Supporting information for

Mechanistic study of the double boron--silicon exchange reaction between dibenzosilole and boron tribromide

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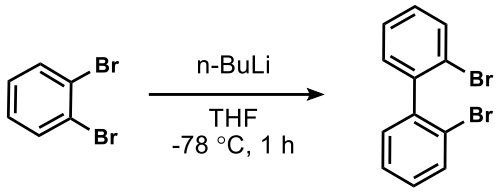
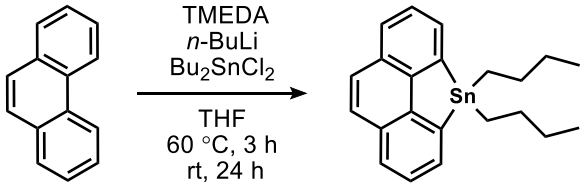
1. Synthetic Procedures

1.1 Synthesis of 2,2'-Dibromo-1,1'-biphenyl



1,2-Dibromobenzene (4.72 g, 20.0 mmol, 1.00 eq.) was dissolved in anhydrous THF (50 mL) in a 100 mL round bottom flask under nitrogen and cooled to -78 °C. *n*-butyllithium (n-BuLi) (1.6 M in hexane, 6.25 mL, 10.0 mmol, 2.00 eq.) was added dropwise. Addition of the *n*-BuLi took place over 5 minutes. The resulting mixture was allowed to warm to room temperature. The reaction was then quenched with a small amount of wet THF, and the organic solvent was removed under reduced pressure by rotary evaporation. The residue was dissolved in dichloromethane (50 mL) and washed with water (25 mL), and then washed with saturated aq. NaCl (2 × 25 mL). The organic layer was dried over anhydrous $MgSO_4$ and filtered. The organic solvent was then removed under reduced pressure by rotary evaporation to give the crude product, which was further purified by silica gel chromatography (10% Et_2O/hexane) and the product was isolated as a colorless oil (2.21 g, 71% yield). ^{1}H NMR (300 MHz, $CDCl_3$) 7.65 (d, J = 8.5 Hz, 2H) 7.38 (m, 2H), 7.25 (m, 4H). ^{1}H NMR matched with the reported product in the literature.

1.2 Synthesis of 4,4-dibutyl-4H-phenanthro[4,5-bcd]stannole

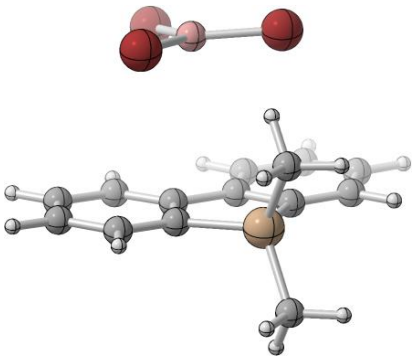


Phenanthrene (1.08 g, 6.00 mmol, 1.00 eq.) and tetramethylethylenediamine (TMEDA) (2.15 mL, 14.4 mmol, 2.40 eq.) were added to a 50 mL round bottom flask under nitrogen. The reaction flask was cooled to 0 °C and *n*-BuLi (2.5 M in hexane, 5.30 mL, 13.2 mmol, 2.20 eq.) was added. The reaction was heated to 60 °C in an oil bath for 3 hours. To the reaction mixture was added 5 mL of dry THF, and the reaction was cooled to -78 °C and dichlorodibutylstannane (Bu_2SnCl_2) (1.23 mL, 10.2 mmol, 1.70 eq.) was then added. The reaction mixture was allowed to warm to room temperature and then was stirred for 24 hours. The reaction was quenched with a small amount of wet THF (5 mL), and the organic solvent was removed under reduced pressure by rotary evaporation. The residue was dissolved in diethyl ether (50 mL) and washed with water (25 mL), back extracted with ether (25 mL) and then washed with saturated aq. NaCl (25 mL). The organic layer was then dried over anhydrous $MgSO_4$ and filtered. The organic solvent was then removed under reduced pressure by rotary evaporation to give the crude product as an orange oil. The crude product which was a single spot by TLC (5% Et_2O/hexane) was purified by silica gel chromatography using only a short column of silica gel with hexanes as the eluent. The pure product was isolated as a colorless oil which later crystallized upon sitting for weeks (0.981 g, 40% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (m, 4H), 7.77 (s, 2H), 7.65 (t, *J* = 7.3 Hz, 2H), 1.71 (t, *J* = 7.5 Hz, 6H) 1.47 (m, 4H). 1.41 (m, 4H) 0.92 (t, *J* = 7.4 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.8, 140.8,

