2.77437	-3.05077	4.92662
H	0.83001	-1.72525	5.77449
H	0.27724	-3.22433	5.01711
Pd	-1.07414	-0.34217	-0.18637
C	-1.44839	1.61103	-0.22728
C	-1.53574	2.34337	0.96296
C	-1.68289	2.26885	-1.44441
C	-1.80525	3.71649	0.94374
H	-1.38451	1.85683	1.92112
C	-1.94698	3.64119	-1.47950
H	-1.64185	1.72180	-2.38009
C	-1.99543	4.34145	-0.28070
H	-1.86108	4.29444	1.86111
H	-2.11326	4.16173	-2.41769
F	-2.24367	5.67722	-0.30767
B	-1.67478	-2.60637	-1.46609
O	-1.14748	-2.77416	-0.36168
C	-3.14917	-0.44039	-0.26882
C	-3.85782	-0.56122	0.92135
C	-3.94120	-0.30779	-1.39584
C	-5.24637	-0.55302	0.99560
C	-5.33117	-0.29953	-1.39179
C	-5.99036	-0.42030	-0.17379
F	-7.33059	-0.41673	-0.12601
F	-3.19251	-0.66983	2.10169
F	-5.88233	-0.66626	2.17380
F	-3.35054	-0.19234	-2.64327
F	-6.03641	-0.18022	-2.52862
O	-2.18392	-2.61047	-2.67631
H	-2.61821	-1.76403	-2.92021

1 ($ArPd^{+}L$-THF)

E: -2203.13462
G: -2202.28174
Esp: -2203.84495
Gcorr: 0.85289
ZPE: 0.91219
Esp + Gcorr: -2202.99206

P	0.73931	-0.15690	0.12544
C	1.06161	1.26994	1.30493
H	0.26232	1.05151	2.02488
C	0.78033	2.70898	0.78563
C	2.38318	1.30428	2.13032
H	-0.09003	2.71105	0.12974
C	1.98051	3.33310	0.04576
C	0.48009	3.56923	2.03331
H	2.67629	0.30127	2.44472
C	3.56132	1.94487	1.37888
C	2.07965	2.15802	3.38324
H	1.70148	4.34751	-0.26795
H	2.22466	2.77949	-0.86542
C	3.21265	3.38102	0.96143
H	-0.39393	3.16627	2.55945
H	0.22596	4.59008	1.71994
C	1.70783	3.59395	2.96404
H	3.82953	1.35103	0.50045
H	4.43731	1.94403	2.04051
H	1.26205	1.70226	3.95788
H	2.96343	2.17630	4.03414
H	4.05738	3.82383	0.41955
C	2.89748	4.22048	2.21267
H	1.47902	4.18785	3.85757
H	3.77708	4.26305	2.86881
H	2.65752	5.25196	1.92248
C	1.39615	0.25521	-1.57658
H	1.16500	1.32611	-1.56583
C	0.58532	-0.31993	-2.76949
C	2.90707	0.10855	-1.87875
H	-0.48389	-0.27406	-2.53673
C	0.96980	-1.76825	-3.10044
C	0.89614	0.56785	-3.99276
H	3.49776	0.45733	-1.02992
C	3.28932	-1.34554	-2.20347
C	3.21352	0.98841	-3.11034

H	0.39349	-2.09818	-3.97491
H	0.69454	-2.43372	-2.27736
C	2.47599	-1.85343	-3.40914
H	0.60285	1.60617	-3.78780
H	0.30588	0.22467	-4.85237
C	2.40008	0.49444	-4.32125
H	3.13981	-1.98924	-1.33248
H	4.36059	-1.38306	-2.43973
H	2.97271	2.03692	-2.89244
H	4.28729	0.94023	-3.33275
H	2.75111	-2.89282	-3.62641
C	2.78382	-0.96601	-4.63126
H	2.61710	1.12656	-5.19094
H	3.85136	-1.02743	-4.88052
H	2.22441	-1.32361	-5.50582
C	1.50544	-1.63008	1.00275
H	2.58395	-1.42674	0.99490
C	1.26759	-2.99793	0.31907
C	1.04632	-1.75664	2.49098
H	1.53947	-2.94650	-0.73224
C	-0.19448	-3.45214	0.44554
C	2.16978	-4.04523	1.00599
H	1.15118	-0.80384	3.01121
C	-0.41384	-2.22681	2.61738
C	1.95954	-2.79939	3.17013
H	-0.33262	-4.40328	-0.08229
H	-0.88387	-2.75307	-0.08756
C	-0.59551	-3.58419	1.92166
H	3.22130	-3.74968	0.90087
H	2.05111	-5.01191	0.50038
C	1.79013	-4.17003	2.49022
H	-1.10047	-1.48512	2.18139
H	-0.66904	-2.30971	3.68117
H	3.00658	-2.47431	3.11433
H	1.69666	-2.86880	4.23334
H	-1.64087	-3.90682	1.99382
C	0.32161	-4.62479	2.59636
H	2.44047	-4.90611	2.97763
H	0.03527	-4.73871	3.64964
H	0.19665	-5.60444	2.11721
Pd	-1.43668	-0.75433	-0.13092
C	-2.00960	1.14099	-0.20532
C	-2.49426	1.72054	0.97353
C	-2.05118	1.86516	-1.40171
C	-3.02471	3.01412	0.96140
H	-2.45200	1.18151	1.91518
C	-2.57693	3.16156	-1.42481
H	-1.66760	1.44260	-2.32380
C	-3.04988	3.71115	-0.24004
H	-3.40056	3.48079	1.86630
H	-2.61350	3.73967	-2.34281
F	-3.54999	4.97022	-0.25576
C	-4.34734	-1.45491	0.76939
O	-3.47416	-1.47330	-0.40420
C	-4.23455	-1.09508	-1.59823
C	-5.56866	-0.58154	-1.07366
C	-5.76066	-1.41090	0.20455
H	-4.11706	-2.34696	1.35604
H	-4.11738	-0.55885	1.35343
H	-3.65614	-0.34884	-2.14389
H	-4.34404	-1.99742	-2.20812
H	-5.49402	0.48393	-0.82918
H	-6.37275	-0.71858	-1.80131
H	-6.46441	-0.95901	0.90840
H	-6.10934	-2.42023	-0.04023

2 ($Ar'B(OH)_2$)

E: -904.42577
G: -904.37590
Esp: -904.85265
Gcorr: 0.04988
ZPE: 0.08464
Esp + Gcorr: -904.80278

B	-2.49540	-0.00000	0.00001
O	-3.21594	1.15514	0.04256
H	-2.65290	1.94247	0.06274
O	-3.21582	-1.15510	-0.04254
H	-2.65270	-1.94242	-0.06289
C	-0.90221	0.00006	-0.00001
C	-0.14920	1.17758	-0.00509
C	-0.14924	-1.17756	0.00508
C	1.23959	1.20260	-0.00573
C	1.23955	-1.20265	0.00574
C	1.93865	-0.00003	-0.00001
F	3.27248	0.00006	0.00000
F	-0.76703	2.38335	-0.00943
F	1.90497	2.36327	-0.01107
F	-0.76703	-2.38335	0.00943
F	1.90483	-2.36336	0.01109

3 (ArPdL-OB(OH)Ar')

E: -2874.64663
G: -2873.84522
Esp: -2875.67854
Gcorr: 0.80142
ZPE: 0.86691
Esp + Gcorr: -2874.87712

P	-1.38915	-0.11291	0.12172
C	-2.37766	1.44751	-0.25743
H	-2.32978	1.38308	-1.35228
C	-1.72331	2.80960	0.10904
C	-3.89239	1.53324	0.09590
H	-0.64676	2.76469	-0.04602
C	-2.01327	3.24824	1.55831
C	-2.32766	3.86197	-0.84599
H	-4.38839	0.57447	-0.06312
C	-4.16457	1.98887	1.53834
C	-4.50002	2.57878	-0.86786
H	-1.52831	4.21833	1.73009
H	-1.58285	2.55042	2.28191
C	-3.52699	3.36291	1.79371
H	-2.10211	3.59173	-1.88516
H	-1.86057	4.83762	-0.65754
C	-3.84996	3.95586	-0.62902
H	-3.78482	1.25434	2.25427
H	-5.25105	2.04230	1.68893
H	-4.35065	2.26037	-1.90835
H	-5.58334	2.64375	-0.70040
H	-3.71753	3.67286	2.82890
C	-4.12549	4.39593	0.82147
H	-4.27708	4.68808	-1.32577
H	-5.20726	4.48767	0.98862
H	-3.68315	5.38435	1.00458
C	-0.64071	0.01487	1.83437
H	-0.39015	1.08162	1.80139
C	0.72124	-0.70791	2.01448
C	-1.49882	-0.22089	3.09974
H	1.30801	-0.60174	1.09879
C	0.56621	-2.20037	2.33571
C	1.44584	-0.02154	3.19224
H	-2.48353	0.23459	2.98029
C	-1.66273	-1.71873	3.41190
C	-0.77019	0.45238	4.28373
H	1.56064	-2.63348	2.48752
H	0.12696	-2.72754	1.48530
C	-0.28312	-2.37613	3.60670
H	1.59271	1.04477	2.97274
H	2.43873	-0.46637	3.32398
C	0.61565	-0.18960	4.47980
H	-2.22398	-2.21982	2.61826
H	-2.25549	-1.82495	4.33013
H	-0.66693	1.52947	4.09800

