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Dissecting Transmetalation Reactions at the Molecular Level: C–B versus F-B Bond Activation in Phenyltrifluoroborate Silver Complexes.

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Supporting Information:

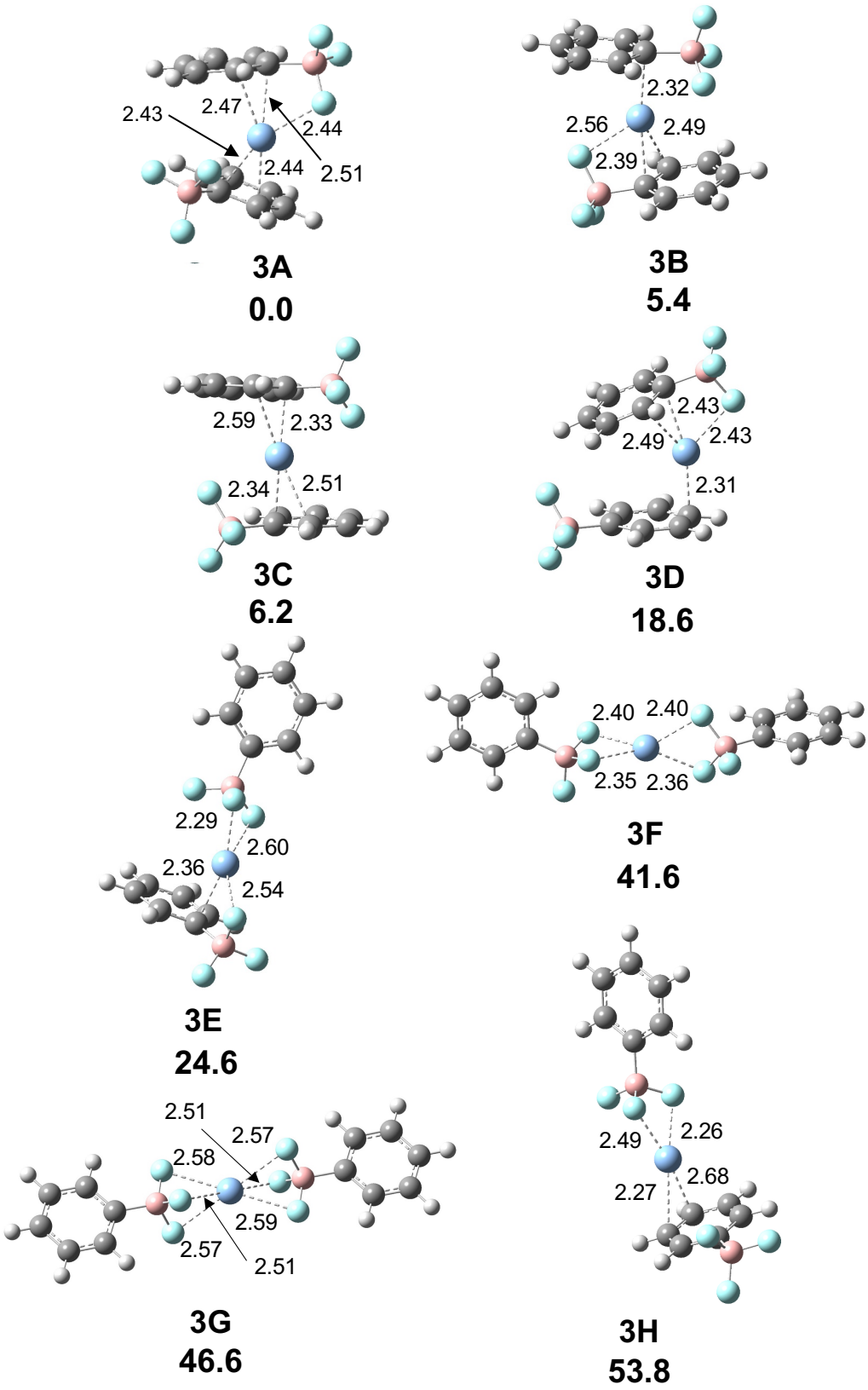


Figure S1: M06/SDD6-31+G(d) DFT calculated structures of isomers of $[Ag(PhBF_3)_2]^-$, **3**. Relative energies are in kJ/mol.

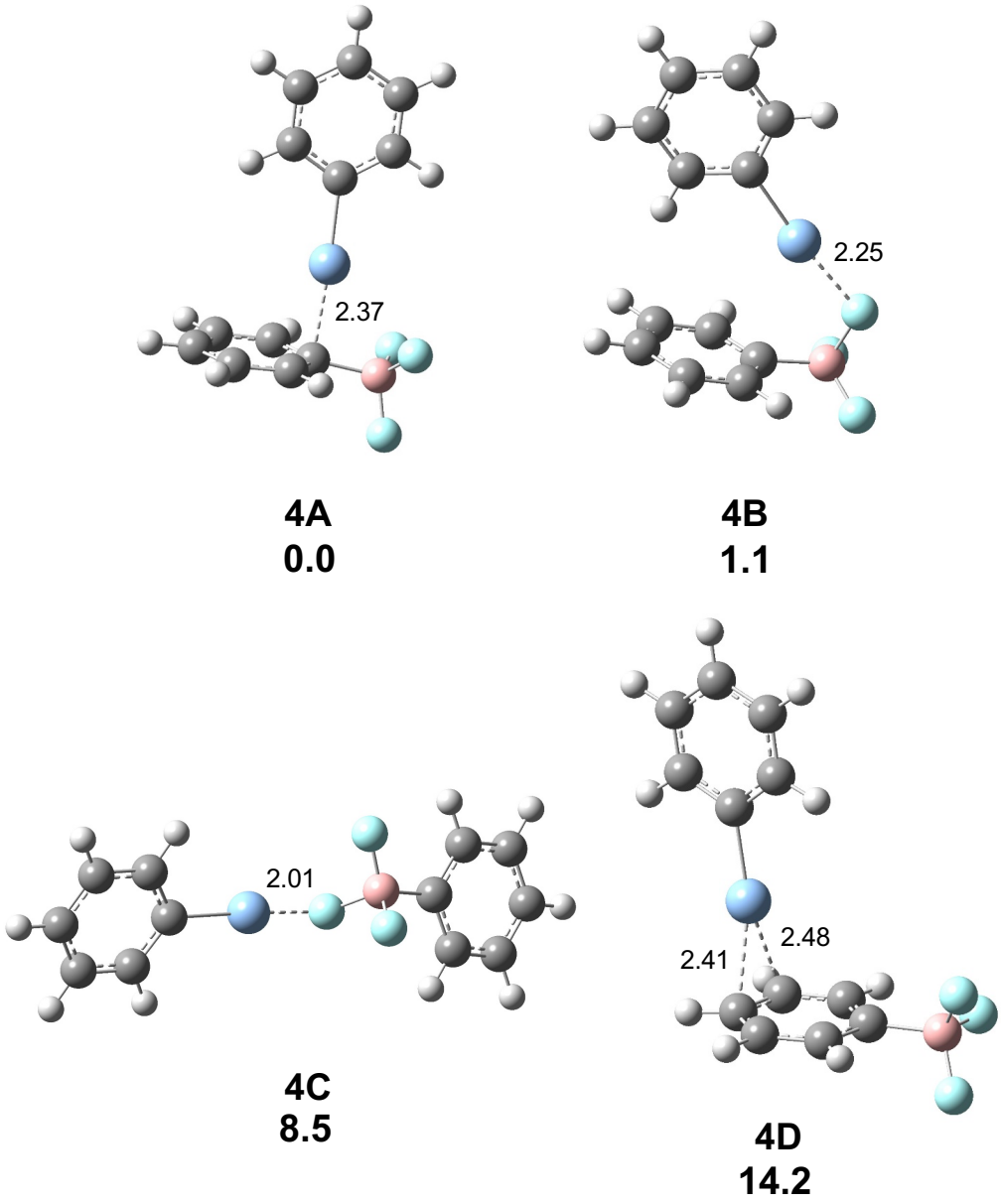


Figure S2: M06/SDD6-31+G(d) DFT calculated structures of isomers of $[PhAg(PhBF_3)]^-$, **4**. Relative energies are in kJ/mol.

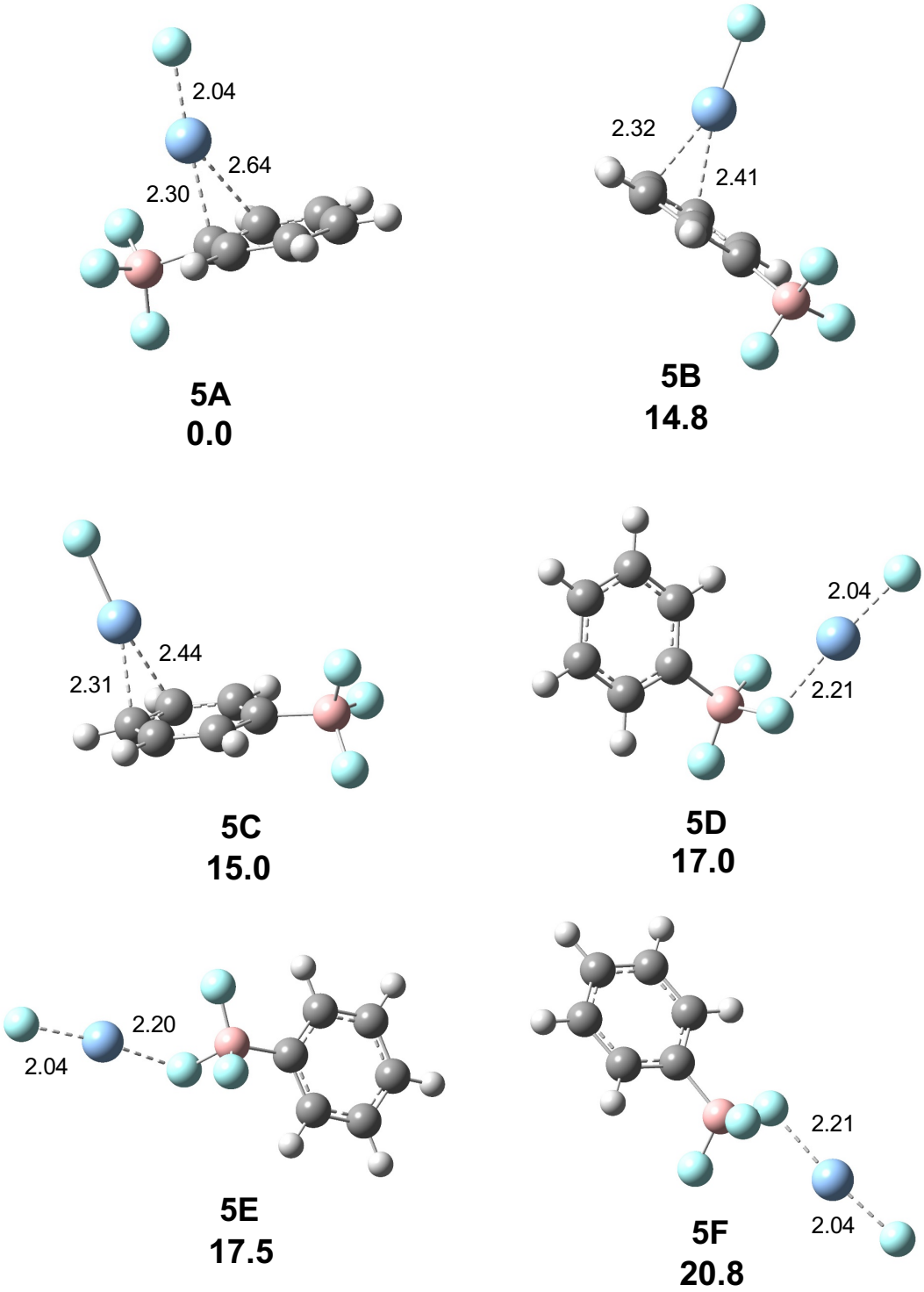
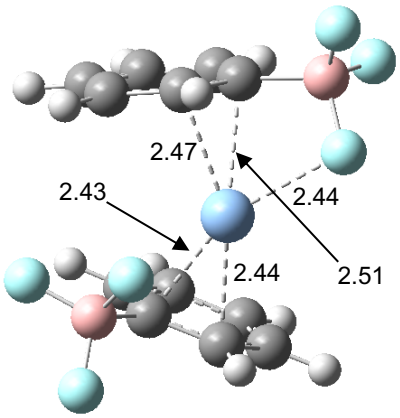


Figure S3: M06/SDD6-31+G(d) DFT calculated structures of isomers of $[FAg(PhBF_3)]^-$, **5**. Relative energies are in kJ/mol.