134.2, 131.2, 127.7, 126.8, 126.6, 29.1, 27.2, 13.6, 12.3. HRMS (ESI-TOF) *m/z* calcd for $C_{22}H_{26}Sn$ 411.1135, found 411.1148 $[M + H]^+$.

2. Cartesian Coordinates for Optimized Stationary Points

DMDBS



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Sum of electronic and thermal Energies = -8653.195680 Hartree

Sum of electronic and thermal Enthalpies = -8653.194736 Hartree

Sum of electronic and thermal Free Energies = -8653.271473 Hartree

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C	1.255618	2.814751	-3.640729	C	0.352857	3.322478	-2.678111
C	-1.099842	2.863680	-0.729375	C	-1.564606	1.886631	0.188538
Si	-0.898913	0.205568	-0.395422	C	-1.463015	4.220987	-0.645534
C	-2.349820	4.596221	0.389118	C	-2.809655	3.654556	1.293579
C	-2.415610	2.300886	1.201809	C	-2.295754	-0.864020	-1.057361
C	0.132302	-0.775680	0.826287	C	-0.022031	4.711713	-2.562437
C	-0.890324	5.137296	-1.602280	H	1.246789	-0.494649	-2.806524
H	2.262961	1.089648	-4.416609	H	1.712145	3.498173	-4.360078
H	-2.655677	5.641034	0.479600	H	-3.483020	3.962431	2.095177
H	-2.795312	1.588993	1.939238	H	-2.953738	-1.194550	-0.239638
H	-1.898041	-1.759114	-1.558561	H	-2.899850	-0.299975	-1.781583
H	0.474321	-1.707460	0.349800	H	1.013366	-0.213106	1.162514
H	-0.464353	-1.047864	1.710137	H	0.407368	5.426445	-3.267792
H	-1.160657	6.193457	-1.537280	Br	0.582148	1.786131	3.470985
B	1.117549	3.041626	2.138817	Br	0.599824	4.859474	2.300086
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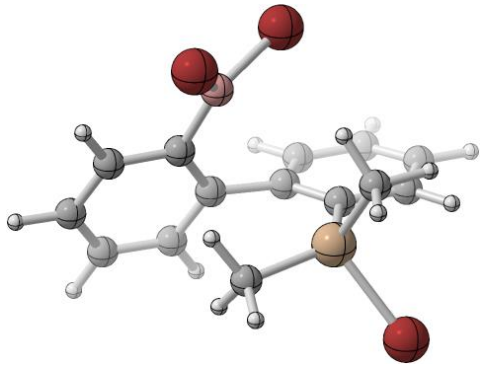
IM-2