H	-1.37140	0.33594	5.19515
H	-0.41229	-3.44419	3.82244
C	0.44089	-1.69111	4.78253
H	1.13147	0.29848	5.31611
H	-0.13584	-1.82136	5.70817
H	1.42183	-2.15843	4.94121
C	-2.66637	-1.47273	-0.11861
H	-3.40456	-1.31127	0.67773
C	-2.12420	-2.91597	0.01417
C	-3.40818	-1.37581	-1.49094
H	-1.57016	-3.02385	0.94294
C	-1.21544	-3.29021	-1.16680
C	-3.32244	-3.88707	0.05098
H	-3.77739	-0.36400	-1.66206
C	-2.50916	-1.77393	-2.67467
C	-4.61037	-2.34283	-1.44193
H	-0.80907	-4.29798	-1.01635
H	-0.32016	-2.63160	-1.19893
C	-1.99134	-3.20743	-2.48954
H	-3.96579	-3.64698	0.90752
H	-2.95445	-4.91085	0.19749
C	-4.11537	-3.78953	-1.26193
H	-1.66247	-1.07721	-2.76861
H	-3.08903	-1.69642	-3.60330
H	-5.28280	-2.06690	-0.61876
H	-5.18335	-2.25206	-2.37389
H	-1.33110	-3.47654	-3.32234
C	-3.19178	-4.17389	-2.43433
H	-4.97379	-4.47171	-1.22874
H	-3.74451	-4.13020	-3.38185
H	-2.84022	-5.20670	-2.31056
Pd	0.28052	-0.56115	-1.37942
C	0.90935	1.31565	-1.34907
C	0.60342	2.12376	-2.45104
C	1.68505	1.84151	-0.30995
C	1.05461	3.44698	-2.51066
H	0.00581	1.73626	-3.27049
C	2.15433	3.15771	-0.36298
H	1.93326	1.24070	0.55510
C	1.82063	3.93834	-1.46165
H	0.81881	4.08712	-3.35512
H	2.76848	3.56991	0.43141
F	2.25926	5.22254	-1.51359
B	2.91853	-1.33738	-2.62836
O	3.78695	-1.86729	-3.56955
H	3.27369	-2.06246	-4.37246
O	1.62280	-1.16852	-2.83536
C	3.62127	-0.93780	-1.24216
C	3.53237	-1.73618	-0.11025
C	4.25814	0.28480	-1.08024
C	4.04940	-1.35709	1.12265
C	4.76312	0.71963	0.14029
C	4.65351	-0.11070	1.25044
F	5.10632	0.29207	2.44685
F	2.88709	-2.92602	-0.17944
F	3.94133	-2.15440	2.20126
F	4.33728	1.13559	-2.12591
F	5.30464	1.94188	0.26922

3'

E: -2049.02167

O	-0.15228	-0.77936	-0.67127
B	0.70046	-0.86206	0.33329
O	0.33467	-1.33775	1.59271
H	1.09038	-1.38955	2.19652
C	2.22593	-0.40183	0.11240
C	2.57010	0.59340	-0.80585
C	3.29426	-0.96157	0.81179
C	3.88499	0.99814	-1.02130
C	4.62046	-0.59258	0.62355
C	4.91523	0.39852	-0.30574
F	1.62831	1.23036	-1.52226
F	3.06152	-1.92460	1.74063
F	5.60844	-1.17385	1.32150
F	4.16956	1.96365	-1.90924
F	6.18331	0.77768	-0.50558
Pd	-2.17226	-1.00348	-0.27354
C	-2.27420	0.98963	0.13330
C	-1.60082	1.49399	1.25732
C	-2.90316	1.89652	-0.73182
C	-1.54834	2.86789	1.51077
H	-1.08827	0.81548	1.93251
C	-2.85312	3.27642	-0.49827
H	-3.43731	1.53963	-1.60886
C	-2.17618	3.73323	0.62328
H	-1.02561	3.26690	2.37502
H	-3.33019	3.98454	-1.16911
P	-4.38289	-1.02874	0.18986
H	-5.20737	-0.15089	-0.53989
H	-5.11324	-2.22745	0.05358
H	-4.74666	-0.67079	1.50196
P	-1.81150	-3.31457	-0.76499
H	-2.81207	-4.31159	-0.74906
H	-1.24624	-3.59192	-2.02684
H	-0.85367	-3.94756	0.05253
F	-2.12696	5.07002	0.86348

4 (ArPdL-(OH)B(OH)(Ar')OB(OH)Ar')
E: -3779.10910
G: -3778.23148
Esp: -3780.55422
Gcorr: 0.87762
ZPE: 0.95411
Esp + Gcorr: -3779.67661

P	2.48949	-0.31855	0.09206
C	3.71216	0.94447	0.74846
H	3.09039	1.35373	1.55448
C	4.08827	2.17423	-0.12599
C	5.01850	0.41900	1.41683
H	3.21745	2.52027	-0.67529
C	5.23935	1.91553	-1.11454
C	4.53876	3.27877	0.85740
H	4.82921	-0.50729	1.96655
C	6.15948	0.17306	0.40938
C	5.47609	1.51712	2.40340
H	5.44277	2.84737	-1.65903
H	4.95891	1.17172	-1.86881
C	6.49636	1.46011	-0.35764
H	3.72087	3.51550	1.54822
H	4.76422	4.19643	0.29811
C	5.78652	2.81730	1.63427
H	5.89907	-0.61480	-0.29797
H	7.04032	-0.17803	0.96336
H	4.69442	1.69560	3.15393
H	6.37180	1.17862	2.94110
H	7.30806	1.26153	-1.06894
C	6.92873	2.55358	0.63518
H	6.08799	3.59770	2.34437
H	7.83395	2.23717	1.17099
H	7.17646	3.47746	0.09543
C	3.37377	-1.26362	-1.27844
H	4.05007	-0.47210	-1.61002
C	2.53160	-1.62519	-2.52709
C	4.26819	-2.48101	-0.91503
H	1.84930	-0.79617	-2.75371
C	1.73783	-2.92799	-2.32823
C	3.51731	-1.81031	-3.70013
H	4.82366	-2.28546	0.00690
C	3.47183	-3.78852	-0.75555
C	5.26043	-2.66331	-2.08733
H	1.14679	-3.13329	-3.23196
H	1.03463	-2.82253	-1.49830
C	2.69549	-4.09766	-2.04573
H	4.07177	-0.87807	-3.87243

H	2.95917	-2.03154	-4.61957
C	4.49018	-2.96388	-3.38883
H	2.78319	-3.73243	0.08929
H	4.17666	-4.60147	-0.53605
H	5.87160	-1.75982	-2.21042
H	5.94627	-3.48996	-1.85974
H	2.11661	-5.02004	-1.91320
C	3.68292	-4.26356	-3.21388
H	5.20244	-3.07689	-4.21565
H	4.36051	-5.10506	-3.01635
H	3.13836	-4.49472	-4.13921
C	2.28137	-1.46674	1.57526
H	3.18483	-2.08510	1.51741
C	1.05439	-2.41771	1.51111
C	2.29102	-0.80100	2.98024
H	0.96432	-2.85272	0.51318
C	-0.25636	-1.69091	1.84768
C	1.27592	-3.53950	2.54709
H	3.11201	-0.08876	3.06831
C	0.96610	-0.08420	3.28759
C	2.51416	-1.92289	4.01734
H	-1.09212	-2.39542	1.75962
H	-0.43724	-0.89675	1.12073
C	-0.19738	-1.08696	3.25545
H	2.19745	-4.09111	2.31810
H	0.44572	-4.25575	2.49009
C	1.35600	-2.93455	3.96166
H	0.78382	0.70568	2.55156
H	1.03605	0.39718	4.27190
H	3.47104	-2.42551	3.82220
H	2.57923	-1.48021	5.02018
H	-1.13757	-0.56630	3.47459
C	0.03807	-2.20492	4.28645
H	1.52816	-3.73316	4.69414
H	0.08240	-1.78405	5.30008
H	-0.80060	-2.91381	4.26578
Pd	0.46519	0.45934	-0.69925
C	0.88730	2.36935	-0.42130
C	0.85450	3.01118	0.82079
C	1.01795	3.14862	-1.58293
C	0.96004	4.40400	0.91209
H	0.75013	2.44074	1.73656
C	1.13181	4.53976	-1.50733
H	1.05095	2.67580	-2.56112
C	1.10447	5.14062	-0.25482
H	0.93560	4.91040	1.87212
H	1.24071	5.14954	-2.39893
F	1.22159	6.49106	-0.17122
O	-0.76738	-1.31964	-1.41692
B	-1.99250	-0.46111	-1.47451
H	-0.49884	-1.55174	-2.32155
O	-1.50489	0.95868	-1.44302
H	-1.45667	1.31870	-2.34397
C	-4.34291	-1.49386	2.19251
C	-4.28899	-2.34867	1.09748
C	-3.53857	-1.97999	-0.01306
C	-2.84832	-0.77393	-0.11796
C	-2.92883	0.04580	1.00466
C	-3.64942	-0.29184	2.14657
O	-2.69630	-0.70464	-2.72386
F	-5.04850	-1.82951	3.28131
B	-3.95281	-0.34670	-3.04936
C	-4.81258	0.51646	-2.01705
C	-5.73818	-0.08008	-1.16880
C	-4.48365	1.83901	-1.74326
C	-6.26518	0.56722	-0.05877
C	-4.99180	2.52767	-0.64904
C	-5.88458	1.88051	0.20091
O	-4.45042	-0.73910	-4.25930
H	-5.35534	-0.41822	-4.39523
F	-6.37220	2.51829	1.27066
F	-3.60246	2.48297	-2.53900
F	-4.62508	3.79153	-0.39661
F	-6.07587	-1.37370	-1.36056
F	-7.10022	-0.06610	0.77791
F	-2.26580	1.22296	1.06885
F	-3.65319	0.52299	3.21652
F	-3.52902	-2.85222	-1.04595
F	-4.95971	-3.51175	1.12302