AgPhBF32 Isomers

Isomer 3A # opt freq M06/gen pseudo=read

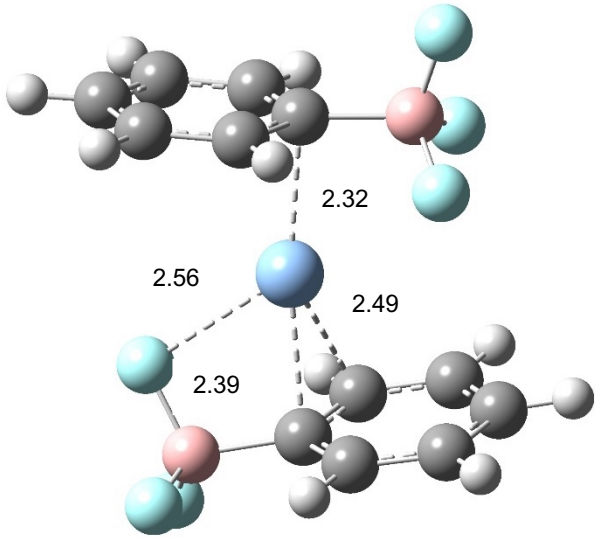


Zero-point correction= 0.205726 (Hartree/Particle)
Thermal correction to Energy= 0.226475
Thermal correction to Enthalpy= 0.227419
Thermal correction to Gibbs Free Energy= 0.152661
Sum of electronic and zero-point Energies= -1258.811075
Sum of electronic and thermal Energies= -1258.790325
Sum of electronic and thermal Enthalpies= -1258.789381
Sum of electronic and thermal Free Energies= -1258.864139
HF = -1259.0168003
Single Point Energy Calculations with extended basis set: HF = -1259.4391946

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-2.738554	-0.919902	-0.719683
C	-2.233310	0.393797	0.122647
C	-1.949613	1.609839	-0.548735
C	-2.106980	0.403239	1.527308
C	-1.573345	2.769173	0.151291
H	-2.110094	1.659474	-1.629119
C	-1.751519	1.553197	2.223532
H	-2.301883	-0.524707	2.065686
C	-1.482183	2.741005	1.537406
H	-1.358966	3.687504	-0.395491
H	-1.666831	1.525533	3.310641
H	-1.188935	3.636306	2.085210
F	-3.952205	-0.639472	-1.359850
F	-1.754680	-1.211343	-1.726203
F	-2.863915	-2.028487	0.127840
Ag	0.079236	0.254231	-0.608364
B	3.132311	0.398235	-0.570102
C	2.234973	-0.578511	0.382306
C	1.542981	-1.681916	-0.172491
C	2.075306	-0.359045	1.763288
C	0.720248	-2.506565	0.608618
H	1.687277	-1.917020	-1.230901
C	1.290678	-1.198055	2.550388
H	2.593308	0.489295	2.212578
C	0.603772	-2.269041	1.973919
H	0.163028	-3.316703	0.139543
H	1.191153	-1.004556	3.619651
H	-0.042825	-2.900972	2.582579
F	4.034339	-0.332815	-1.345299
F	2.207920	1.064155	-1.481213
F	3.785857	1.377143	0.180815

Isomer 3B # opt freq M06/gen pseudo=read



Zero-point correction= 0.205469 (Hartree/Particle)
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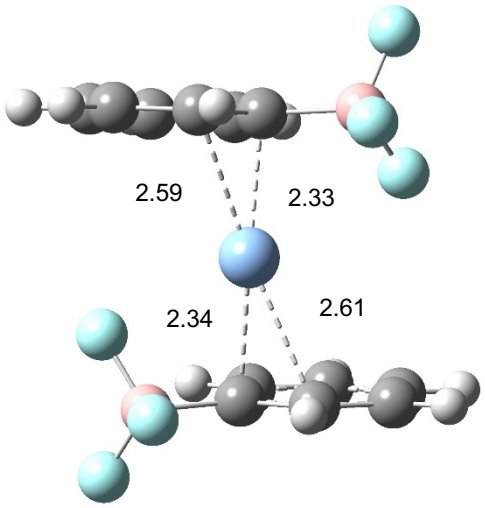
Thermal correction to Enthalpy= 0.227343
Thermal correction to Gibbs Free Energy= 0.151017
Sum of electronic and zero-point Energies= -1258.809015
Sum of electronic and thermal Energies= -1258.788086
Sum of electronic and thermal Enthalpies= -1258.787142
Sum of electronic and thermal Free Energies= -1258.863467
HF = -1259.0144845

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	2.557199	1.357549	-0.036871
C	2.309085	-0.269209	-0.036543
C	2.131556	-0.990968	-1.242045
C	2.348886	-1.033349	1.153405
C	2.053259	-2.387178	-1.262283
H	2.096679	-0.430358	-2.178020
C	2.273285	-2.425428	1.137537
H	2.464294	-0.501635	2.099027
C	2.134975	-3.104778	-0.072714
H	1.916638	-2.910045	-2.208818
H	2.308263	-2.984004	2.073020
H	2.061460	-4.191776	-0.084331
F	1.728254	1.943268	-1.027843
F	2.214426	1.879995	1.227108
F	3.899258	1.635676	-0.327127
Ag	-0.007957	-0.132075	0.006398
B	-2.854332	-1.202163	0.028882
C	-2.354291	0.359776	0.022339
C	-2.383387	1.162543	-1.137855
C	-1.888328	0.978743	1.209450
C	-2.007905	2.503764	-1.112112
H	-2.733580	0.707809	-2.065147
C	-1.493740	2.323805	1.234575
H	-1.890860	0.397775	2.135001
C	-1.563250	3.087389	0.074952
H	-2.038270	3.095516	-2.027156
H	-1.116141	2.761726	2.158021
H	-1.235580	4.125924	0.085780
F	-3.389418	-1.548708	-1.217585
F	-1.705849	-2.034172	0.286326
F	-3.783797	-1.417285	1.052415

Isomer 3C # opt freq M06/gen pseudo=read



Zero-point correction= 0.205356 (Hartree/Particle)
Thermal correction to Energy= 0.226269
Thermal correction to Enthalpy= 0.227213
Thermal correction to Gibbs Free Energy= 0.151486
Sum of electronic and zero-point Energies= -1258.808728
Sum of electronic and thermal Energies= -1258.787815
Sum of electronic and thermal Enthalpies= -1258.786871
Sum of electronic and thermal Free Energies= -1258.862599
HF = -1259.0140843

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-2.774754	-1.070180	-0.424256
C	-2.280733	0.409443	0.087000
C	-2.065417	1.497486	-0.789099
C	-2.081573	0.657628	1.466810
C	-1.715057	2.767770	-0.313498
H	-2.221776	1.336675	-1.856913
C	-1.743640	1.920798	1.943612
H	-2.223797	-0.171353	2.163261
C	-1.566463	2.981022	1.051420
H	-1.543740	3.582286	-1.016559
H	-1.603642	2.081605	3.012911
H	-1.278456	3.964065	1.422305
F	-2.882869	-1.081782	-1.823868
F	-1.778529	-2.021900	-0.031032
F	-3.988926	-1.418234	0.176199
Ag	-0.013023	-0.046069	-0.286808
B	2.730242	1.118189	-0.438138
C	2.267718	-0.372317	0.078633
C	2.092861	-1.468999	-0.797109
C	2.086418	-0.631884	1.459569
C	1.799562	-2.753989	-0.321820
H	2.233456	-1.300712	-1.865900
C	1.804018	-1.909030	1.936023
H	2.194445	0.200961	2.157276
C	1.666000	-2.974947	1.043413
H	1.659605	-3.573861	-1.025722
H	1.676127	-2.076611	3.005833
H	1.423475	-3.970175	1.414591
F	2.589287	1.194008	-1.837247
F	1.885654	2.086161	0.169087
F	4.057249	1.365575	-0.063011

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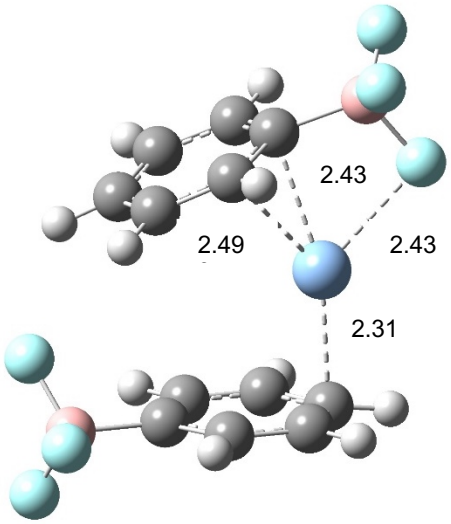
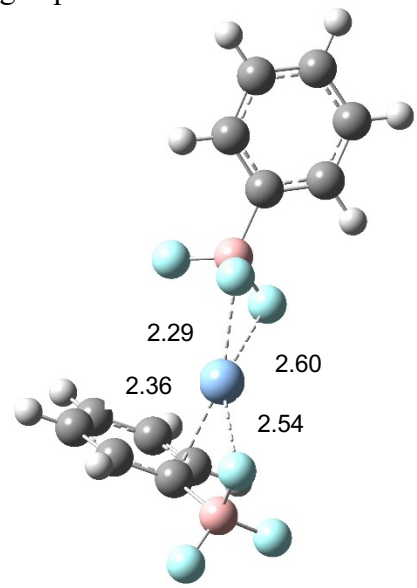


Zero-point correction= 0.205551 (Hartree/Particle)
Thermal correction to Energy= 0.226345
Thermal correction to Enthalpy= 0.227289
Thermal correction to Gibbs Free Energy= 0.150874
Sum of electronic and zero-point Energies= -1258.804005
Sum of electronic and thermal Energies= -1258.783211
Sum of electronic and thermal Enthalpies= -1258.782267
Sum of electronic and thermal Free Energies= -1258.858682
HF = -1259.0095562

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	3.527112	0.305075	0.476985
C	2.156440	1.124263	0.121055
C	1.086425	1.231813	1.046225
C	1.954883	1.711576	-1.146343
C	-0.118952	1.868952	0.711225
H	1.228979	0.842538	2.056992
C	0.773461	2.376894	-1.466994
H	2.763454	1.652634	-1.876841
C	-0.273132	2.445761	-0.544434
H	-0.946718	1.902262	1.419904
H	0.655548	2.828611	-2.453060
H	-1.224553	2.909796	-0.799780
F	3.762597	0.279049	1.851623
F	3.309895	-1.079877	0.047292
F	4.622974	0.798344	-0.225345
Ag	0.895272	-0.929984	-0.165800
B	-3.837012	0.644337	0.362201
C	-2.713800	-0.488732	0.001527
C	-2.261165	-1.424204	0.942733
C	-2.157335	-0.551180	-1.284414
C	-1.309199	-2.392515	0.627353
H	-2.673942	-1.380834	1.951007
C	-1.205125	-1.509014	-1.633687
H	-2.483821	0.174815	-2.031519
C	-0.768569	-2.454741	-0.674951
H	-0.992758	-3.123475	1.372429
H	-0.818766	-1.561953	-2.652550
H	-0.137900	-3.294834	-0.973259
F	-4.158059	0.580107	1.730797
F	-3.315118	1.926528	0.059383
F	-4.986890	0.426891	-0.420686

Isomer 3E # opt freq M06/gen pseudo=read

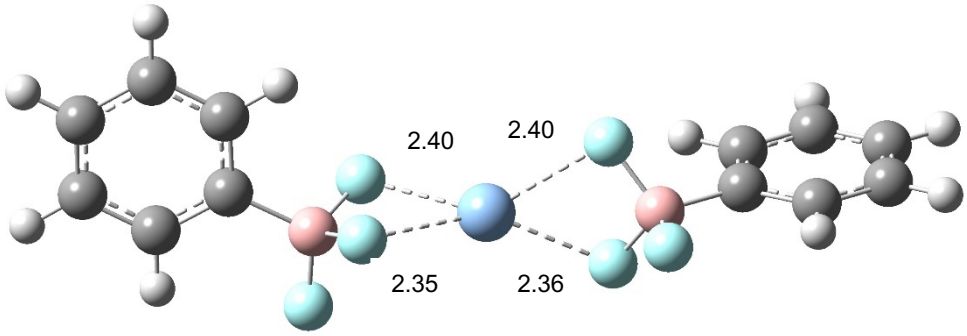


Zero-point correction= 0.205182 (Hartree/Particle)
Thermal correction to Energy= 0.226218
Thermal correction to Enthalpy= 0.227163
Thermal correction to Gibbs Free Energy= 0.149753
Sum of electronic and zero-point Energies= -1258.801708
Sum of electronic and thermal Energies= -1258.780671
Sum of electronic and thermal Enthalpies= -1258.779727
Sum of electronic and thermal Free Energies= -1258.857136
HF = -1259.0068895

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-3.646880	-1.128156	0.011230
C	-2.962724	0.348545	-0.192284
C	-2.387731	0.767910	-1.414294
C	-2.930759	1.278393	0.874944
C	-1.837932	2.046002	-1.568194
H	-2.407147	0.076679	-2.258340
C	-2.398697	2.555730	0.720383
H	-3.362533	0.978472	1.832061
C	-1.853233	2.942608	-0.505413
H	-1.384157	2.330688	-2.517013
H	-2.392824	3.249567	1.561280
H	-1.414944	3.933454	-0.620252
F	-3.684790	-1.820741	-1.203831
F	-2.805562	-1.865608	0.927741
F	-4.918650	-1.018686	0.574936
Ag	-0.794602	-0.458498	0.263189
B	1.992543	0.270620	-0.005179
C	3.572654	0.005031	-0.046751
C	4.168122	-0.824424	-1.004092
C	4.412828	0.585749	0.912317
C	5.541532	-1.068818	-1.006727
H	3.538069	-1.285614	-1.766119
C	5.785926	0.348794	0.923359
H	3.972802	1.243855	1.664154
C	6.356422	-0.483139	-0.039716
H	5.978223	-1.720016	-1.765709
H	6.415514	0.814142	1.683492
H	7.430748	-0.672468	-0.037049
F	1.329880	-0.104875	-1.203991
F	1.366535	-0.568956	1.025278
F	1.651009	1.587093	0.313441