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C	4.712413	0.523661	1.452522	C	3.815238	1.588837	1.437108
C	1.983277	2.924121	0.430475	C	2.517936	4.217803	0.355864
C	1.688916	5.333376	0.339824	C	0.306767	5.165570	0.416912
C	-0.224564	3.885582	0.535119	C	0.591487	2.740374	0.548360
Si	-0.330232	1.100931	0.768851	C	-1.513796	0.843028	-0.657185
C	0.671271	-0.433054	1.140094	Br	-1.638737	1.423005	2.595097
B	2.115394	1.048137	-2.026187	Br	1.704076	2.722229	-2.843994
Br	1.475556	-0.532051	-2.925564	H	3.901566	-0.903531	-1.514139
H	5.435171	-1.215879	0.392077	H	5.381426	0.388959	2.303976
H	3.768840	2.280065	2.280868	H	3.600214	4.336956	0.272857
H	2.120095	6.332492	0.260709	H	-0.355742	6.032119	0.402386
H	-1.307160	3.775749	0.644129	H	-2.174818	1.713886	-0.770405
H	-2.137324	-0.044434	-0.476364	H	-0.966666	0.699381	-1.601507
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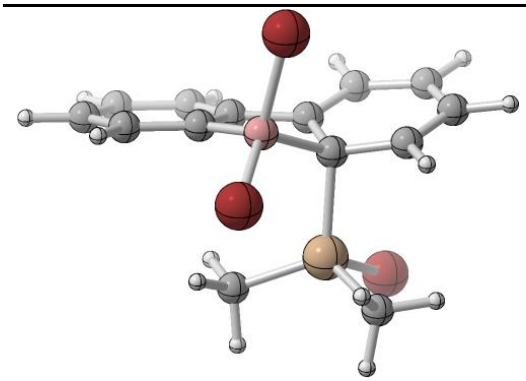
IM-3



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C	4.996934	0.495977	1.367480	C	4.102159	1.546061	1.538216
C	2.087721	2.775355	0.524822	C	2.089870	4.001228	1.194677
C	1.112998	4.936586	0.882924	C	0.138680	4.700989	-0.112036
C	0.113821	3.488004	-0.758497	C	1.035849	2.440740	-0.411610
Si	-0.140008	1.122815	0.513321	C	-1.761131	0.940844	-0.388948
C	0.740041	-0.447911	0.982607	Br	-0.694743	2.099837	2.482938
B	1.912627	1.506060	-1.579914	Br	2.629507	2.873913	-2.899245
Br	0.910444	0.058559	-2.578270	H	3.934488	-0.710187	-1.659652
H	5.645378	-1.127270	0.103489	H	5.748505	0.290622	2.130793
H	4.132958	2.162077	2.439319	H	2.880071	4.242842	1.906433
H	1.120581	5.901642	1.394138	H	-0.578714	5.481986	-0.363076
H	-0.633299	3.288595	-1.531592	H	-2.356506	1.858276	-0.287514
H	-2.317794	0.119692	0.087277	H	-1.612910	0.700174	-1.449012
H	1.602323	-0.248507	1.632781	H	1.068400	-1.003258	0.095070
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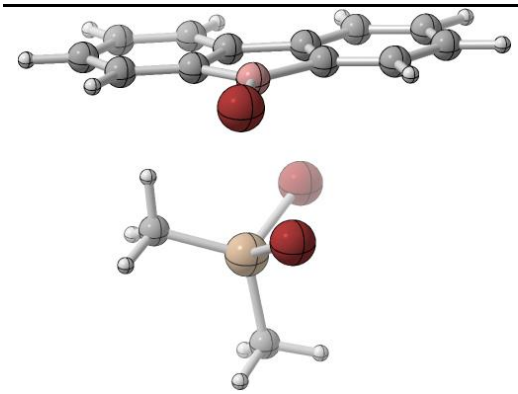