4'

E: -2953.48562
G: -2953.25025
Esp: -2954.57168
Gcorr: 0.23538
Esp + Gcorr: -2954.33630

Pd	3.38728	-0.38006	0.02934
C	2.51100	1.45503	-0.14332
C	2.16980	2.13302	1.03506
C	2.06001	1.95548	-1.37148
C	1.34027	3.25603	0.99777
H	2.50286	1.76033	1.99872
C	1.22564	3.07706	-1.42545
H	2.30992	1.45113	-2.30021
C	0.86908	3.69200	-0.23449
H	1.03624	3.76861	1.90497
H	0.82787	3.44505	-2.36572
F	0.01085	4.74297	-0.26985
O	1.73726	-0.95423	1.34426
B	0.49735	-1.32300	0.52714
H	1.95046	-1.71207	1.91328
O	0.87142	-1.72467	-0.81025
H	1.06083	-2.67512	-0.79421
C	-2.19261	2.26424	0.65673
C	-1.76735	1.62983	1.81828
C	-0.91441	0.53711	1.72169
C	-0.44890	0.01630	0.51460
C	-0.90127	0.68543	-0.61896
C	-1.75087	1.78846	-0.56873
O	-0.09992	-2.45123	1.27557
F	-3.00938	3.32677	0.72135
B	-1.34611	-2.93638	1.20940
C	-2.42579	-2.25354	0.25013
C	-3.33783	-1.32684	0.74059
C	-2.35370	-2.38418	-1.13142
C	-4.10753	-0.52062	-0.08749
C	-3.11097	-1.60293	-1.99682
C	-3.98690	-0.66039	-1.46694
O	-1.67435	-4.01811	1.98552
H	-2.59814	-4.28125	1.85451
F	-4.70479	0.12116	-2.28248
F	-1.49839	-3.27488	-1.67214
F	-2.99869	-1.73602	-3.32640
F	-3.42596	-1.12654	2.07409
F	-4.92373	0.41523	0.42082
F	-0.54569	0.29329	-1.85995
F	-2.14178	2.39779	-1.70323
F	-0.55736	-0.04340	2.89023
F	-2.18737	2.07635	3.01601
P	4.32662	-2.58881	0.20526
H	5.72156	-2.79680	0.19497
H	3.99208	-3.35792	1.34063
H	3.95793	-3.50855	-0.79878
P	5.06814	0.59224	-1.09328
H	6.18640	-0.19706	-1.42790
H	4.75740	1.15586	-2.34369
H	5.70132	1.67861	-0.46412

TS-5

E: -3779.09536
G: -3778.21851
Esp: -3780.53858
Gcorr: 0.87685
ZPE: 0.95315

Esp + Gcorr: -3779.66173

P	2.49897	-0.19584	0.09165
C	3.18256	1.47636	0.64146
H	2.28856	1.83611	1.15461
C	3.44280	2.50661	-0.49054
C	4.32275	1.60739	1.69241
H	2.70423	2.37916	-1.28812
C	4.86654	2.41517	-1.07632
C	3.27324	3.90638	0.14018
H	4.22700	0.85168	2.47344
C	5.73517	1.52951	1.09426
C	4.14087	3.00430	2.33295
H	4.97574	3.18938	-1.84754
H	5.03999	1.45659	-1.56838
C	5.91833	2.61996	0.02626
H	2.25797	4.01671	0.53390
H	3.40907	4.67700	-0.63045
C	4.31020	4.10171	1.26406
H	5.92287	0.53899	0.66879
H	6.46732	1.66758	1.90117
H	3.14922	3.07535	2.79920
H	4.88528	3.14122	3.12864
H	6.92326	2.54694	-0.40838
C	5.72750	4.00553	0.66953
H	4.16728	5.08688	1.72578
H	6.47846	4.16300	1.45564
H	5.87427	4.79218	-0.08280
C	3.44305	-0.69870	-1.45982
H	3.48439	0.29077	-1.92911
C	2.65889	-1.58796	-2.45421
C	4.89486	-1.22988	-1.35898
H	1.63283	-1.21227	-2.52734
C	2.68092	-3.06179	-2.01957
C	3.31988	-1.45745	-3.84163
H	5.46297	-0.63405	-0.64340
C	4.93989	-2.70946	-0.94626
C	5.54683	-1.09967	-2.75447
H	2.11871	-3.66646	-2.74476
H	2.18253	-3.18130	-1.05377
C	4.13799	-3.56129	-1.94880
H	3.28714	-0.41096	-4.17343
H	2.74996	-2.04799	-4.57103
C	4.77477	-1.95217	-3.77777
H	4.56277	-2.83783	0.06978
H	5.98616	-3.04245	-0.93627
H	5.55871	-0.04995	-3.07460
H	6.59158	-1.43190	-2.69487
H	4.14943	-4.61122	-1.63106
C	4.78797	-3.42959	-3.33963
H	5.24261	-1.85407	-4.76532
H	5.82008	-3.80351	-3.30789
H	4.24274	-4.04129	-4.07088
C	2.79986	-1.22732	1.63603
H	3.88591	-1.12845	1.76544
C	2.48799	-2.74730	1.67490
C	2.11339	-0.57975	2.88123
H	2.89085	-3.23995	0.79153
C	0.98652	-3.06014	1.77552
C	3.19584	-3.31466	2.92612
H	2.23149	0.50565	2.87058
C	0.61034	-0.90733	2.94772
C	2.81055	-1.14501	4.13569
H	0.85959	-4.15130	1.80522
H	0.45756	-2.70445	0.89222
C	0.39453	-2.42442	3.04080
H	4.27733	-3.13097	2.86652
H	3.05309	-4.40281	2.95818
C	2.61450	-2.67060	4.19903
H	0.09623	-0.52384	2.05904
H	0.17576	-0.39880	3.81910
H	3.88041	-0.89675	4.11352
H	2.38629	-0.67342	5.03207
H	-0.67889	-2.64136	3.09220
C	1.10745	-2.98047	4.28645
H	3.12862	-3.07126	5.08195
H	0.68603	-2.53314	5.19720
H	0.95020	-4.06543	4.35540
Pd	0.23801	-0.11777	-0.47305
C	0.11459	1.83395	-0.08109
C	-0.12850	2.31751	1.21263
C	0.05122	2.73734	-1.15289
C	-0.44821	3.66106	1.43694
H	-0.09008	1.64803	2.06550
C	-0.26262	4.08517	-0.94689
H	0.23708	2.39779	-2.16768
C	-0.51313	4.51973	0.34779
H	-0.64806	4.03560	2.43623
H	-0.31655	4.78636	-1.77405
F	-0.82821	5.82503	0.55522
O	-0.24553	-2.21609	-1.09115
B	-1.69431	-2.09886	-1.11894
H	0.06699	-2.37357	-1.99688
O	-2.20043	-2.44440	-2.37418
H	-3.16248	-2.53854	-2.34276
C	-3.67574	2.18241	-1.14240
C	-3.46204	1.57552	0.09058
C	-2.63277	0.46584	0.15047
C	-1.99484	-0.09623	-0.95335
C	-2.22274	0.57323	-2.15723
C	-3.04579	1.68314	-2.28083
O	-2.28308	-2.63620	0.04793
F	-4.46284	3.25847	-1.23168
B	-3.35405	-2.62723	0.85311
C	-4.66389	-1.75540	0.56749
C	-5.18158	-0.91637	1.55537
C	-5.29265	-1.67859	-0.67115
C	-6.20670	-0.00780	1.32021
C	-6.32224	-0.78996	-0.95275
C	-6.77619	0.05784	0.05306
O	-3.28352	-3.38382	1.99233
H	-4.07635	-3.29616	2.54295
F	-7.76289	0.92304	-0.19563
F	-4.91922	-2.50919	-1.67723
F	-6.88611	-0.75031	-2.16648
F	-4.65057	-0.93567	2.79443
F	-6.63931	0.80678	2.28927
F	-1.57446	0.18189	-3.27931
F	-3.21821	2.30727	-3.45851
F	-2.41468	-0.04383	1.39074
F	-4.04327	2.07919	1.19416