Isomer 3F # opt freq M06/gen pseudo=read



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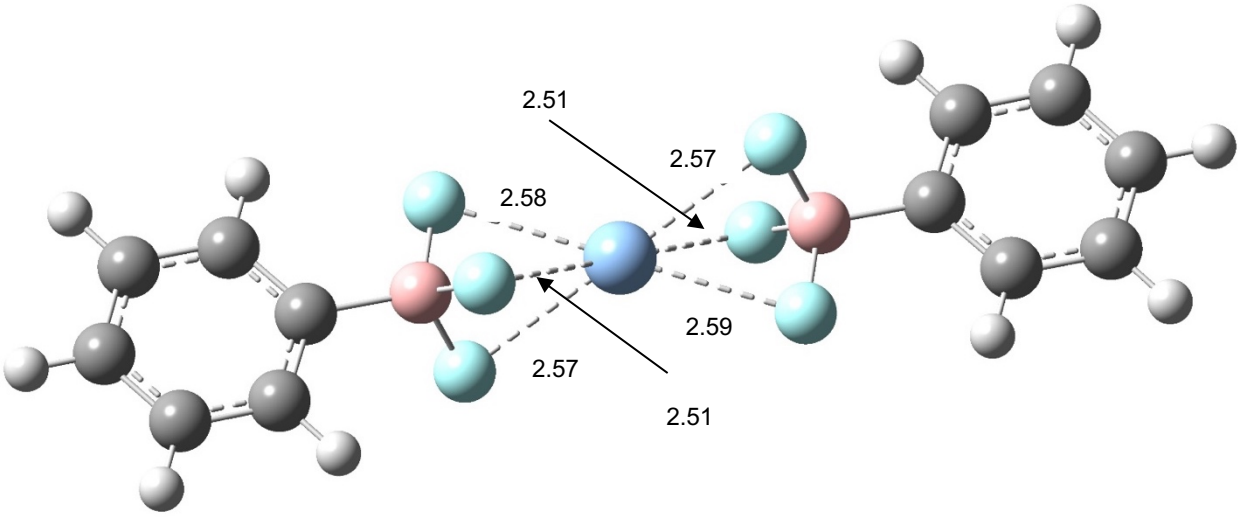
Thermal correction to Enthalpy= 0.227241
Thermal correction to Gibbs Free Energy= 0.149858
Sum of electronic and zero-point Energies= -1258.795228
Sum of electronic and thermal Energies= -1258.774301
Sum of electronic and thermal Enthalpies= -1258.773357
Sum of electronic and thermal Free Energies= -1258.850740
HF = -1259.0005979

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-2.864022	-0.455825	-0.549084
C	-4.441197	1.088785	0.836945
C	-5.486338	-0.372018	-0.742675
C	-5.685030	1.589799	1.212816
H	-3.538747	1.472860	1.317546
C	-6.739551	0.120398	-0.376499
H	-5.411562	-1.142770	-1.511147
C	-6.842812	1.104431	0.604432
H	-5.755954	2.360452	1.981880
H	-7.639668	-0.265430	-0.857916
H	-7.820127	1.492363	0.894719
F	-1.988284	0.613008	-0.977689
F	-2.168503	-0.991306	0.608610
F	-2.878475	-1.432588	-1.536498
Ag	0.000068	-0.302780	-0.000820
B	2.864153	-0.456552	0.549493
C	5.486557	-0.373134	0.741825
C	4.440657	1.090418	-0.834741
C	6.739613	0.119757	0.375750
H	5.412123	-1.145158	1.509051
C	5.684327	1.591934	-1.210487
H	3.537963	1.475409	-1.314153
C	6.842412	1.105409	-0.603604
H	7.639971	-0.266980	0.855989
H	5.754892	2.363866	-1.978301
H	7.819601	1.493721	-0.893809
F	2.879138	-1.434149	1.536043
F	1.988117	0.611610	0.978904
F	2.168706	-0.991381	-0.608668
C	-4.311963	0.098563	-0.145925
C	4.311886	0.098566	0.146547

Isomer 3G # opt freq M06/gen pseudo=read



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Thermal correction to Enthalpy= 0.227031
Thermal correction to Gibbs Free Energy= 0.145822
Sum of electronic and zero-point Energies= -1258.793326
Sum of electronic and thermal Energies= -1258.771948
Sum of electronic and thermal Enthalpies= -1258.771004
Sum of electronic and thermal Free Energies= -1258.852212
HF = -1258.9980346

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	2.748368	0.041973	0.037484
C	5.103169	1.202753	0.001804
C	5.044442	-1.189557	0.004248
C	6.497617	1.174661	-0.021468
H	4.580493	2.160333	0.010776
C	6.436455	-1.232482	-0.019322
H	4.474722	-2.121330	0.015364
C	7.169826	-0.045848	-0.032332
H	7.062913	2.107934	-0.030924
H	6.954096	-2.193025	-0.027430
H	8.260079	-0.074186	-0.050681
F	2.200425	1.354015	0.074974
F	2.170891	-0.593411	-1.110308
F	2.198123	-0.657627	1.153421
Ag	-0.000062	0.000567	0.000712
B	-2.748364	-0.042394	-0.039149
C	-5.103130	-1.203128	-0.001832
C	-5.044393	1.189179	-0.004347
C	-6.497554	-1.175033	0.022476
H	-4.580472	-2.160714	-0.011230
C	-6.436395	1.232106	0.020283
H	-4.474707	2.120967	-0.015960
C	-7.169756	0.045482	0.033858
H	-7.062850	-2.108301	0.032333
H	-6.954010	2.192660	0.028772
H	-8.259996	0.073809	0.053028
F	-2.200432	-1.354325	-0.078028
F	-2.198714	0.658512	-1.154400
F	-2.170211	0.591808	1.109244
C	4.347259	0.025996	0.014767
C	-4.347222	-0.026371	-0.015354

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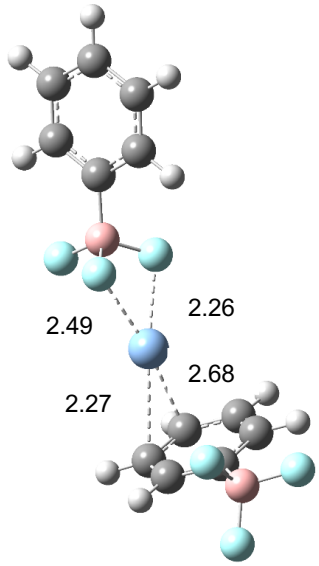

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Thermal correction to Energy= 0.226617
Thermal correction to Enthalpy= 0.227561
Thermal correction to Gibbs Free Energy= 0.149282
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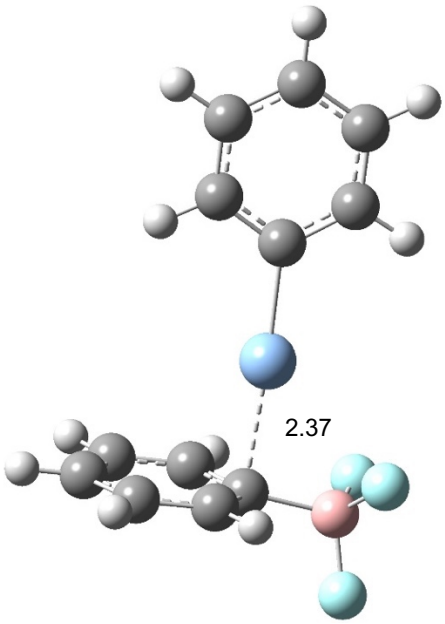
Sum of electronic and thermal Energies= -1258.769664
Sum of electronic and thermal Enthalpies= -1258.768720
Sum of electronic and thermal Free Energies= -1258.847000
HF = -1258.9962812

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-4.799764	1.442880	-0.279993
C	-3.766152	0.230420	0.094490
C	-3.170979	0.104631	1.358222
C	-3.445662	-0.737268	-0.870236
C	-2.320951	-0.953713	1.672220
H	-3.398297	0.857042	2.113593
C	-2.598506	-1.807006	-0.590963
H	-3.888582	-0.646142	-1.863304
C	-2.027046	-1.937617	0.698960
H	-1.902982	-1.054820	2.674588
H	-2.404803	-2.574679	-1.341391
H	-1.515003	-2.859887	0.984841
F	-5.003177	2.265063	0.843340
F	-4.253843	2.194076	-1.340001
F	-6.024434	0.878585	-0.695696
Ag	-0.176686	-0.827643	0.011731
B	2.700104	-0.616416	-0.152732
C	4.016495	0.285120	-0.075975
C	3.958324	1.567451	0.485689
C	5.255823	-0.154238	-0.552836
C	5.085763	2.380365	0.570009
H	3.001948	1.934605	0.863994
C	6.393845	0.649332	-0.474300
H	5.329649	-1.148947	-0.994574
C	6.311645	1.920905	0.088659
H	5.010331	3.375470	1.010374
H	7.348201	0.281471	-0.854187
H	7.198236	2.553093	0.150403
F	2.054441	-0.756343	1.120570
F	1.661210	0.050627	-0.957792
F	2.884499	-1.880963	-0.698829

PhAgPhBF3- Isomers

Isomer 4A # opt freq M06/gen pseudo=read

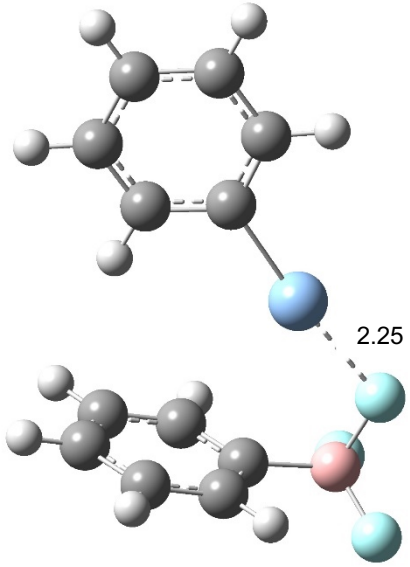


Zero-point correction= 0.190784 (Hartree/Particle)
Thermal correction to Energy= 0.207500
Thermal correction to Enthalpy= 0.208444
Thermal correction to Gibbs Free Energy= 0.141220
Sum of electronic and zero-point Energies= -934.298901
Sum of electronic and thermal Energies= -934.282186
Sum of electronic and thermal Enthalpies= -934.281241
Sum of electronic and thermal Free Energies= -934.348466
HF = -934.4896853
Single Point Energy Calculations with extended basis set: HF = -934.7993853

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	2.468963	-1.493601	0.015663
C	2.165331	0.120739	0.013622
C	2.078806	0.871457	1.205206
C	2.110634	0.849079	-1.195590
C	2.000955	2.266489	1.195099
H	2.105978	0.330358	2.152144
C	2.033562	2.242188	-1.215321
H	2.161721	0.292415	-2.133315
C	1.992997	2.953753	-0.016587
H	1.944449	2.816538	2.135204
H	2.003303	2.774220	-2.166929
H	1.933604	4.042569	-0.028636
F	2.179457	-2.024517	1.286969
F	1.658482	-2.120870	-0.960913
F	3.822200	-1.710774	-0.301797
Ag	-0.198400	-0.041318	-0.003237
C	-4.437426	-1.306465	-0.019013
C	-3.041116	-1.276538	-0.015952
C	-2.312307	-0.072971	0.002999
C	-3.079881	1.106111	0.019013
C	-4.476596	1.093684	0.014957
C	-5.165549	-0.117858	-0.003998
H	-4.960315	-2.265515	-0.034128
H	-2.504712	-2.228104	-0.029915
H	-2.574930	2.075318	0.034941
H	-5.030194	2.035579	0.026727
H	-6.256647	-0.136010	-0.007190

Isomer 4B # opt freq M06/gen pseudo=read

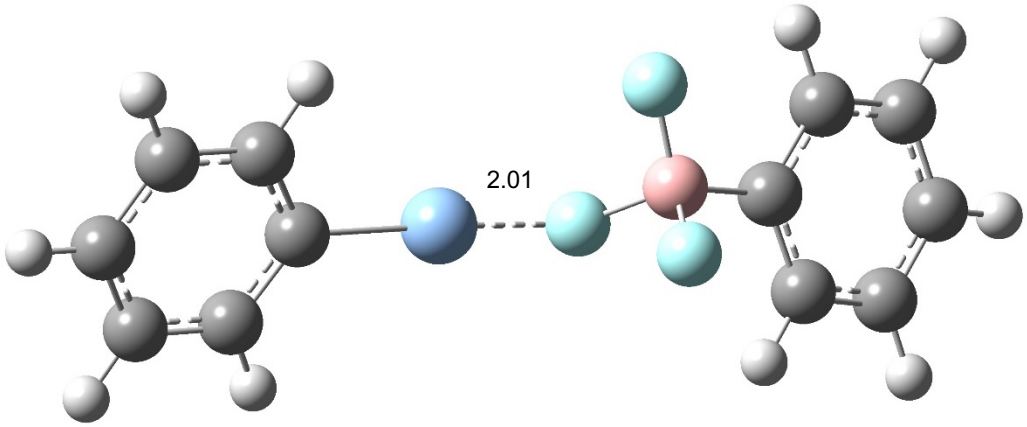


Zero-point correction= 0.191147 (Hartree/Particle)
Thermal correction to Energy= 0.207687
Thermal correction to Enthalpy= 0.208631
Thermal correction to Gibbs Free Energy= 0.142178
Sum of electronic and zero-point Energies= -934.298368
Sum of electronic and thermal Energies= -934.281828
Sum of electronic and thermal Enthalpies= -934.280884
Sum of electronic and thermal Free Energies= -934.347338
HF = -934.4895155
Single Point Energy Calculations with extended basis set: HF = -934.7988821

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	2.940069	-0.739436	0.169738
C	2.224594	0.706093	0.034049
C	1.662346	1.356046	1.143143
C	2.058387	1.317764	-1.217302
C	0.959788	2.554005	1.012869
H	1.778218	0.902490	2.129331
C	1.354493	2.512053	-1.361925
H	2.487028	0.832427	-2.096564
C	0.800379	3.134633	-0.243973
H	0.524733	3.030619	1.893145
H	1.229082	2.957400	-2.350191
H	0.239334	4.063712	-0.353669
F	3.361043	-1.007267	1.472993
F	1.910327	-1.757765	-0.160825
F	3.976916	-0.919401	-0.744361
Ag	-0.195152	-0.970390	-0.075679
C	-3.897846	1.317066	0.412814
C	-4.930977	0.432845	0.106368
C	-4.613595	-0.874920	-0.255984
C	-3.279074	-1.285470	-0.309032
C	-2.213268	-0.419677	-0.005776
C	-2.568495	0.892932	0.355958
H	-4.127885	2.346481	0.696829
H	-5.971541	0.758875	0.148669
H	-5.409947	-1.582333	-0.498801
H	-3.068853	-2.318313	-0.596642
H	-1.783351	1.613817	0.598580

Isomer 4C # opt freq M06/gen pseudo=read

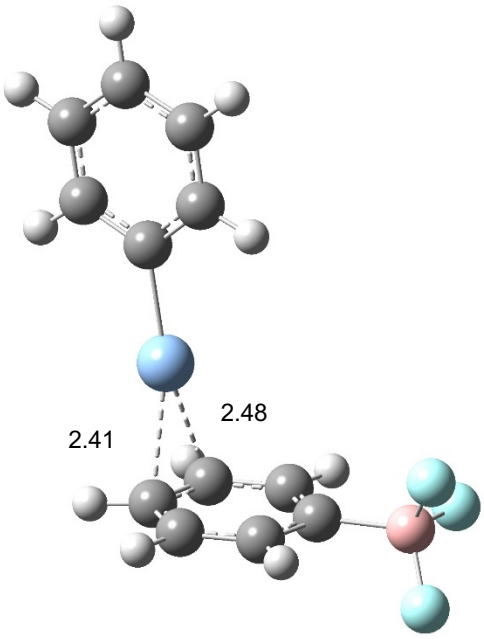


Zero-point correction= 0.191213 (Hartree/Particle)
Thermal correction to Energy= 0.207726
Thermal correction to Enthalpy= 0.208670
Thermal correction to Gibbs Free Energy= 0.142025
Sum of electronic and zero-point Energies= -934.295647
Sum of electronic and thermal Energies= -934.279134
Sum of electronic and thermal Enthalpies= -934.278190
Sum of electronic and thermal Free Energies= -934.344835
HF = -934.4868602

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	1.887351	0.442060	0.443949
C	3.435572	0.125520	0.138256
C	4.311024	1.093490	-0.365698
C	3.959696	-1.153427	0.370949
C	5.650788	0.803945	-0.628430
H	3.926185	2.097464	-0.552235
C	5.293914	-1.458847	0.111077
H	3.296604	-1.926018	0.766625
C	6.147626	-0.476246	-0.391379
H	6.311390	1.579766	-1.020031
H	5.673158	-2.464761	0.300107
H	7.194009	-0.707959	-0.596584
F	1.542135	1.776011	0.215298
F	1.055423	-0.363455	-0.482339
F	1.495617	0.048263	1.728897
Ag	-1.118646	-0.126976	-0.183352
C	-5.374635	-1.221599	-0.099720
C	-3.979295	-1.240813	-0.155760
C	-3.204832	-0.068338	-0.086379
C	-3.922603	1.134627	0.042494
C	-5.317671	1.169715	0.099593
C	-6.053940	-0.011511	0.028397
H	-5.933977	-2.158123	-0.157002
H	-3.483444	-2.208989	-0.257857
H	-3.380612	2.080920	0.103089
H	-5.832260	2.127774	0.201918
H	-7.143910	0.011032	0.072632

Isomer 4D # opt freq M06/gen pseudo=read



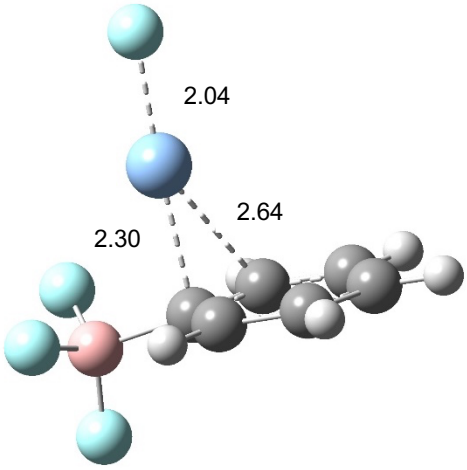
Zero-point correction= 0.191351 (Hartree/Particle)
Thermal correction to Energy= 0.207810
Thermal correction to Enthalpy= 0.208754
Thermal correction to Gibbs Free Energy= 0.142716
Sum of electronic and zero-point Energies= -934.293483
Sum of electronic and thermal Energies= -934.277024
Sum of electronic and thermal Enthalpies= -934.276080
Sum of electronic and thermal Free Energies= -934.342118
HF = -934.4848339

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	3.785837	1.221576	-0.130473
C	2.752417	-0.036326	0.007407
C	2.126408	-0.627470	-1.091693
C	2.470614	-0.579192	1.275064
C	1.271977	-1.733194	-0.952486
H	2.326075	-0.221981	-2.084068
C	1.618897	-1.662300	1.446556
H	2.946793	-0.125823	2.146585
C	1.011775	-2.261632	0.327075
H	0.861719	-2.225702	-1.836374
H	1.424111	-2.064757	2.441306
H	0.427359	-3.176503	0.439565
F	3.954448	1.564593	-1.486559
F	3.275472	2.324966	0.585763
F	5.031189	0.853862	0.429446
Ag	-0.850321	-0.789790	-0.087739
C	-2.704450	0.198728	-0.008207
C	-3.917986	-0.449459	-0.298989
C	-2.796854	1.559128	0.336259
C	-5.147579	0.211806	-0.252114
H	-3.914065	-1.506824	-0.575070
C	-4.019027	2.232745	0.387547
H	-1.889477	2.119207	0.571203
C	-5.203734	1.560652	0.092584
H	-6.066166	-0.330091	-0.487701
H	-4.044304	3.290027	0.658607
H	-6.160873	2.082956	0.130177

FAgPhBF3 Isomers

Isomer 5A # opt freq M06/gen pseudo=read

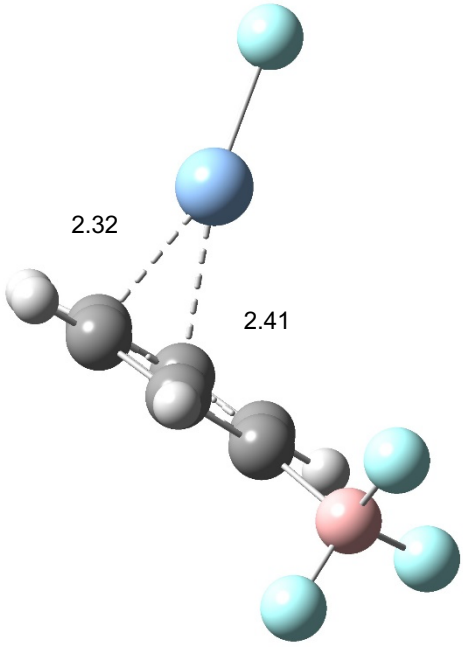


Zero-point correction= 0.103765 (Hartree/Particle)
Thermal correction to Energy= 0.116288
Thermal correction to Enthalpy= 0.117233
Thermal correction to Gibbs Free Energy= 0.061655
Sum of electronic and zero-point Energies= -802.773997
Sum of electronic and thermal Energies= -802.761474
Sum of electronic and thermal Enthalpies= -802.760530
Sum of electronic and thermal Free Energies= -802.816107
HF = -802.8777625
Single Point Energy Calculations with extended basis set: HF = -803.1400284

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	1.902765	-0.798418	0.001151
C	0.923872	0.523972	0.010773
C	0.591622	1.205851	1.205499
C	0.517830	1.140604	-1.197392
C	-0.036302	2.452075	1.193390
H	0.877668	0.747553	2.153097
C	-0.113113	2.387857	-1.215735
H	0.754732	0.636228	-2.135907
C	-0.373593	3.051737	-0.019576
H	-0.265317	2.956029	2.132971
H	-0.401031	2.839296	-2.165627
H	-0.862429	4.026320	-0.030453
F	1.838239	-1.441975	1.250829
F	1.478884	-1.681387	-1.018397
F	3.222448	-0.387387	-0.259418
Ag	-1.086062	-0.580798	-0.002527
F	-2.943397	-1.432408	0.060004

Isomer 5B # opt freq M06/gen pseudo=read

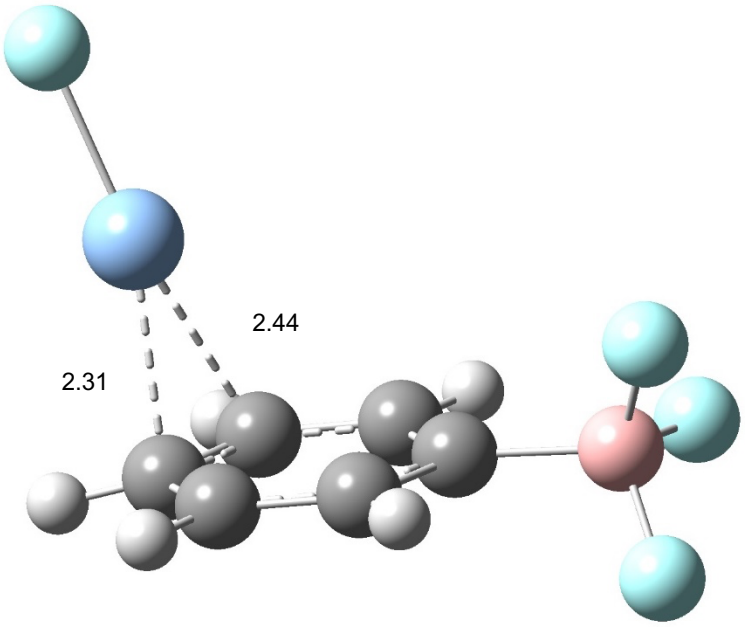


Zero-point correction= 0.103719 (Hartree/Particle)
Thermal correction to Energy= 0.116110
Thermal correction to Enthalpy= 0.117055
Thermal correction to Gibbs Free Energy= 0.061554
Sum of electronic and zero-point Energies= -802.768373
Sum of electronic and thermal Energies= -802.755982
Sum of electronic and thermal Enthalpies= -802.755037
Sum of electronic and thermal Free Energies= -802.810538
HF = -802.872092

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	3.132494	-0.470309	-0.074650
C	1.680041	0.263289	0.084557
C	0.869406	0.106001	1.208160
C	1.224914	1.140999	-0.919927
C	-0.330879	0.821531	1.364413
H	1.198397	-0.570316	1.997564
C	0.037236	1.846552	-0.807781
H	1.844245	1.269583	-1.809281
C	-0.757397	1.708934	0.349956
H	-0.877414	0.775292	2.308687
H	-0.281073	2.530432	-1.595278
H	-1.599166	2.382919	0.521856
F	3.354740	-1.346773	1.004851
F	3.175143	-1.177492	-1.293114
F	4.132407	0.529810	-0.093373
Ag	-2.045026	-0.188743	-0.002751
F	-3.570198	-1.393243	-0.573616

Isomer 5C # opt freq M06/gen pseudo=read

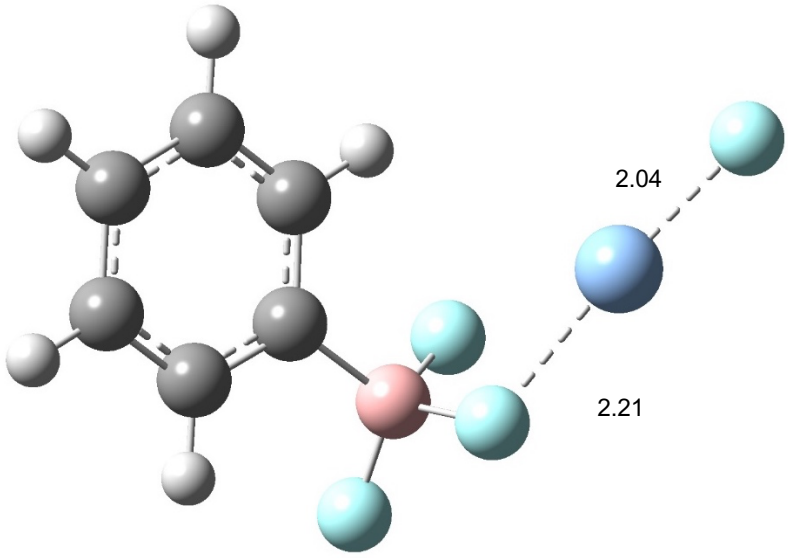


Zero-point correction= 0.103725 (Hartree/Particle)
Thermal correction to Energy= 0.116148
Thermal correction to Enthalpy= 0.117093
Thermal correction to Gibbs Free Energy= 0.061123
Sum of electronic and zero-point Energies= -802.768285
Sum of electronic and thermal Energies= -802.755862
Sum of electronic and thermal Enthalpies= -802.754918
Sum of electronic and thermal Free Energies= -802.810887
HF = -802.8720104