6 (ArAr'PdL-(OH)B(OH)OB(OH)Ar')

E: -3779.12406
G: -3778.24764
Esp: -3780.56386
Gcorr: 0.87642
ZPE: 0.95406
Esp + Gcorr: -3779.68744

P	2.19695	-0.36606	0.14282
C	3.50967	0.95247	0.38242
H	2.97082	1.55398	1.12574
C	3.76308	1.92872	-0.80107
C	4.88664	0.61043	1.02010
H	2.83263	2.10618	-1.33642
C	4.83833	1.46179	-1.80077
C	4.25147	3.24915	-0.16385
H	4.78158	-0.16081	1.78819
C	5.94204	0.14648	-0.00268
C	5.38830	1.92045	1.67101
H	4.95843	2.24276	-2.56390
H	4.53170	0.55562	-2.33373
C	6.17015	1.22117	-1.07578
H	3.48558	3.63708	0.51710

H	4.40325	4.00610	-0.94479
C	5.57581	3.00536	0.58948
H	5.64241	-0.78699	-0.48162
H	6.87897	-0.05810	0.53291
H	4.67127	2.25812	2.43126
H	6.34336	1.73993	2.18273
H	6.92596	0.87225	-1.79101
C	6.64213	2.52782	-0.41378
H	5.90483	3.93878	1.06362
H	7.59878	2.36455	0.10102
H	6.81159	3.29777	-1.17858
C	2.90319	-1.54705	-1.14773
H	3.49286	-0.81716	-1.70738
C	1.91565	-2.13416	-2.18444
C	3.89549	-2.66491	-0.72608
H	1.16674	-1.37905	-2.43890
C	1.22588	-3.41387	-1.68073
C	2.73822	-2.47963	-3.44463
H	4.55683	-2.30880	0.06855
C	3.19639	-3.95183	-0.25195
C	4.73021	-3.00737	-1.98213
H	0.53153	-3.77814	-2.45042
H	0.63260	-3.20190	-0.78866
C	2.27244	-4.49189	-1.35562
H	3.21179	-1.57144	-3.84078
H	2.07194	-2.86616	-4.22746
C	3.80656	-3.53521	-3.09938
H	2.62454	-3.77589	0.66144
H	3.96464	-4.69714	-0.00612
H	5.27344	-2.11849	-2.32823
H	5.48094	-3.76816	-1.72976
H	1.76680	-5.39895	-1.00090
C	3.10177	-4.81426	-2.61095
H	4.40464	-3.75867	-3.99171
H	3.84378	-5.59095	-2.38176
H	2.45068	-5.20971	-3.40225
C	2.23617	-1.25732	1.80327
H	3.14852	-1.86214	1.74070
C	1.04858	-2.22551	2.04870
C	2.38294	-0.36283	3.06587
H	0.87143	-2.83412	1.15764
C	-0.24681	-1.48201	2.41664
C	1.42836	-3.15015	3.22470
H	3.17532	0.37372	2.92789
C	1.07491	0.37019	3.40053
C	2.76915	-1.28291	4.24309
H	-1.04537	-2.21239	2.57182
H	-0.56059	-0.81349	1.60601
C	-0.04367	-0.64238	3.68337
H	2.33613	-3.71718	2.97976
H	0.62437	-3.87938	3.39173
C	1.65214	-2.31110	4.49737
H	0.78473	1.00395	2.55896
H	1.23522	1.02520	4.26717
H	3.71634	-1.79363	4.02320
H	2.93025	-0.67457	5.14311
H	-0.97532	-0.11471	3.92089
C	0.35367	-1.56138	4.85189
H	1.93839	-2.97054	5.32636
H	0.49938	-0.97023	5.76610
H	-0.45356	-2.27834	5.05390
Pd	0.00612	0.57862	-0.38287
C	0.50757	2.51116	-0.21965
C	0.46692	3.19617	1.00221
C	0.79361	3.25441	-1.37803
C	0.74840	4.56611	1.08371
H	0.19435	2.67903	1.91441
C	1.07819	4.62106	-1.31756
H	0.80275	2.77029	-2.34870
C	1.05560	5.25296	-0.08076
H	0.71956	5.09207	2.03322
H	1.31107	5.18974	-2.21267
F	1.33277	6.58215	-0.01319
B	-1.63892	-1.68771	-2.05294
O	-1.01148	-1.44269	-0.84376
H	-1.28800	-2.02450	-0.11554
C	-1.85894	1.40788	-0.66543
C	-2.74018	1.55981	0.39450
C	-2.32071	1.87479	-1.88623
C	-3.99646	2.14241	0.26878
C	-3.58207	2.42991	-2.07791
C	-4.43169	2.56032	-0.98418
F	-5.65648	3.08805	-1.13181
F	-2.38844	1.14377	1.64463
F	-4.81257	2.28159	1.33144
F	-1.51542	1.81048	-2.98847
F	-3.98909	2.84243	-3.29140
O	-1.34578	-0.94366	-3.14198
H	-0.80195	-0.16372	-2.93479
O	-2.54510	-2.71683	-2.19825
B	-3.79216	-2.88446	-1.67088
C	-4.29492	-2.02269	-0.44212
C	-5.36768	-1.13975	-0.51830
C	-3.67747	-2.13149	0.79776
C	-5.81198	-0.41454	0.58270
C	-4.08243	-1.42744	1.92154
C	-5.17211	-0.56869	1.80903
O	-4.63058	-3.82383	-2.16848
H	-4.23798	-4.28215	-2.93277
F	-5.99476	-0.94688	-1.69122
F	-6.82220	0.45365	0.46479
F	-5.58107	0.12652	2.87047
F	-3.44528	-1.55198	3.09177
F	-2.60436	-2.96558	0.91744

TS'-A^{+}

E: -3186.37019
G: -3186.01032
Esp: -3187.53719
Gcorr: 0.35986
Esp + Gcorr: -3187.17733

Pd	-3.05545	-2.08426	-0.18163
C	-3.56220	-0.10986	-0.26467
C	-3.47323	0.51841	-1.51551
C	-3.82001	0.66989	0.86994
C	-3.58809	1.90543	-1.62868
H	-3.26693	-0.06284	-2.40868
C	-3.93715	2.06101	0.77315
H	-3.89324	0.21449	1.85273
C	-3.80354	2.65017	-0.47528
H	-3.48920	2.40749	-2.58590
H	-4.09674	2.67944	1.65028
F	-3.86293	4.00145	-0.57374
O	-1.22043	-1.59780	-1.25713
B	-0.09462	-1.04451	-0.40994
H	-0.88407	-2.33792	-1.78854
O	-0.12960	-1.53596	0.94410
H	0.09458	-2.47990	0.93934
C	-0.42452	3.42238	-0.60340
C	-0.00864	2.68306	-1.70387
C	0.07284	1.29769	-1.60010
C	-0.22375	0.58463	-0.43802
C	-0.63237	1.37128	0.63596
C	-0.73735	2.75865	0.57526
O	1.13437	-1.52549	-1.11859
F	-0.53028	4.75383	-0.68028
B	2.40794	-1.18899	-0.99713
C	2.95525	-0.23947	0.24338
C	2.95144	1.16603	-0.05318
C	2.46038	-0.58379	1.54508
C	2.55500	2.12032	0.85429
C	2.03960	0.34941	2.46490
C	2.08666	1.70091	2.10651
O	3.39075	-1.57179	-1.86056
H	3.01648	-2.06884	-2.60927

F	1.66988	2.60868	2.96581
F	2.49275	-1.86377	1.89159
F	1.58175	0.00099	3.66383
F	3.36916	1.55695	-1.25150
F	2.55353	3.41909	0.55691
F	-0.93590	0.82537	1.83258
F	-1.15163	3.45531	1.64515
F	0.47749	0.64310	-2.71241
F	0.29859	3.30615	-2.85226
P	-2.39570	-4.40150	-0.07031
H	-3.36595	-5.42361	-0.04505
H	-1.56264	-4.90555	-1.09252
H	-1.63055	-4.79121	1.04918
P	-5.10701	-2.34259	0.69334
H	-5.50046	-3.64745	1.04737
H	-5.38445	-1.64210	1.88011
H	-6.18878	-1.94955	-0.11325
C	6.31099	-0.47689	-0.78345
O	5.52012	-0.98218	0.34265
C	5.65872	-2.43675	0.43791
C	6.35689	-2.86429	-0.84673
C	7.21959	-1.63648	-1.17586
H	5.62099	-0.20463	-1.58613
H	6.83989	0.41101	-0.43126
H	6.25891	-2.64133	1.32988
H	4.66031	-2.85916	0.57286
H	6.94477	-3.77492	-0.70543
H	5.62029	-3.03620	-1.63642
H	8.12913	-1.63151	-0.56564
H	7.50782	-1.58512	-2.22905
H	4.13202	-0.59530	0.23976