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	3.130126	-0.467626	-0.068101
C	1.688059	0.286500	0.088740
C	0.889762	0.160363	1.225615
C	1.212543	1.119627	-0.943521
C	-0.318587	0.862837	1.365950
H	1.237302	-0.481178	2.035879
C	0.018351	1.816277	-0.843889
H	1.820777	1.221084	-1.843919
C	-0.764982	1.709444	0.325463
H	-0.863273	0.835102	2.311794
H	-0.314165	2.470089	-1.650852
H	-1.610572	2.382317	0.483680
F	3.459558	-1.130126	1.130495
F	3.058091	-1.393489	-1.129163
F	4.117576	0.497674	-0.370470
Ag	-2.042787	-0.185717	-0.004512
F	-3.553066	-1.428598	-0.530216

Isomer 5D # opt freq M06/gen pseudo=read

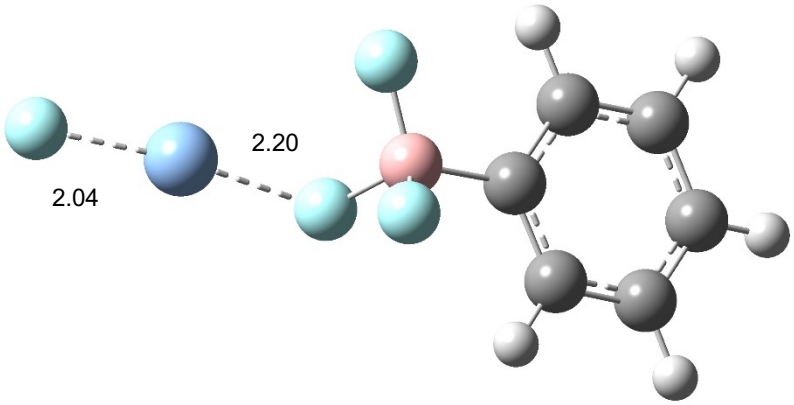


Zero-point correction= 0.103880 (Hartree/Particle)
Thermal correction to Energy= 0.116323
Thermal correction to Enthalpy= 0.117268
Thermal correction to Gibbs Free Energy= 0.060277
Sum of electronic and zero-point Energies= -802.767520
Sum of electronic and thermal Energies= -802.755076
Sum of electronic and thermal Enthalpies= -802.754132
Sum of electronic and thermal Free Energies= -802.811122
HF = -802.8713995
Single Point Energy Calculations with extended basis set: HF = -803.1326796

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-0.607369	1.451971	0.290329
C	-1.732575	0.305363	0.164046
C	-1.567488	-0.951131	0.762214
C	-2.899738	0.506852	-0.584772
C	-2.515402	-1.963843	0.617942
H	-0.676293	-1.139386	1.365540
C	-3.857628	-0.494616	-0.735096
H	-3.058595	1.478719	-1.055569
C	-3.667482	-1.738134	-0.133323
H	-2.355223	-2.932689	1.093606
H	-4.757422	-0.305560	-1.323434
H	-4.413289	-2.525948	-0.249499
F	0.150994	1.329679	1.466536
F	0.374907	1.249115	-0.810236
F	-1.107819	2.738602	0.139472
Ag	1.916552	-0.209618	-0.208045
F	3.433207	-1.536274	0.087534

Isomer 5E # opt freq M06/gen pseudo=read

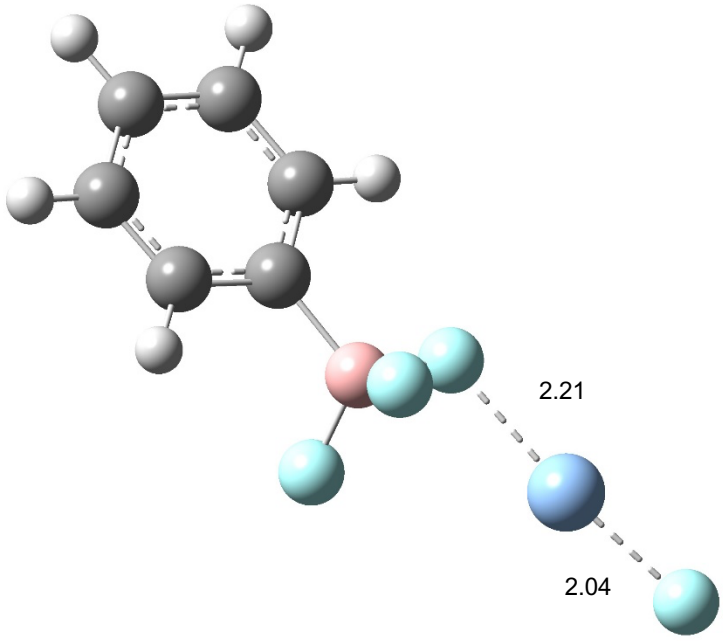


Zero-point correction= 0.103608 (Hartree/Particle)
Thermal correction to Energy= 0.116193
Thermal correction to Enthalpy= 0.117138
Thermal correction to Gibbs Free Energy= 0.059620
Sum of electronic and zero-point Energies= -802.767333
Sum of electronic and thermal Energies= -802.754747
Sum of electronic and thermal Enthalpies= -802.753803
Sum of electronic and thermal Free Energies= -802.811320
HF = -802.8709406

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	0.570551	0.065277	0.567908
C	2.129820	0.042967	0.179563
C	2.864330	1.214106	-0.036055
C	2.808951	-1.174840	0.037431
C	4.216788	1.178145	-0.377680
H	2.360169	2.175511	0.072912
C	4.158259	-1.226919	-0.305756
H	2.259715	-2.103809	0.205234
C	4.869764	-0.045303	-0.514998
H	4.764164	2.108966	-0.536856
H	4.659231	-2.191002	-0.410226
H	5.926983	-0.078779	-0.782504
F	0.075649	1.350600	0.820094
F	-0.215792	-0.433969	-0.586135
F	0.256991	-0.792486	1.626045
Ag	-2.355451	-0.052261	-0.224356
F	-4.383993	0.130308	-0.164269

Isomer 5F # opt freq M06/gen pseudo=read



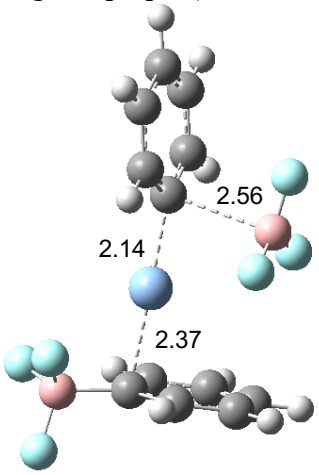
Zero-point correction= 0.103913 (Hartree/Particle)
Thermal correction to Energy= 0.116377
Thermal correction to Enthalpy= 0.117321
Thermal correction to Gibbs Free Energy= 0.061300
Sum of electronic and zero-point Energies= -802.766088
Sum of electronic and thermal Energies= -802.753624
Sum of electronic and thermal Enthalpies= -802.752679
Sum of electronic and thermal Free Energies= -802.808701
HF = -802.8700003

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-0.590732	-0.505132	0.023118
C	-2.146500	-0.095704	-0.000238
C	-2.606128	1.226033	0.011566
C	-3.116009	-1.108626	-0.018397
C	-3.968779	1.528335	0.005855
H	-1.876721	2.037314	0.023570
C	-4.479279	-0.822689	-0.024086
H	-2.785484	-2.149590	-0.030162
C	-4.912381	0.503347	-0.011997
H	-4.295681	2.569688	0.014571
H	-5.209024	-1.634129	-0.039414
H	-5.978407	0.735630	-0.017141
F	0.246788	0.700266	-0.116624
F	-0.207360	-1.099869	1.233253
F	-0.237695	-1.351103	-1.035992
Ag	2.392571	0.190772	-0.016939
F	4.423002	0.041403	0.025240

Species associated with Figure 2

TS3a-6 #m06 genecp opt=(ts,calcfc,noeigentest,maxstep=1) nosymm test freq



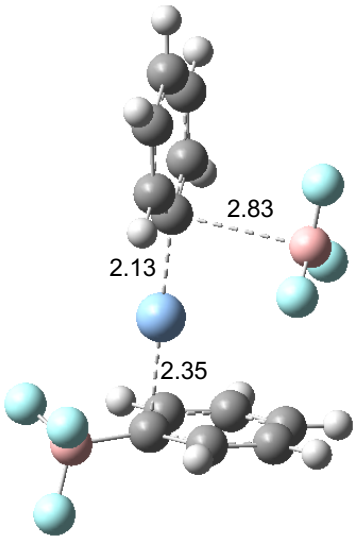
Zero-point correction= 0.204210 (Hartree/Particle)
Thermal correction to Energy= 0.225192
Thermal correction to Enthalpy= 0.226137
Thermal correction to Gibbs Free Energy= 0.149982
Sum of electronic and zero-point Energies= -1258.774716
Sum of electronic and thermal Energies= -1258.753733
Sum of electronic and thermal Enthalpies= -1258.752789
Sum of electronic and thermal Free Energies= -1258.828943
HF = -1258.9789253

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-2.531931	-0.852001	0.199079
C	-1.286920	1.351242	0.591856
C	-1.732834	2.124387	-0.498183
C	-1.846350	1.671050	1.843718
C	-2.679228	3.139081	-0.357120
H	-1.336485	1.918089	-1.495317
C	-2.795995	2.680891	2.002489
H	-1.546193	1.097459	2.724459
C	-3.216313	3.419678	0.898152
H	-3.001605	3.711180	-1.229136
H	-3.213326	2.889459	2.989523
H	-3.962671	4.206950	1.014565
F	-3.716586	-0.254156	0.221422
F	-2.019588	-1.185884	-0.980430
F	-2.138006	-1.502500	1.288046
Ag	0.483544	0.176323	0.380611
B	3.393074	0.054890	-0.544598
C	2.478225	-1.070144	0.227077
C	1.686110	-1.984737	-0.504253
C	2.528819	-1.260046	1.625740
C	1.030115	-3.053479	0.112891
H	1.618894	-1.859018	-1.586769
C	1.881195	-2.328355	2.247957
H	3.120357	-0.557207	2.214371
C	1.141041	-3.234235	1.488999
H	0.419125	-3.733029	-0.481953
H	1.948779	-2.451324	3.329573
H	0.623832	-4.061283	1.975848
F	4.480094	-0.581236	-1.168777
F	2.604053	0.694362	-1.534514
F	3.853324	1.006608	0.382470

Imaginary Vibrational Frequency = -46.0907 cm-1

6 # opt freq nosymm M06/gen pseudo=read

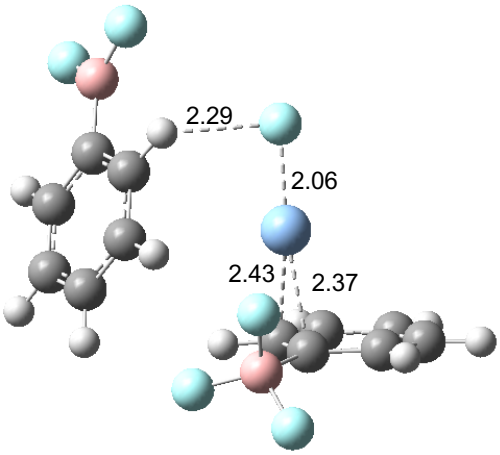


Zero-point correction= 0.204900 (Hartree/Particle)
Thermal correction to Energy= 0.226575
Thermal correction to Enthalpy= 0.227519
Thermal correction to Gibbs Free Energy= 0.148889
Sum of electronic and zero-point Energies= -1258.774268
Sum of electronic and thermal Energies= -1258.752594
Sum of electronic and thermal Enthalpies= -1258.751650
Sum of electronic and thermal Free Energies= -1258.830279
HF = -1258.9791685

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-2.639618	-0.943823	0.202322
C	-1.191249	1.448002	0.642172
C	-1.704490	2.166482	-0.455608
C	-1.790684	1.720363	1.886843
C	-2.739645	3.093798	-0.326146
H	-1.282554	1.997304	-1.449276
C	-2.829120	2.642210	2.032949
H	-1.442945	1.188775	2.776279
C	-3.307617	3.335941	0.923246
H	-3.105499	3.628283	-1.205090
H	-3.267642	2.818212	3.017422
H	-4.118801	4.057540	1.030967
F	-3.793231	-0.304057	0.249229
F	-2.100761	-1.212369	-0.973121
F	-2.210102	-1.569814	1.283351
Ag	0.557728	0.259231	0.433873
B	3.439186	0.036512	-0.537216
C	2.482808	-1.072105	0.211009
C	1.674306	-1.963945	-0.529765
C	2.522032	-1.275521	1.608789
C	0.994544	-3.023858	0.075448
H	1.607703	-1.825434	-1.610024
C	1.848318	-2.334505	2.220320
H	3.123447	-0.592634	2.210999
C	1.094079	-3.218663	1.450631
H	0.374705	-3.687656	-0.528325
H	1.907483	-2.466501	3.301340
H	0.557934	-4.039267	1.928000
F	4.642484	-0.579637	-0.926274
F	2.771880	0.527498	-1.682344
F	3.711870	1.098653	0.347796

TS3a-7 #m06 genecp opt=(ts,calcfc,noeigentest) freq test nosymm



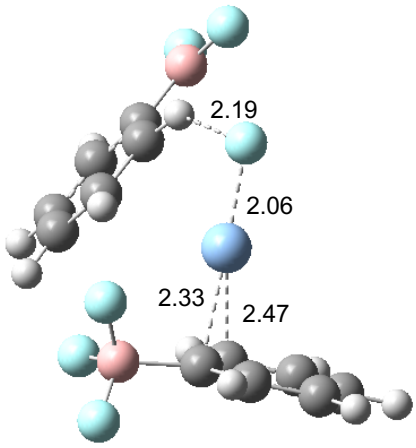
Zero-point correction= 0.205887 (Hartree/Particle)
Thermal correction to Energy= 0.226561
Thermal correction to Enthalpy= 0.227505
Thermal correction to Gibbs Free Energy= 0.152371
Sum of electronic and zero-point Energies= -1258.762729
Sum of electronic and thermal Energies= -1258.742055
Sum of electronic and thermal Enthalpies= -1258.741111
Sum of electronic and thermal Free Energies= -1258.816245
HF = -1258.9686159

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-2.784821	-0.719426	-0.533092
C	-2.367816	0.790325	-0.036176
C	-2.881654	1.920789	-0.718306
C	-1.602494	1.052621	1.124754
C	-2.704781	3.213329	-0.242373
H	-3.471151	1.746698	-1.619834
C	-1.406853	2.363585	1.600737
H	-1.233342	0.209785	1.712638
C	-1.971259	3.437791	0.928779
H	-3.138058	4.056771	-0.781017
H	-0.822929	2.525971	2.506838
H	-1.832009	4.452272	1.302500
F	-4.155423	-0.746406	-0.827323
F	-2.052506	-1.053635	-1.703478
F	-2.484251	-1.661393	0.471853
Ag	-0.124375	0.879773	-0.794258
B	4.277475	-0.724982	0.832172
C	2.878838	-1.320851	1.054223
C	1.971192	-1.434334	-0.012803
C	2.484260	-1.756550	2.329757
C	0.700691	-1.969241	0.195462
H	2.241471	-1.038966	-0.993773
C	1.220736	-2.299494	2.535726
H	3.179144	-1.664397	3.165763
C	0.328254	-2.403021	1.468163
H	-0.022475	-2.032530	-0.619914
H	0.923260	-2.633076	3.530187
H	-0.676981	-2.794420	1.617760
F	4.765387	-0.448695	-0.367607
F	1.660110	1.023221	-1.804007
F	5.102353	-0.489969	1.859786

Imaginary Vibrational Frequency = -14.0565 cm-1

7 # opt freq nosymm M06/gen pseudo=read

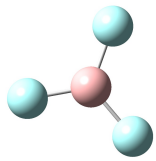


Zero-point correction= 0.205850 (Hartree/Particle)
Thermal correction to Energy= 0.227434
Thermal correction to Enthalpy= 0.228378
Thermal correction to Gibbs Free Energy= 0.149759
Sum of electronic and zero-point Energies= -1258.763192
Sum of electronic and thermal Energies= -1258.741608
Sum of electronic and thermal Enthalpies= -1258.740664
Sum of electronic and thermal Free Energies= -1258.819283
HF = -1258.969042

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-2.894109	-0.675694	-0.295013
C	-2.467513	0.879450	0.027486
C	-3.005997	1.940056	-0.743524
C	-1.674207	1.249823	1.138736
C	-2.829471	3.272052	-0.388995
H	-3.610963	1.682667	-1.614988
C	-1.482250	2.596858	1.492776
H	-1.272422	0.458393	1.774355
C	-2.074782	3.602965	0.742033
H	-3.278813	4.061600	-0.992141
H	-0.877095	2.845869	2.364687
H	-1.936907	4.647822	1.020580
F	-4.291766	-0.765483	-0.367601
F	-2.338780	-1.072411	-1.538373
F	-2.400689	-1.522520	0.718344
Ag	-0.335985	0.902736	-0.916530
B	4.487177	-0.853498	1.127018
C	3.073277	-1.447594	1.180873
C	2.159840	-1.235186	0.132794
C	2.671772	-2.216636	2.287136
C	0.882875	-1.790133	0.196816
H	2.415345	-0.606934	-0.725931
C	1.391680	-2.753808	2.354197
H	3.374202	-2.386366	3.104466
C	0.493868	-2.537447	1.307478
H	0.175931	-1.643478	-0.622608
H	1.087589	-3.337621	3.223184
H	-0.521771	-2.927743	1.352238
F	4.940856	-0.153443	0.095749
F	1.422217	0.890244	-1.981955
F	5.356884	-1.022996	2.129848

BF_3 # opt freq M06/6-31+G(d)

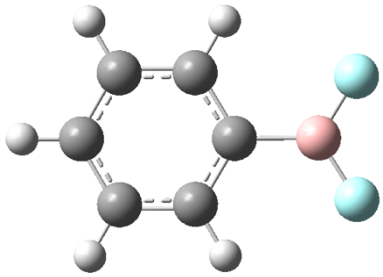


Zero-point correction= 0.012561 (Hartree/Particle)
Thermal correction to Energy= 0.016054
Thermal correction to Enthalpy= 0.016998
Thermal correction to Gibbs Free Energy= -0.011891
Sum of electronic and zero-point Energies= -324.466679
Sum of electronic and thermal Energies= -324.463187
Sum of electronic and thermal Enthalpies= -324.462243
Sum of electronic and thermal Free Energies= -324.491131
HF = -324.4792407

Optimized Geometry:
Charge = 0 Multiplicity = 1

B	0.000000	0.000000	0.000000
F	0.000000	1.311704	0.000000
F	1.135969	-0.655852	0.000000
F	-1.135969	-0.655852	0.000000

$PhBF_2$ # opt freq M06/6-31+G(d)

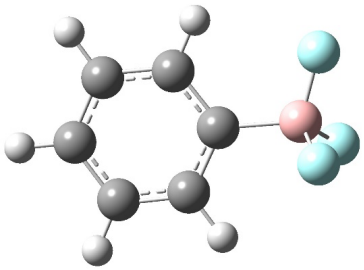


Zero-point correction= 0.100543 (Hartree/Particle)
Thermal correction to Energy= 0.107871
Thermal correction to Enthalpy= 0.108816
Thermal correction to Gibbs Free Energy= 0.067973
Sum of electronic and zero-point Energies= -455.983713
Sum of electronic and thermal Energies= -455.976384
Sum of electronic and thermal Enthalpies= -455.975440
Sum of electronic and thermal Free Energies= -456.016283
HF = -456.0842558

Optimized Geometry:
Charge = 0 Multiplicity = 1

B	1.731856	-0.000015	0.000053
F	2.429032	-1.127995	0.000308
F	2.428895	1.128052	-0.000298
C	0.190478	-0.000064	-0.000019
C	-0.525178	1.206396	0.000053
C	-0.525230	-1.206454	-0.000133
C	-1.915090	1.208644	0.000231
H	0.018317	2.151050	0.000036
C	-1.915146	-1.208625	-0.000230
H	0.018232	-2.151132	-0.000121
C	-2.609378	0.000026	0.000031
H	-2.460649	2.150963	0.000284
H	-2.460734	-2.150922	-0.000241
H	-3.698525	0.000066	0.000082

$PhBF_3^-$ # opt freq M06/6-31+G(d)

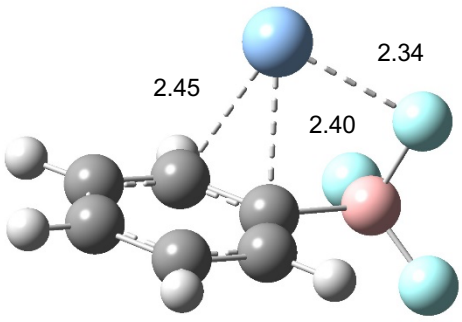


Zero-point correction= 0.101611 (Hartree/Particle)
Thermal correction to Energy= 0.109990
Thermal correction to Enthalpy= 0.110934
Thermal correction to Gibbs Free Energy= 0.067476
Sum of electronic and zero-point Energies= -555.922210
Sum of electronic and thermal Energies= -555.913831
Sum of electronic and thermal Enthalpies= -555.912887
Sum of electronic and thermal Free Energies= -555.956345
HF = -556.0238207

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	1.570504	0.010533	0.000006
C	-0.058017	0.025566	0.000049
C	-0.809530	1.206142	0.000058
C	-0.776861	-1.178710	0.000040
C	-2.205442	1.194707	0.000003
H	-0.274560	2.157673	0.000077
C	-2.169642	-1.209759	0.000014
H	-0.215522	-2.116058	0.000050
C	-2.894299	-0.016882	-0.000023
H	-2.760896	2.135353	-0.000025
H	-2.697024	-2.166374	0.000008
H	-3.985694	-0.033654	-0.000072
F	2.082001	1.329285	0.000047
F	2.045972	-0.673382	1.146754
F	2.045797	-0.673235	-1.146902

8 # opt freq M06/gen pseudo=read



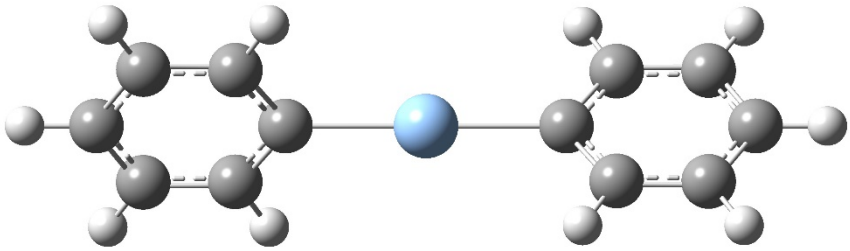
Zero-point correction= 0.102905 (Hartree/Particle)
Thermal correction to Energy= 0.113372
Thermal correction to Enthalpy= 0.114316
Thermal correction to Gibbs Free Energy= 0.064370
Sum of electronic and zero-point Energies= -702.823063
Sum of electronic and thermal Energies= -702.812596
Sum of electronic and thermal Enthalpies= -702.811652
Sum of electronic and thermal Free Energies= -702.861598
HF = -702.925968

Optimized Geometry:

Charge = 0 Multiplicity = 1
B -1.470547 -1.078720 0.172631
C 0.168727 -0.946896 0.161067
C 0.876498 -0.299808 1.211836
C 0.933662 -1.420356 -0.926347
C 2.276815 -0.154648 1.173418
H 0.324216 -0.022841 2.113684
C 2.317330 -1.297302 -0.950263
H 0.413546 -1.923559 -1.742493
C 2.992502 -0.659576 0.097400
H 2.794820 0.325066 2.003395
H 2.883949 -1.699766 -1.789468
H 4.077208 -0.567205 0.070215
F -1.964960 -0.768717 1.434713
F -1.955653 -0.016653 -0.742240
F -1.900327 -2.288978 -0.311019
Ag -0.173314 1.396224 -0.203282

Species associated with Figure 3

9 # opt freq M06/gen pseudo=read

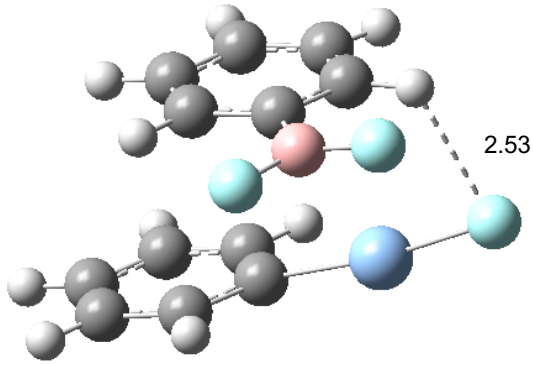


Zero-point correction= 0.176293 (Hartree/Particle)
Thermal correction to Energy= 0.188374
Thermal correction to Enthalpy= 0.189318
Thermal correction to Gibbs Free Energy= 0.134656
Sum of electronic and zero-point Energies= -609.781744
Sum of electronic and thermal Energies= -609.769663
Sum of electronic and thermal Enthalpies= -609.768719
Sum of electronic and thermal Free Energies= -609.823380
HF = -609.9580364

Optimized Geometry:
Charge = -1 Multiplicity = 1
C -4.293480 -0.854100 -0.839943
C -2.895940 -0.845948 -0.832266
C -2.133420 -0.000258 -0.000521
C -2.893918 0.846209 0.832322
C -4.291424 0.855774 0.842067
C -5.004034 0.001179 0.001585
H -4.832371 -1.532353 -1.507026
H -2.379753 -1.533682 -1.508984
H -2.376036 1.533442 1.508255
H -4.828638 1.534558 1.509957
H -6.095748 0.001692 0.002397
Ag 0.000000 -0.000690 -0.000904
C 2.133418 -0.000392 -0.000400
C 2.894828 -0.832460 0.845990
C 2.895030 0.832325 -0.845971
C 4.292350 -0.840525 0.855659
H 2.377707 -1.509105 1.533094

C 4.292556 0.841667 -0.854035
H 2.378084 1.508474 -1.533694
C 5.004036 0.000911 0.001234
H 4.830313 -1.507833 1.534424
H 4.830696 1.509482 -1.532162
H 6.095749 0.001455 0.001895

TS4b-10 #m06 genecp freq opt=(ts,calcfc,noeigentest) test nosymm

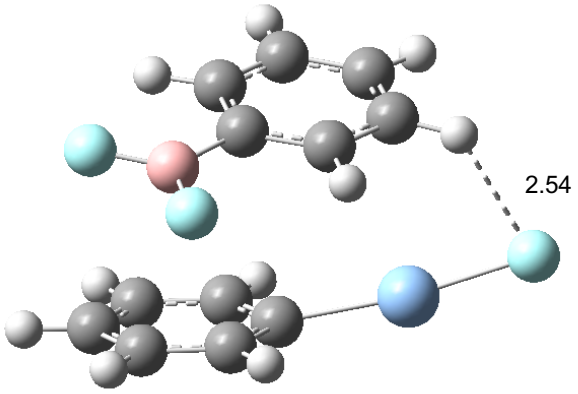


Zero-point correction= 0.190918 (Hartree/Particle)
Thermal correction to Energy= 0.207287
Thermal correction to Enthalpy= 0.208231
Thermal correction to Gibbs Free Energy= 0.143066
Sum of electronic and zero-point Energies= -934.249743
Sum of electronic and thermal Energies= -934.233374
Sum of electronic and thermal Enthalpies= -934.232429
Sum of electronic and thermal Free Energies= -934.297595
HF = -934.4406605