IM-B^{+}

E: -2953.88340
G: -2953.63609
Esp: -2954.95734
Gcorr: 0.24731
Esp + Gcorr: -2954.71003

Pd	-3.19639	-0.60426	-0.18598
C	-2.54580	1.32425	-0.07197
C	-2.17108	1.94533	-1.27202
C	-2.28939	1.97638	1.14089
C	-1.50278	3.17141	-1.26310
H	-2.35518	1.45760	-2.22421
C	-1.62022	3.20500	1.16637
H	-2.56687	1.52185	2.08691
C	-1.22726	3.76825	-0.03869
H	-1.17741	3.64836	-2.18219
H	-1.37801	3.70047	2.10083
F	-0.52773	4.92980	-0.02315
O	-1.41399	-1.08185	-1.35563
B	-0.13070	-1.28687	-0.59468
H	-1.54455	-1.81080	-1.98392
O	-0.34332	-1.86372	0.70702
H	-0.74480	-2.74109	0.60268
C	2.01357	2.64366	-0.38529
C	1.90832	1.94330	-1.58088
C	1.21998	0.73405	-1.60436
C	0.62955	0.15326	-0.48164
C	0.76098	0.89519	0.68930
C	1.43222	2.11381	0.75832
O	0.64213	-2.23366	-1.47081
F	2.65347	3.81692	-0.33961
B	1.88698	-2.64756	-1.50943
C	2.96158	-2.56623	-0.17541
C	3.77903	-1.36927	-0.30901
C	2.27465	-2.70673	1.09510
C	3.80829	-0.39269	0.65193
C	2.30282	-1.73817	2.06695
C	3.07009	-0.58908	1.83390
O	2.52376	-3.22233	-2.55974
H	1.95646	-3.21510	-3.35169
F	3.08164	0.35616	2.74380
F	1.61707	-3.82730	1.30733
F	1.62176	-1.85293	3.19744
F	4.48494	-1.21955	-1.41170
F	4.49904	0.73235	0.50079
F	0.25642	0.45150	1.86131
F	1.51055	2.77963	1.91968
F	1.15136	0.11508	-2.80499
F	2.45686	2.44294	-2.69852
P	-3.89289	-2.91168	-0.28346
H	-5.23612	-3.26563	-0.04582
H	-3.67228	-3.63261	-1.47671
H	-3.26344	-3.79057	0.62432
P	-5.03890	0.20357	0.81008
H	-6.07392	-0.70843	1.09142
H	-4.86384	0.81934	2.06139
H	-5.74113	1.19921	0.10985
H	3.54608	-3.47169	-0.39728

TS'-C^{+}

E: -2953.87639
G: -2953.63152
Esp: -2954.95398
Gcorr: 0.24487
Esp + Gcorr: -2954.70911

Pd	-3.18498	-0.77893	-0.19876
C	-2.65368	1.18661	-0.15159
C	-2.25819	1.77024	-1.36339
C	-2.50487	1.91357	1.03645
C	-1.67293	3.03801	-1.38630
H	-2.36139	1.22525	-2.29660
C	-1.92359	3.18603	1.02893
H	-2.80101	1.48843	1.99020
C	-1.50618	3.71443	-0.18377
H	-1.33181	3.48984	-2.31235
H	-1.76597	3.74316	1.94645
F	-0.89176	4.92254	-0.19615
O	-1.33616	-1.21362	-1.30263
B	-0.09033	-1.31918	-0.48917
H	-1.45453	-2.00458	-1.85456
O	-0.23064	-1.98032	0.75417
H	-0.55191	-2.88705	0.62938
C	1.75901	2.73343	-0.14828
C	1.79948	2.03526	-1.34939
C	1.20830	0.78031	-1.42007
C	0.58988	0.14478	-0.34459
C	0.57751	0.88479	0.83620
C	1.13878	2.15382	0.94932
O	0.81173	-2.23336	-1.41855
F	2.29744	3.95329	-0.05589
B	1.99396	-2.25951	-1.85996
C	3.47365	-2.44946	-0.18431
C	4.09548	-1.19006	-0.29670
C	2.70510	-2.70427	0.96671
C	3.89602	-0.20195	0.65621
C	2.50535	-1.73587	1.93347
C	3.12068	-0.49256	1.77739
O	2.86289	-2.35559	-2.84447
H	2.49236	-2.14479	-3.72524
F	2.91829	0.44864	2.69254
F	2.12048	-3.89183	1.10914
F	1.74476	-1.96417	2.99985
F	4.88380	-0.92826	-1.33558
F	4.43754	1.00991	0.51895
F	0.00990	0.39740	1.95539
F	1.07450	2.82126	2.10930
F	1.26929	0.16452	-2.63220
F	2.38613	2.58078	-2.42472
P	-3.78723	-3.11965	-0.21229
H	-5.14113	-3.49739	-0.31205

H	-3.24186	-3.94830	-1.21697
H	-3.42223	-3.87596	0.92096
P	-5.11432	-0.02189	0.66880
H	-6.11435	-0.97489	0.93985
H	-5.03517	0.65868	1.89565
H	-5.82531	0.90035	-0.11721
H	3.85405	-3.29173	-0.75793

7 (PdLArAr')

E: -2698.59829
G: -2697.81972
Esp: -2699.54894
Gcorr: 0.77857
ZPE: 0.84127
Esp + Gcorr: -2698.77037

P	1.26298	-0.36762	0.14365
C	2.13460	0.82304	1.29771
H	1.56441	0.60066	2.20737
C	1.92624	2.34505	1.07544
C	3.63006	0.57254	1.62825
H	0.89651	2.53751	0.78702
C	2.87812	2.93939	0.02384
C	2.20502	3.03312	2.42968
H	3.82705	-0.50154	1.71980
C	4.57176	1.17817	0.56799
C	3.91358	1.26163	2.98173
H	2.68443	4.01711	-0.05726
H	2.68647	2.51560	-0.96830
C	4.33830	2.69315	0.44125
H	1.50733	2.65515	3.18920
H	2.02574	4.11235	2.33423
C	3.66122	2.77817	2.86233
H	4.42848	0.70255	-0.40382
H	5.61062	0.98223	0.86588
H	3.27232	0.83032	3.76218
H	4.95496	1.07835	3.27895
H	5.01612	3.10478	-0.31740
C	4.60736	3.36766	1.79906
H	3.84889	3.25723	3.83168
H	5.65324	3.20955	2.09559
H	4.45249	4.45205	1.71885
C	2.13980	-0.35459	-1.51508
H	2.49626	0.67973	-1.51885
C	1.20153	-0.47290	-2.74464
C	3.38524	-1.25052	-1.74905
H	0.28402	0.09149	-2.55881
C	0.83143	-1.92962	-3.06022
C	1.95635	0.12505	-3.94944
H	4.03117	-1.24035	-0.86544
C	3.02010	-2.70654	-2.09081
C	4.14224	-0.65125	-2.95629
H	0.18106	-1.94945	-3.94481
H	0.24989	-2.35918	-2.23735
C	2.10580	-2.75131	-3.32793
H	2.20097	1.17770	-3.75319
H	1.31351	0.10061	-4.83931
C	3.24234	-0.68407	-4.20867
H	2.54545	-3.20423	-1.24358
H	3.94678	-3.25886	-2.29673
H	4.44621	0.38075	-2.73590
H	5.05865	-1.22795	-3.13906
H	1.83685	-3.79199	-3.54848
C	2.85906	-2.14275	-4.52654
H	3.78483	-0.25095	-5.05838
H	3.76142	-2.73158	-4.73957
H	2.22898	-2.17640	-5.42545
C	1.53868	-2.02284	1.00811
H	2.57891	-2.30020	0.79994
C	0.61613	-3.15010	0.47476
C	1.36429	-1.95873	2.55097
H	0.68422	-3.21387	-0.60999
C	-0.85006	-2.92946	0.86733
C	1.07158	-4.49418	1.08223
H	1.99743	-1.17546	2.97253
C	-0.10630	-1.70117	2.93029
C	1.81562	-3.30576	3.15164
H	-1.46215	-3.74954	0.47182
H	-1.29009	-2.03158	0.37329
C	-0.99390	-2.83730	2.39208
H	2.11218	-4.69700	0.79768
H	0.45758	-5.30540	0.67003
C	0.93671	-4.44621	2.61386
H	-0.45125	-0.73898	2.52766
H	-0.19613	-1.64429	4.02267
H	2.86970	-3.48910	2.90426
H	1.74311	-3.25451	4.24604
H	-2.04063	-2.64590	2.65435
C	-0.53283	-4.18018	2.99618
H	1.26279	-5.40127	3.04393
H	-0.63752	-4.15066	4.08856
H	-1.17144	-4.99500	2.63042
Pd	-1.08479	-0.10742	-0.02412
C	-1.14190	1.87295	-0.25595
C	-1.65100	2.64659	0.79998
C	-0.62967	2.52666	-1.38359
C	-1.58952	4.04282	0.76209
H	-2.08206	2.16624	1.67215
C	-0.57162	3.92393	-1.43911
H	-0.24259	1.96200	-2.22378
C	-1.04063	4.65554	-0.35702
H	-1.96400	4.64764	1.58231
H	-0.16094	4.43717	-2.30328
F	-0.97046	6.01193	-0.39795
C	-3.13528	-0.05907	-0.17044
C	-3.94969	-0.04869	0.95137
C	-3.79652	-0.04617	-1.38871
C	-5.33942	-0.03157	0.89199
C	-5.18268	-0.02801	-1.50895
C	-5.95910	-0.02108	-0.35407
F	-7.29974	-0.00895	-0.44149
F	-3.39163	-0.04738	2.19695
F	-6.09164	-0.02593	2.00884
F	-3.08285	-0.04812	-2.54918
F	-5.78422	-0.02003	-2.71350