Optimized Geometry:
Charge = -1 Multiplicity = 1
B 2.908437 -0.579217 1.032402
C 1.957832 0.558490 0.634931
C 0.990516 1.027763 1.538889
C 2.017726 1.125575 -0.647494
C 0.114150 2.043748 1.180273
H 0.913302 0.569799 2.525822
C 1.147054 2.151829 -1.003125
H 2.696725 0.711028 -1.392649
C 0.199824 2.610353 -0.091286
H -0.658881 2.373727 1.873672
H 1.175957 2.552579 -2.015712
H -0.510430 3.382703 -0.386760
F 2.800856 -1.198723 2.212737
F 1.614769 -0.923939 -2.995258
F 3.914632 -0.982368 0.266871
Ag -0.207262 -0.656869 -2.055988
C -3.922473 1.268172 -0.696098
C -4.144453 0.760968 0.584042
C -3.281553 -0.218457 1.074885
C -2.214042 -0.670339 0.294956
C -1.949210 -0.179898 -0.999862
C -2.850574 0.800659 -1.460952
H -4.589796 2.033286 -1.101484
H -4.979705 1.120136 1.188271
H -3.437865 -0.631161 2.074997
H -1.550717 -1.426598 0.724238
H -2.708067 1.231039 -2.456561

Imaginary Vibrational Frequency = -19.7627 cm-1

10 #m06 genecp freq opt nosymm test

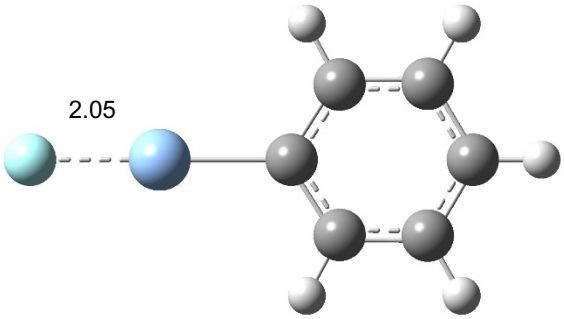


Zero-point correction= 0.191393 (Hartree/Particle)
Thermal correction to Energy= 0.208395
Thermal correction to Enthalpy= 0.209339
Thermal correction to Gibbs Free Energy= 0.143336
Sum of electronic and zero-point Energies= -934.253184
Sum of electronic and thermal Energies= -934.236182
Sum of electronic and thermal Enthalpies= -934.235238
Sum of electronic and thermal Free Energies= -934.301241
HF = -934.444577

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	0.779385	-0.325090	1.993809
C	0.971938	0.805584	0.971786
C	0.389904	2.063811	1.185251
C	1.677355	0.584065	-0.220483
C	0.503986	3.067334	0.229432
H	-0.184063	2.239819	2.095840
C	1.783757	1.578149	-1.186956
H	2.101060	-0.402146	-0.414846
C	1.196589	2.822117	-0.955266
H	0.027625	4.034132	0.393417
H	2.256677	1.374133	-2.147547
H	1.248960	3.586927	-1.729871
F	0.176026	-0.126589	3.166769
F	0.947816	0.865190	-4.258574
F	1.274705	-1.548643	1.804796
Ag	-0.501274	0.370128	-2.865322
C	-3.422797	0.685033	0.419986
C	-3.162694	-0.422485	1.224947
C	-2.218934	-1.355799	0.794477
C	-1.546787	-1.167578	-0.415969
C	-1.767732	-0.052777	-1.252033
C	-2.737824	0.855854	-0.786767
H	-4.157728	1.428407	0.739365
H	-3.682759	-0.556434	2.174950
H	-1.997286	-2.232073	1.409754
H	-0.802052	-1.914610	-0.707256
H	-2.961902	1.747328	-1.379234

11 # opt freq M06/gen pseudo=read

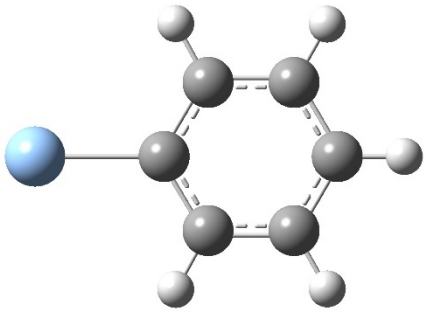


Zero-point correction= 0.089635 (Hartree/Particle)
Thermal correction to Energy= 0.097486
Thermal correction to Enthalpy= 0.098430
Thermal correction to Gibbs Free Energy= 0.055320
Sum of electronic and zero-point Energies= -478.264650
Sum of electronic and thermal Energies= -478.256798
Sum of electronic and thermal Enthalpies= -478.255854
Sum of electronic and thermal Free Energies= -478.298965
HF = -478.3542844

Optimized Geometry:
Charge = -1 Multiplicity = 1

Ag	-1.332267	0.000002	-0.000016
C	0.757921	0.000004	-0.000024
C	1.516935	-1.188366	-0.000008
C	1.516945	1.188371	-0.000006
C	2.913836	-1.199026	0.000016
H	0.998934	-2.151215	-0.000011
C	2.913838	1.199020	0.000017
H	0.998932	2.151219	-0.000015
C	3.625554	-0.000007	0.000015
H	3.451186	-2.151036	0.000036
H	3.451204	2.151021	0.000032
H	4.717185	-0.000001	0.000040
F	-3.385674	-0.000009	0.000068

12 # opt freq M06/gen pseudo=read



Zero-point correction= 0.088701 (Hartree/Particle)
Thermal correction to Energy= 0.094874
Thermal correction to Enthalpy= 0.095819
Thermal correction to Gibbs Free Energy= 0.056716
Sum of electronic and zero-point Energies= -378.337153
Sum of electronic and thermal Energies= -378.330980
Sum of electronic and thermal Enthalpies= -378.330036

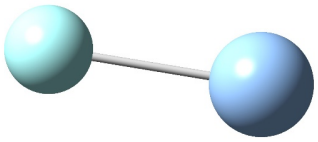
Sum of electronic and thermal Free Energies= -378.369139
HF = -378.4258545

Optimized Geometry:
Charge = 0 Multiplicity = 1

Ag	-1.661190	0.000000	-0.000020
C	0.433612	0.000001	0.000005
C	1.146472	-1.203752	0.000014
C	1.146474	1.203754	0.000013
C	2.542636	-1.203163	0.000031
H	0.622004	-2.159486	0.000008
C	2.542637	1.203162	0.000029
H	0.622006	2.159487	0.000005
C	3.243917	-0.000001	0.000039
H	3.082056	-2.150807	0.000037
H	3.082059	2.150805	0.000035
H	4.333332	-0.000001	0.000052

Species associated with Figures 4 and 5

AgF # opt freq M06/gen pseudo=read

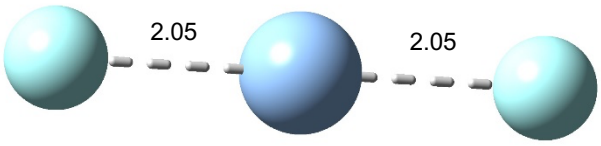


Zero-point correction= 0.001129 (Hartree/Particle)
Thermal correction to Energy= 0.003717
Thermal correction to Enthalpy= 0.004661
Thermal correction to Gibbs Free Energy= -0.022112
Sum of electronic and zero-point Energies= -246.795344
Sum of electronic and thermal Energies= -246.792756
Sum of electronic and thermal Enthalpies= -246.791812
Sum of electronic and thermal Free Energies= -246.818585
HF = -246.7964729

Optimized Geometry:
Charge = 0 Multiplicity = 1

Ag	0.000000	0.000000	0.323065
F	0.000000	0.000000	-1.687117

14 # opt freq M06/gen pseudo=read

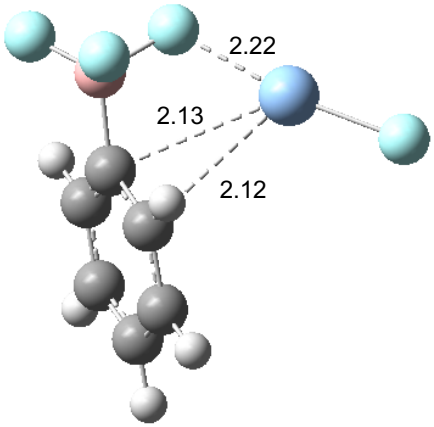


Zero-point correction= 0.002685 (Hartree/Particle)
Thermal correction to Energy= 0.006902
Thermal correction to Enthalpy= 0.007846
Thermal correction to Gibbs Free Energy= -0.022440
Sum of electronic and zero-point Energies= -346.737834
Sum of electronic and thermal Energies= -346.733617
Sum of electronic and thermal Enthalpies= -346.732673
Sum of electronic and thermal Free Energies= -346.762959
HF = -346.7405193

Optimized Geometry:

Charge = -1 Multiplicity = 1
Ag 0.000000 0.000000 0.000000
F 0.000000 0.000000 2.045325
F 0.000000 0.000000 -2.045325

TS5a-5c #m06 genecp opt=(ts,calcfc,noeigentest) nosymm test freq

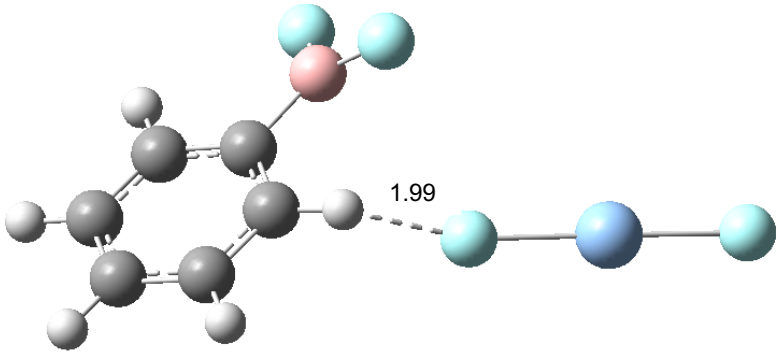


Zero-point correction= 0.103759 (Hartree/Particle)
Thermal correction to Energy= 0.115386
Thermal correction to Enthalpy= 0.116330
Thermal correction to Gibbs Free Energy= 0.063222
Sum of electronic and zero-point Energies= -802.767577
Sum of electronic and thermal Energies= -802.755951
Sum of electronic and thermal Enthalpies= -802.755007
Sum of electronic and thermal Free Energies= -802.808114
HF = -802.8713364

Optimized Geometry:
Charge = -1 Multiplicity = 1
B -2.025548 -0.021218 -1.110457
C -0.749304 -0.905030 -0.664554
C 0.034780 -1.576759 -1.613236
C -0.330427 -0.967645 0.672148
C 1.182281 -2.278363 -1.249993
H -0.272370 -1.544854 -2.660398
C 0.821635 -1.659757 1.048817
H -0.928552 -0.466932 1.436600
C 1.582091 -2.318870 0.086331
H 1.772951 -2.792217 -2.010492
H 1.128355 -1.677756 2.095202
H 2.484927 -2.859403 0.373877
F -2.705878 -0.540457 -2.206378
F -2.888305 0.243110 -0.043736
F -1.493608 1.303850 -1.538440
Ag -0.124495 2.080231 0.028436
F 1.067271 3.076836 1.348896

Imaginary Vibrational Frequency = -23.7766 cm-1

TS5c-14 #m06 genecp freq opt=(ts,calcfc,noeigentest) nosymm test



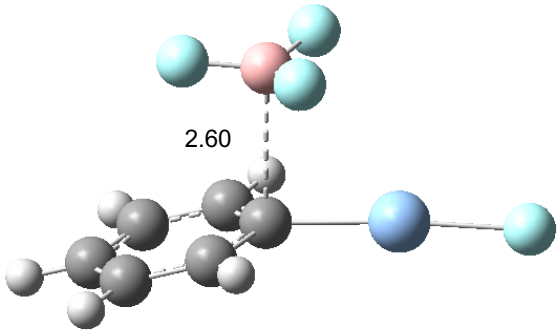
Zero-point correction= 0.103691 (Hartree/Particle)
Thermal correction to Energy= 0.115992
Thermal correction to Enthalpy= 0.116936
Thermal correction to Gibbs Free Energy= 0.061005
Sum of electronic and zero-point Energies= -802.720143
Sum of electronic and thermal Energies= -802.707842
Sum of electronic and thermal Enthalpies= -802.706898
Sum of electronic and thermal Free Energies= -802.762830
HF = -802.8238345

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	-1.981585	-0.557007	-0.983528
C	-0.649464	-1.308158	-0.761586
C	-0.273587	-2.341428	-1.633155
C	0.182905	-0.991972	0.323276
C	0.891626	-3.069894	-1.416135
H	-0.907204	-2.577557	-2.489432
C	1.356159	-1.714189	0.531189
H	-0.064622	-0.121359	0.939039
C	1.704923	-2.755596	-0.327223
H	1.170446	-3.876212	-2.094931
H	2.009024	-1.451091	1.362960
H	2.623501	-3.318409	-0.155638
F	-2.591259	-0.605697	-2.173520
F	-2.637731	0.057917	-0.020074
F	-0.189401	1.847021	0.673412
Ag	-0.801047	3.812073	0.735263
F	-1.390078	5.765323	0.786106