8 ($B(OH)_2OB(OH)Ar'$)

E: -1080.49120
G: -1080.42100
Esp: -1081.00378
Gcorr: 0.07020
ZPE: 0.10899
Esp + Gcorr: -1080.93358

B	3.06137	-0.35360	-0.49070
O	2.67116	0.70756	0.29582
B	1.47597	1.34843	0.42852
O	4.12300	-1.13220	-0.11886
H	4.47139	-0.86097	0.74506
O	2.42360	-0.57675	-1.67909
H	2.79987	-1.34504	-2.13685
O	1.53129	2.67083	0.74195
H	0.65154	3.07185	0.81369
C	0.09348	0.58796	0.27033
C	-0.03319	-0.79392	0.43436
C	-1.08805	1.26462	-0.04073
C	-1.23883	-1.46759	0.28072
C	-2.31235	0.63061	-0.20836
C	-2.38462	-0.74878	-0.04468
F	1.03547	-1.54388	0.76827
F	-1.07432	2.60926	-0.19655
F	-3.41348	1.32744	-0.51482
F	-1.31001	-2.79388	0.45030
F	-3.55104	-1.38038	-0.19381

TS-9

E: -2698.57222
G: - 2697.79436
Esp: -2699.51927
Gcorr: 0.77787
ZPE: 0.84011
Esp + Gcorr: -2698.74140

P	-1.29923	-0.36386	-0.12849
C	-2.08175	1.11088	-0.98018
H	-1.60001	1.01058	-1.95984
C	-1.63405	2.50535	-0.46844
C	-3.61114	1.13717	-1.23151
H	-0.57096	2.47984	-0.23050
C	-2.42890	2.98023	0.76028
C	-1.87922	3.50603	-1.61801
H	-3.96547	0.14339	-1.52857
C	-4.40102	1.61343	0.00350
C	-3.85996	2.13826	-2.38227
H	-2.08312	3.98542	1.03659
H	-2.23678	2.33990	1.62813
C	-3.93226	3.01681	0.43023
H	-1.28864	3.21529	-2.49706
H	-1.53791	4.50533	-1.31599
C	-3.38016	3.54445	-1.96765
H	-4.29653	0.91057	0.83299
H	-5.46949	1.64162	-0.24993
H	-3.33063	1.80821	-3.28637
H	-4.93089	2.16654	-2.62526
H	-4.49838	3.33865	1.31370
C	-4.17200	4.00367	-0.72804
H	-3.54886	4.24618	-2.79454
H	-5.24396	4.05383	-0.96309
H	-3.85592	5.01359	-0.43373
C	-2.14487	-0.56008	1.54201
H	-2.48406	0.46364	1.70912
C	-1.15439	-0.85898	2.69473
C	-3.39082	-1.46671	1.69682
H	-0.25009	-0.25453	2.55403
C	-0.77740	-2.34738	2.73239
C	-1.84270	-0.47192	4.01843
H	-4.08272	-1.30002	0.86307
C	-3.02484	-2.96021	1.77537
C	-4.07827	-1.07397	3.02476
H	-0.06809	-2.52564	3.55179
H	-0.26437	-2.62721	1.80397
C	-2.04249	-3.20377	2.93566
H	-2.09165	0.59798	4.01041
H	-1.15516	-0.63936	4.85855
C	-3.11743	-1.31542	4.20695
H	-2.59680	-3.31189	0.83591
H	-3.94224	-3.54152	1.93978
H	-4.38089	-0.01873	2.99547
H	-4.99146	-1.66981	3.15669
H	-1.76857	-4.26604	2.96617
C	-2.72489	-2.80473	4.25807
H	-3.61350	-1.03136	5.14374
H	-3.61675	-3.42513	4.42021
H	-2.04675	-2.98345	5.10349
C	-1.78875	-1.79921	-1.24863
H	-2.81331	-2.07075	-0.96779
C	-0.88672	-3.05366	-1.05943
C	-1.80283	-1.45701	-2.76390
H	-0.80887	-3.30579	0.00023
C	0.53046	-2.84184	-1.61856
C	-1.53622	-4.23264	-1.81293
H	-2.41186	-0.56923	-2.94688
C	-0.37611	-1.22593	-3.29839
C	-2.44552	-2.63840	-3.51946
H	1.12109	-3.75326	-1.45652
H	1.05294	-2.03389	-1.07600
C	0.46631	-2.50125	-3.11442
H	-2.54272	-4.42233	-1.41631
H	-0.94515	-5.14339	-1.64814
C	-1.61018	-3.91325	-3.31742
H	0.10395	-0.39021	-2.77183
H	-0.42624	-0.95601	-4.36163
H	-3.47176	-2.79377	-3.16032
H	-2.50917	-2.39493	-4.58866
H	1.47988	-2.33213	-3.49893
C	-0.19043	-3.67472	-3.86716
H	-2.07754	-4.75117	-3.85010
H	-0.23769	-3.45404	-4.94218
H	0.41745	-4.58179	-3.74848
Pd	1.05397	-0.09209	0.04401
C	1.91586	1.78812	0.13667
C	1.97260	2.49696	-1.08193
C	1.70188	2.51471	1.32685
C	1.75391	3.87371	-1.12010
H	2.16860	1.97319	-2.00771
C	1.47927	3.89100	1.29296
H	1.68467	2.00497	2.28069
C	1.49487	4.54585	0.06733
H	1.76986	4.41864	-2.05856
H	1.28430	4.44992	2.20286
F	1.25449	5.88017	0.02974
C	3.07411	0.23805	0.23845
C	3.89388	-0.03580	-0.86729
C	3.66695	-0.01630	1.48452
C	5.20390	-0.47866	-0.75699
C	4.97456	-0.45732	1.63345
C	5.75602	-0.68264	0.50451
F	7.01785	-1.11575	0.62941
F	3.40959	0.10902	-2.12546
F	5.93804	-0.73478	-1.85251
F	2.95518	0.15782	2.62459
F	5.48738	-0.68794	2.85342

10 (ArAr')

E: -1058.71003
G: -1058.61477
Esp: -1059.18225
Gcorr: 0.09526
ZPE: 0.13282
Esp + Gcorr: -1059.08699

C	2.00618	-0.93907	-0.76257
C	3.39883	-0.94423	-0.76701
C	4.06986	-0.00002	0.00000
C	3.39888	0.94423	0.76701
C	2.00622	0.93910	0.76260
C	1.29273	0.00002	0.00003
H	1.47218	-1.66614	-1.36393
H	3.96013	-1.66207	-1.35556
H	3.96020	1.66207	1.35553
H	1.47226	1.66618	1.36398
C	-0.18942	0.00002	0.00005
C	-0.92995	-1.18156	0.12835
C	-0.92997	1.18158	-0.12829
C	-2.31995	-1.19417	0.12743
C	-2.31998	1.19416	-0.12740
C	-3.02022	-0.00001	0.00001
F	-0.30334	2.36187	-0.27486
F	-2.98699	2.34849	-0.26036
F	-4.35744	-0.00003	-0.00003
F	-2.98695	-2.34852	0.26031
F	-0.30329	-2.36185	0.27485
F	5.42202	-0.00000	-0.00006

11^{+} (ArPdL^{+}-O(B(OH)$_2$)-B(OH)Ar')

E: -3051.16895
G: -3050.33178

Esp: -3052.2821
Gcorr: 0.83716
ZPE: 0.90373
Esp + Gcorr: -3051.44492

P	1.39516	-0.29597	-0.08680
C	2.74446	0.98606	-0.29218
H	2.97590	1.12406	0.76963
C	2.40407	2.40875	-0.80191
C	4.05457	0.51443	-0.98687
H	1.46394	2.73885	-0.37145
C	2.33362	2.49447	-2.33441
C	3.53089	3.33685	-0.29681
H	4.28573	-0.51972	-0.70903
C	3.97934	0.63242	-2.52282
C	5.18175	1.44363	-0.48383
H	2.08328	3.52398	-2.62097
H	1.53035	1.85568	-2.72098
C	3.68489	2.08056	-2.94188
H	3.56630	3.31475	0.80100
H	3.30775	4.37005	-0.59334
C	4.88266	2.90080	-0.88866
H	3.20970	-0.02070	-2.93484
H	4.93702	0.30114	-2.94506
H	5.27484	1.36217	0.60736
H	6.13814	1.12275	-0.91672
H	3.63309	2.13917	-4.03614
C	4.80331	3.00231	-2.42340
H	5.67987	3.55433	-0.51350
H	5.76306	2.71227	-2.87142
H	4.60634	4.04111	-2.71990
C	0.89031	-1.01636	-1.73573
H	0.98733	-0.11024	-2.34414
C	-0.58617	-1.47873	-1.89768
C	1.81471	-2.08643	-2.38481
H	-1.25714	-0.80280	-1.35672
C	-0.84005	-2.91447	-1.41220
C	-0.89000	-1.42858	-3.41112
H	2.86520	-1.84361	-2.20859
C	1.54312	-3.51222	-1.87174
C	1.51474	-2.04349	-3.90122
H	-1.87541	-3.18102	-1.63734
H	-0.72845	-2.99067	-0.32754
C	0.08334	-3.90379	-2.13560
H	-0.74842	-0.40727	-3.78963
H	-1.94053	-1.69784	-3.58225
C	0.03886	-2.40998	-4.15749
H	1.76740	-3.60093	-0.80535
H	2.21978	-4.20080	-2.39406
H	1.73422	-1.04455	-4.29927
H	2.16955	-2.75282	-4.42330
H	-0.10134	-4.91836	-1.76229
C	-0.21213	-3.84096	-3.64545
H	-0.16693	-2.35930	-5.23345
H	0.42877	-4.54970	-4.18607
H	-1.25362	-4.13239	-3.83503
C	2.24409	-1.60340	0.97026
H	2.85097	-2.16182	0.24829
C	1.25327	-2.58296	1.64517
C	3.20193	-1.05478	2.06147
H	0.54458	-2.96373	0.91150
C	0.48861	-1.91263	2.79458
C	2.05223	-3.76688	2.22985
H	3.91995	-0.35764	1.62582
C	2.41532	-0.36538	3.19084
C	3.99494	-2.24596	2.63998
H	-0.21916	-2.62506	3.23385
H	-0.17203	-1.08393	2.44310
C	1.45727	-1.37095	3.85145
H	2.59112	-4.28197	1.42465
H	1.35462	-4.49037	2.67038
C	3.03809	-3.25512	3.29367
H	1.84431	0.48877	2.80181
H	3.11830	0.02873	3.93540
H	4.57240	-2.73001	1.84150
H	4.71380	-1.87028	3.37930
H	0.89116	-0.87599	4.64643
C	2.25920	-2.55745	4.42497
H	3.60970	-4.09695	3.70229
H	2.95429	-2.19631	5.19375
H	1.57865	-3.26923	4.90987
Pd	-0.38534	0.38588	1.13591
C	-0.72345	2.00178	0.01959
C	-0.65171	3.21254	0.72701
C	-1.12837	2.01341	-1.31803
C	-0.99283	4.41887	0.11235
H	-0.29847	3.23833	1.75388
C	-1.47162	3.21593	-1.94437
H	-1.18644	1.10076	-1.89558
C	-1.39680	4.39530	-1.21723
H	-0.93866	5.36076	0.64865
H	-1.79171	3.23760	-2.98108
F	-1.72382	5.56114	-1.82185
B	-3.24391	1.27223	1.68774
O	-3.93868	2.43029	1.84221
H	-4.68578	2.53746	1.22980
O	-2.14150	1.06380	2.49839
C	-3.59944	0.16657	0.63975
C	-3.41085	-1.19352	0.89453
C	-4.06366	0.50228	-0.63188
C	-3.67948	-2.17097	-0.05248
C	-4.28707	-0.44324	-1.62335
C	-4.10389	-1.78912	-1.32188
F	-4.29410	-2.71321	-2.26517
F	-2.95003	-1.60391	2.09132
F	-3.49316	-3.46547	0.22920
F	-4.27123	1.79740	-0.93973
F	-4.66179	-0.07924	-2.85395
B	-1.75235	1.81440	3.62566
O	-2.46050	2.86480	4.10449
H	-3.21664	3.08558	3.53131
O	-0.58952	1.39775	4.19462
H	-0.33451	1.95285	4.94987

11'$^{+}$●BF_4^-

E: -2650.16579

B	-1.44727	-1.33994	-0.81034
O	-0.83686	-0.50008	0.14020
B	0.13845	-0.83659	1.07277
O	-2.07733	-0.76275	-1.87575
H	-2.08888	0.20724	-1.82608
O	-1.31713	-2.67958	-0.65963
H	-2.13736	-3.10413	-0.98617
O	-0.20410	-0.65654	2.36913
H	0.52899	-0.84068	2.97866
C	1.58426	-1.24603	0.60942
C	1.94979	-1.35372	-0.73623
C	2.63932	-1.35939	1.52142
C	3.26381	-1.53353	-1.15261
C	3.96192	-1.54329	1.14789
C	4.27637	-1.62394	-0.20575
F	1.03329	-1.24459	-1.71289
F	2.40143	-1.25176	2.85186
F	4.93132	-1.62490	2.06640
F	3.56215	-1.57980	-2.45603
F	5.54280	-1.78049	-0.58976
Pd	-1.33648	1.68712	0.12892
C	0.64570	1.99813	-0.22091
C	1.50916	2.13821	0.87297
C	1.17437	1.80852	-1.50290
C	2.89163	2.00647	0.70570
H	1.11379	2.31367	1.86976
C	2.55380	1.67789	-1.68450
H	0.51922	1.71885	-2.36456

C	3.38040	1.75777	-0.56962
H	3.57591	2.07600	1.54514
H	2.98309	1.48399	-2.66217
P	-1.38421	3.90741	-0.11748
H	-0.94164	4.40391	-1.35436
H	-2.63890	4.53204	0.00985
H	-0.60272	4.64742	0.78506
P	-3.67249	1.37426	0.68419
H	-4.37427	2.58509	0.85976
H	-4.55909	0.68476	-0.15868
H	-3.94641	0.75572	1.91573
F	4.71175	1.56475	-0.73237
B	-4.57070	-2.28811	-0.08755
F	-3.93821	-3.15393	-1.02348
F	-3.56622	-1.56703	0.61635
F	-5.31255	-3.04340	0.81498
F	-5.38856	-1.37934	-0.77037

12 (ArPdL$^+$-O(B(OH)F)-B(OH)Ar′)

E: -3151.18526
G: -3150.34802
Esp: -3152.35699
Gcorr: 0.83724
ZPE: 0.90482
Esp + Gcorr: -3151.51975