Imaginary Vibrational Frequency = -26.1944 cm-1

TS5a-13 #m06 genecp opt=(ts,calcfc,noeigentest,maxstep=5) nosymm test freq



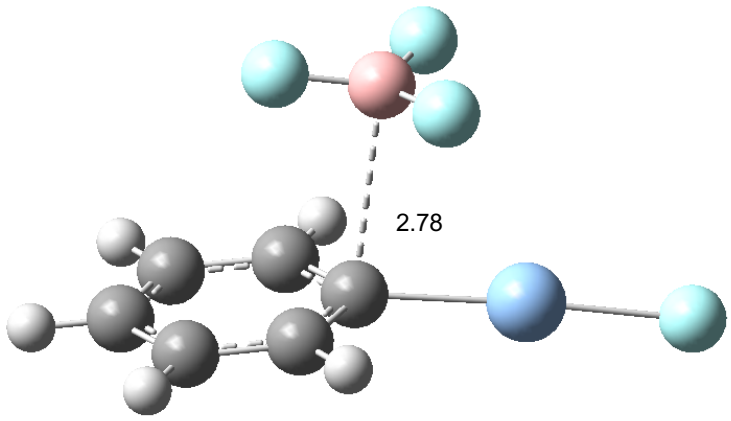
Zero-point correction= 0.102507 (Hartree/Particle)
Thermal correction to Energy= 0.114964
Thermal correction to Enthalpy= 0.115908
Thermal correction to Gibbs Free Energy= 0.060537
Sum of electronic and zero-point Energies= -802.740565
Sum of electronic and thermal Energies= -802.728109
Sum of electronic and thermal Enthalpies= -802.727165
Sum of electronic and thermal Free Energies= -802.782536
HF = -802.8430725

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	0.599038	1.823528	0.347855
C	-0.883013	-0.267901	-0.079638
C	-1.468895	0.122662	-1.302036
C	-1.721259	-0.166852	1.050042
C	-2.782326	0.583421	-1.397303
H	-0.866872	0.082467	-2.213803
C	-3.037867	0.289003	0.975294
H	-1.321879	-0.439209	2.030699
C	-3.575547	0.667662	-0.253973
H	-3.188340	0.884330	-2.365634
H	-3.646434	0.355300	1.879912
H	-4.601595	1.033856	-0.319234
F	1.343333	1.776291	-0.748839
F	-0.451811	2.637306	0.352641
F	1.118038	1.473035	1.516691
Ag	0.899899	-1.390011	-0.025793
F	2.552949	-2.598971	0.000425

Imaginary Vibrational Frequency = -43.5212 cm-1

13 #m06 genecp opt nosymm test freq

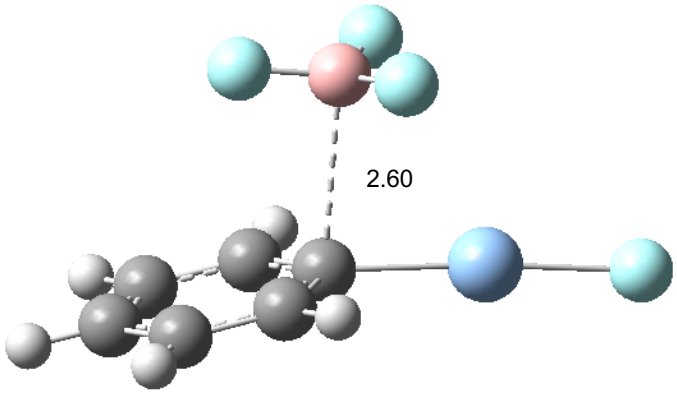


Zero-point correction= 0.103164 (Hartree/Particle)
Thermal correction to Energy= 0.116216
Thermal correction to Enthalpy= 0.117161
Thermal correction to Gibbs Free Energy= 0.060710
Sum of electronic and zero-point Energies= -802.740023
Sum of electronic and thermal Energies= -802.726971
Sum of electronic and thermal Enthalpies= -802.726027
Sum of electronic and thermal Free Energies= -802.782477
HF = -802.8431872

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	0.596973	1.934557	0.341941
C	-0.904416	-0.368151	-0.079707
C	-1.467230	0.071397	-1.296620
C	-1.740885	-0.237874	1.049088
C	-2.758154	0.594057	-1.389715
H	-0.867434	0.013078	-2.208882
C	-3.034768	0.281370	0.976270
H	-1.364846	-0.550376	2.026982
C	-3.552224	0.699255	-0.248837
H	-3.145691	0.925205	-2.355918
H	-3.642101	0.362739	1.880689
H	-4.561274	1.110300	-0.312837
F	1.285008	1.853484	-0.782751
F	-0.481587	2.701231	0.373726
F	1.144843	1.566883	1.486047
Ag	0.887346	-1.463523	-0.020791
F	2.573860	-2.627716	0.008622

TS13-15 #m06 genecp opt=(ts,calcfc,noeigentest,maxstep=5) nosymm test freq



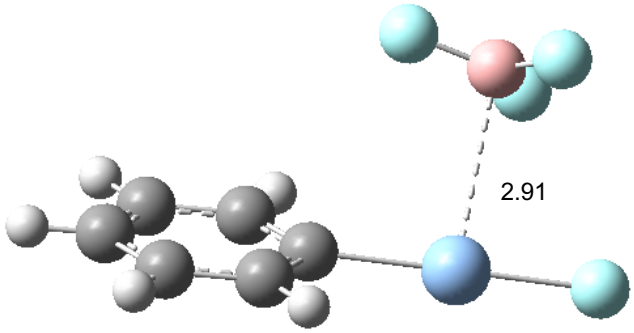
Zero-point correction= 0.103085 (Hartree/Particle)
Thermal correction to Energy= 0.115378
Thermal correction to Enthalpy= 0.116323
Thermal correction to Gibbs Free Energy= 0.061109
Sum of electronic and zero-point Energies= -802.737268
Sum of electronic and thermal Energies= -802.724975
Sum of electronic and thermal Enthalpies= -802.724030
Sum of electronic and thermal Free Energies= -802.779244
HF = -802.8403529

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	1.759770	1.745363	-0.176773
C	-1.279044	-0.299914	0.166642
C	-1.802448	0.333334	-0.977619
C	-2.198999	-0.518454	1.209841
C	-3.139142	0.723309	-1.078855
H	-1.141753	0.540275	-1.823640
C	-3.540254	-0.136209	1.125554
H	-1.861187	-1.005209	2.128418
C	-4.020275	0.489104	-0.024055
H	-3.494864	1.215010	-1.987492
H	-4.214922	-0.327793	1.963539
H	-5.066272	0.792566	-0.096040
F	2.157977	1.379483	-1.381931
F	0.644800	2.446918	-0.058935
F	2.589340	1.687373	0.845249
Ag	0.698881	-0.936666	0.280457
F	2.635813	-1.572573	0.352948

Imaginary Vibrational Frequency = -27.4698 cm-1

15 #m06 genecp opt freq test nosymm

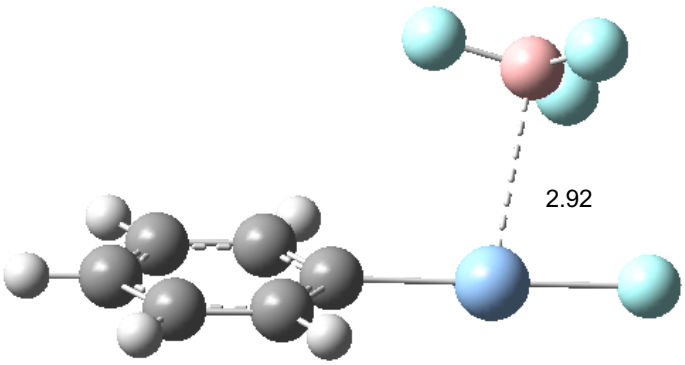


Zero-point correction= 0.103263 (Hartree/Particle)
Thermal correction to Energy= 0.116406
Thermal correction to Enthalpy= 0.117351
Thermal correction to Gibbs Free Energy= 0.059260
Sum of electronic and zero-point Energies= -802.737112
Sum of electronic and thermal Energies= -802.723969
Sum of electronic and thermal Enthalpies= -802.723025
Sum of electronic and thermal Free Energies= -802.781115
HF = -802.8403752

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	1.844307	1.729808	-0.177015
C	-1.301077	-0.282724	0.156321
C	-1.841481	0.348871	-0.980868
C	-2.209496	-0.516112	1.206475
C	-3.184206	0.720888	-1.069952
H	-1.190719	0.567174	-1.831535
C	-3.556109	-0.150601	1.134854
H	-1.857875	-1.001676	2.120507
C	-4.053742	0.471567	-0.009000
H	-3.554068	1.209890	-1.974407
H	-4.221081	-0.353780	1.977850
H	-5.104390	0.760614	-0.071957
F	2.384792	1.337118	-1.314921
F	0.717805	2.422881	-0.213322
F	2.545666	1.709312	0.938914
Ag	0.683034	-0.901206	0.253981
F	2.626059	-1.516106	0.321381

TS15-16 #m06 genecp opt=(ts,calcfc,noeigentest,maxstep=1) freq test nosymm



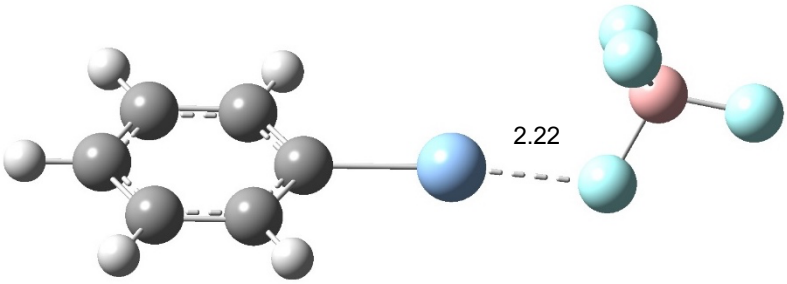
Zero-point correction= 0.102953 (Hartree/Particle)
Thermal correction to Energy= 0.115451
Thermal correction to Enthalpy= 0.116395
Thermal correction to Gibbs Free Energy= 0.059770
Sum of electronic and zero-point Energies= -802.737391
Sum of electronic and thermal Energies= -802.724893
Sum of electronic and thermal Enthalpies= -802.723948
Sum of electronic and thermal Free Energies= -802.780574
HF = -802.8403438

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	1.941078	1.698806	-0.155849
C	-1.349851	-0.323390	0.154619
C	-1.892962	0.372743	-0.942875
C	-2.260166	-0.633848	1.183142
C	-3.240116	0.732345	-1.015890
H	-1.240722	0.653103	-1.773818
C	-3.610774	-0.280525	1.127825
H	-1.907232	-1.172412	2.066524
C	-4.111066	0.406737	0.022927
H	-3.611882	1.272950	-1.889672
H	-4.276415	-0.543402	1.953656
H	-5.164898	0.686657	-0.026932
F	2.498259	1.343319	-1.297024
F	0.806721	2.380442	-0.189863
F	2.623962	1.653818	0.969654
Ag	0.650116	-0.894198	0.229102
F	2.615967	-1.436827	0.277982

Imaginary Vibrational Frequency = -42.4673 cm-1

16 #m06 genecp opt freq test nosymm

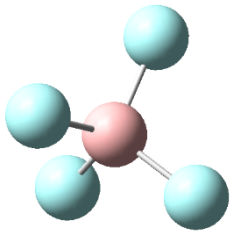


Zero-point correction= 0.103579 (Hartree/Particle)
Thermal correction to Energy= 0.115089
Thermal correction to Enthalpy= 0.116033
Thermal correction to Gibbs Free Energy= 0.062857
Sum of electronic and zero-point Energies= -802.799974
Sum of electronic and thermal Energies= -802.788465
Sum of electronic and thermal Enthalpies= -802.787521
Sum of electronic and thermal Free Energies= -802.840697
HF = -802.9035538

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	3.206849	1.077113	0.063996
C	-1.783212	-0.005497	0.063832
C	-2.516440	0.499064	-1.025600
C	-2.542800	-0.504191	1.137858
C	-3.912905	0.508348	-1.046444
H	-1.986077	0.904012	-1.890229
C	-3.939482	-0.501210	1.131489
H	-2.034011	-0.909145	2.015631
C	-4.634459	0.006693	0.035427
H	-4.440283	0.912256	-1.913504
H	-4.487708	-0.897135	1.989324
H	-5.725491	0.012686	0.024841
F	2.838741	1.662787	-1.141317
F	2.760028	1.833226	1.141526
F	4.564375	0.829730	0.128526
Ag	0.305900	-0.004652	0.091143
F	2.513194	-0.212968	0.136412

BF_4^- # opt freq M06/gen



Zero-point correction= 0.014203 (Hartree/Particle)
Thermal correction to Energy= 0.018579
Thermal correction to Enthalpy= 0.019523
Thermal correction to Gibbs Free Energy= -0.011063
Sum of electronic and zero-point Energies= -424.420313
Sum of electronic and thermal Energies= -424.415938
Sum of electronic and thermal Enthalpies= -424.414994
Sum of electronic and thermal Free Energies= -424.445579
HF = -424.4345166

Optimized Geometry:
Charge = -1 Multiplicity = 1

B	0.00000000	0.00000000	0.00000000
F	0.81187900	0.81187900	0.81187900
F	-0.81187900	-0.81187900	0.81187900
F	0.81187900	-0.81187900	-0.81187900
F	-0.81187900	0.81187900	-0.81187900