P	2.03075	-0.19652	0.06054
C	3.06432	1.32622	-0.30874
H	2.96163	1.81903	0.66600
C	2.55344	2.37365	-1.33814
C	4.59203	1.13016	-0.55016
H	1.47595	2.47818	-1.25983
C	2.92292	2.05232	-2.79690
C	3.22060	3.71417	-0.95412
H	4.98562	0.32828	0.08107
C	4.94191	0.82119	-2.01985
C	5.26902	2.46603	-0.16746
H	2.53760	2.85774	-3.43642
H	2.43850	1.12940	-3.13580
C	4.44801	1.94193	-2.94565
H	2.93769	3.98944	0.06909
H	2.85065	4.50890	-1.61541
C	4.75140	3.59700	-1.07940
H	4.51196	-0.12816	-2.33895
H	6.03225	0.71679	-2.10033
H	5.06424	2.70197	0.88537
H	6.35790	2.37019	-0.27313
H	4.70487	1.69941	-3.98461
C	5.10822	3.27231	-2.54194
H	5.21945	4.54498	-0.78531
H	6.19814	3.20017	-2.65822
H	4.76361	4.08071	-3.20073
C	2.16013	-1.31178	-1.45306
H	2.28756	-0.53550	-2.21253
C	0.87738	-2.07698	-1.86255
C	3.37423	-2.27136	-1.59635
H	0.00074	-1.44064	-1.69897
C	0.72222	-3.39421	-1.08341
C	1.00273	-2.39880	-3.36667
H	4.28822	-1.78791	-1.24010
C	3.18765	-3.60222	-0.84454
C	3.50750	-2.58728	-3.10475
H	-0.21454	-3.88523	-1.37987
H	0.67368	-3.19731	-0.00798
C	1.92240	-4.31952	-1.34100
H	1.08677	-1.46579	-3.93969
H	0.09437	-2.91062	-3.71055
C	2.23340	-3.29315	-3.61134
H	3.12341	-3.44177	0.23402
H	4.07170	-4.22920	-1.02045
H	3.67734	-1.66294	-3.67169
H	4.38115	-3.23222	-3.26726
H	1.78852	-5.25605	-0.78578
C	2.04722	-4.61556	-2.84507
H	2.33252	-3.49670	-4.68483
H	2.90145	-5.28168	-3.02615
H	1.14803	-5.13413	-3.20356
C	2.99465	-0.99180	1.47349
H	3.80421	-1.50902	0.94528
C	2.20835	-2.05667	2.28810
C	3.67382	-0.02726	2.48497
H	1.66370	-2.72153	1.61336
C	1.21301	-1.42201	3.27641
C	3.23669	-2.88139	3.09116
H	4.20847	0.76821	1.96539
C	2.65472	0.59712	3.45176
C	4.70268	-0.85192	3.28787
H	0.68849	-2.22305	3.81301
H	0.44772	-0.85036	2.74049
C	1.95026	-0.50422	4.26082
H	3.94606	-3.36868	2.40911
H	2.71583	-3.67651	3.64059
C	3.98995	-1.96541	4.07417
H	1.90973	1.17300	2.89174
H	3.17262	1.29655	4.12114
H	5.44868	-1.28117	2.60557
H	5.23902	-0.18762	3.97851
H	1.22898	-0.05042	4.95191
C	2.98773	-1.32239	5.05144
H	4.72842	-2.55386	4.63311
H	3.52015	-0.67532	5.76179
H	2.48069	-2.10031	5.63772
Pd	-0.19034	0.09885	0.60342
C	-0.18571	2.05144	0.30686
C	0.31798	2.98707	1.21760
C	-0.92441	2.51116	-0.79738
C	0.10874	4.35804	1.02794
H	0.88651	2.66605	2.08348
C	-1.13740	3.87733	-1.00195
H	-1.32254	1.80641	-1.52219
C	-0.60891	4.77635	-0.08389
H	0.49909	5.09134	1.72698
H	-1.69959	4.24193	-1.85616
F	-0.80315	6.10599	-0.27973
O	-1.19624	-1.90110	1.00532
B	-2.51706	-1.29220	0.71434
H	-1.02778	-2.61303	0.37114
O	-2.28551	0.12637	1.12455
H	-2.78734	0.77061	0.60095
O	-2.78098	-1.42700	-0.71652
B	-3.90697	-1.23126	-1.41300
C	-5.19448	-0.53088	-0.77647
C	-6.37211	-1.23481	-0.54753
C	-5.19931	0.80476	-0.39748
C	-7.49367	-0.65327	0.03402
C	-6.29313	1.43091	0.18516
C	-7.45155	0.68930	0.39866
O	-3.93275	-1.62850	-2.72460
H	-4.77818	-1.42174	-3.15168
F	-8.52181	1.26567	0.95567
F	-4.07669	1.55469	-0.58405
F	-6.24830	2.72278	0.53453
F	-6.44342	-2.53725	-0.88794
F	-8.60890	-1.36524	0.24394
F	-3.54033	-1.86380	1.47221

12'

E: -2325.56232

B	0.58224	-1.70949	1.65384
O	0.57222	-1.31521	0.13096
B	-0.40320	-1.19486	-0.79183
O	1.23004	-0.63432	2.35374
H	0.65779	0.14526	2.30328

O	-0.73936	-1.98832	2.11683
H	-1.08141	-2.77867	1.67408
O	-0.05395	-1.37884	-2.10930
H	-0.80839	-1.27270	-2.70868
C	-1.90367	-0.82727	-0.42282
C	-2.22706	0.09324	0.57585
C	-2.98451	-1.38752	-1.10154
C	-3.53770	0.42573	0.89489
C	-4.31020	-1.09193	-0.80596
C	-4.58475	-0.17630	0.20331
F	-1.26412	0.73776	1.25683
F	-2.76015	-2.27082	-2.10245
F	-5.31454	-1.66927	-1.48128
F	-3.80484	1.32216	1.85536
F	-5.85057	0.13378	0.50171
Pd	2.46787	-0.18601	-0.19044
C	1.41363	1.55953	-0.28614
C	0.59637	1.83041	-1.39173
C	1.36596	2.41852	0.82038
C	-0.29977	2.90436	-1.37352
H	0.62606	1.18818	-2.26620
C	0.47821	3.49841	0.85269
H	2.00795	2.24372	1.67945
C	-0.34462	3.71276	-0.24507
H	-0.95203	3.11429	-2.21571
H	0.41989	4.16095	1.71074
P	4.16127	1.15250	-0.76004
H	4.46950	2.19532	0.13225
H	5.43168	0.56896	-0.93795
H	4.03125	1.86765	-1.96368
P	3.68176	-2.25508	-0.06957
H	4.88037	-2.36017	-0.81016
H	4.16106	-2.68677	1.18087
H	3.03724	-3.42448	-0.51010
F	1.43222	-2.84883	1.67484
F	-1.21429	4.75404	-0.21986

BF_4^-

E: -424.58174
G: -424.58985
Esp: -424.81973
Gcorr: -0.00811
ZPE: 0.01419
Esp + Gcorr: -424.82783

B	0.00000	0.00000	0.00000
F	0.81256	0.81256	0.81256
F	-0.81256	-0.81256	0.81256
F	-0.81256	0.81256	-0.81256
F	0.81256	-0.81256	-0.81256

THF

E: -232.46692
G: -232.37196
Esp: -232.56510
Gcorr: 0.09496
ZPE: 0.11745
Esp + Gcorr: -232.47014

C	1.16535	-0.42702	-0.13350
O	-0.00009	-1.25403	-0.00026
C	-1.16533	-0.42689	0.13382
C	-0.73151	0.99451	-0.23156
C	0.73155	0.99455	0.23142
H	1.95280	-0.82022	0.52031
H	1.52928	-0.47350	-1.17149
H	-1.95325	-0.82016	-0.51936
H	-1.52852	-0.47318	1.17210
H	-0.78638	1.14399	-1.31654
H	-1.34491	1.76007	0.25292
H	1.34498	1.75992	-0.25331
H	0.78641	1.14439	1.31634

$THFH^+$

E: -232.87871
G: -232.77326
Esp: -232.97547
Gcorr: 0.10546
ZPE: 0.13037
Esp + Gcorr: -232.87001

C	1.23071	-0.38551	-0.13107
O	-0.02920	-1.22094	0.09375
C	-1.25353	-0.30048	0.14992
C	-0.69469	1.04451	-0.26417
C	0.76028	1.00572	0.23320
H	1.98027	-0.83039	0.52008
H	1.48710	-0.50117	-1.18431
H	-1.99609	-0.74390	-0.51159
H	-1.56415	-0.35508	1.19193
H	-0.73118	1.15844	-1.35166
H	-1.26755	1.85321	0.19557
H	1.38570	1.75655	-0.25552
H	0.80951	1.15692	1.31557
H	-0.12663	-1.91257	-0.59729

BF_4^-•$(THF)H^+$

E: -657.51577
G: -657.40200
Esp: -657.83172
Gcorr: 0.11376
ZPE: 0.14687
Esp + Gcorr: -657.71795

B	-1.79646	0.02136	-0.14757
F	-1.28574	-0.72703	1.01854
F	-1.65154	1.37276	0.14928
F	-0.98241	-0.33677	-1.22627
F	-3.10884	-0.34220	-0.33971
C	1.75216	-1.27240	-0.01650
O	1.15328	-0.42347	1.07457
C	1.44984	1.02966	0.80653
C	1.94246	1.04044	-0.62767
C	2.66402	-0.31069	-0.75798
H	2.24945	-2.09713	0.49109
H	0.91369	-1.61816	-0.61844
H	0.51991	1.56434	0.98880
H	2.21385	1.29717	1.53617
H	1.09248	1.08942	-1.31256
H	2.60404	1.89060	-0.81022
H	2.78733	-0.62174	-1.79820
H	3.65011	-0.27294	-0.28415
H	0.13111	-0.57345	1.10587

$(BO_2H)_3$

E: -528.19226
G: -528.14892
Esp: -528.45227
Gcorr: 0.04335
ZPE: 0.07316
Esp + Gcorr: -528.40893

B	0.41171	-1.31614	-0.00002
B	-1.34587	0.30149	0.00005
B	0.93404	1.01474	0.00002
O	0.85076	-2.60070	-0.00019
H	0.10521	-3.22280	-0.00012
O	-2.67780	0.56379	-0.00015
H	-2.84406	1.52043	0.00008

O	1.82731	2.03685	-0.00014
H	2.73872	1.70191	0.00036
O	1.34967	-0.30307	0.00014
O	-0.93764	-1.01730	0.00026
O	-0.41221	1.32044	0.00001