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C	3.948915	0.559108	2.150911	C	3.254192	1.776716	2.118007
C	2.187819	3.585688	0.588001	C	1.734445	4.551927	1.474860
C	1.101502	5.691941	0.961133	C	0.927657	5.861285	-0.411896
C	1.386305	4.884336	-1.303651	C	2.016260	3.748897	-0.807137
Si	-0.768860	0.412915	1.051034	C	-2.498119	-0.257215	1.200095
C	0.583902	-0.844747	1.224328	Br	-0.508229	1.975405	2.636068
B	2.604092	2.470553	-1.477988	Br	2.647655	2.061661	-3.341147
Br	-0.587887	1.385467	-0.958724	H	4.084997	-0.146327	-1.187839
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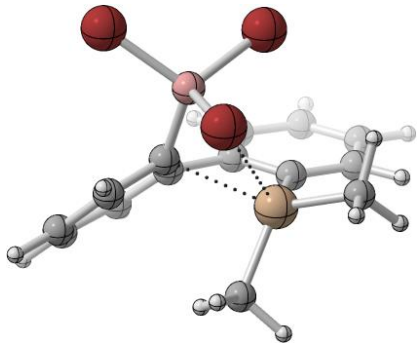

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C	1.977094	-3.072005	-1.356941	C	1.389605	-1.812328	-1.389713
C	-0.145516	-0.130544	-0.253797	C	-0.342748	0.461202	1.029536
Si	-0.816234	-1.612525	2.078476	C	-0.822184	0.352533	-1.383487
C	-1.772632	1.354567	-1.258610	C	-2.078865	1.875750	0.006815
C	-1.376482	1.440013	1.113414	C	-2.642517	-1.450815	1.734685
C	-0.491254	-2.618342	3.617960	Br	-0.224191	0.531082	4.006134
B	0.828947	0.741291	2.190757	Br	1.452296	2.641994	2.021472
Br	2.424114	-0.468389	2.256227	H	0.722418	-4.238375	1.586347
H	2.195717	-4.929274	-0.275604	H	2.648687	-3.377457	-2.160599
H	1.609969	-1.118592	-2.203099	H	-0.650615	-0.126711	-2.348917
H	-2.311614	1.705158	-2.140535	H	-2.847719	2.641400	0.114277
H	-1.573290	1.905594	2.080829	H	-3.089600	-0.742630	2.446851
H	-3.115825	-2.434823	1.877178	H	-2.827732	-1.095543	0.712231
H	-0.695853	-3.672907	3.363024	H	0.556719	-2.521059	3.931538
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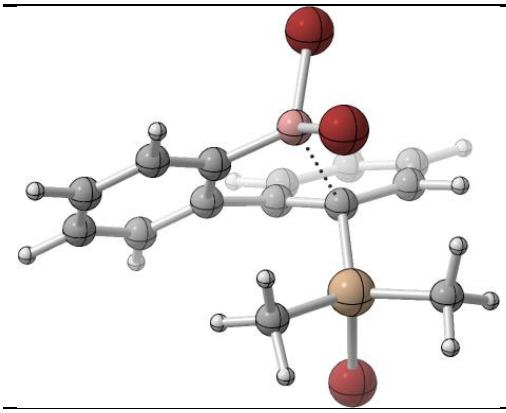
TS-3



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Sum of electronic and thermal Free Energies = -8577.130018 Hartree

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C	3.539946	-1.582801	0.916558	C	2.657578	-0.519837	1.093750
C	0.761770	0.853465	0.020789	C	0.958156	2.156859	0.476378
C	0.067475	3.152501	0.091084	C	-1.028918	2.868892	-0.740454
C	-1.269116	1.565690	-1.129175	C	-0.395327	0.507725	-0.751904
Si	-1.371594	-1.050920	-0.181008	C	-2.977477	-1.207766	-1.121899
C	-0.445489	-2.653114	0.037341	Br	-1.974567	-0.453725	1.928954
B	0.819497	-0.268830	-2.240905	Br	1.458789	1.341902	-3.197993
Br	-0.170626	-1.516803	-3.418640	H	2.732235	-2.504411	-2.277414
H	4.262797	-3.121096	-0.412179	H	4.210187	-1.872582	1.727043
H	2.612928	0.018082	2.042808	H	1.850950	2.403239	1.053228
H	0.244477	4.181456	0.410142	H	-1.694693	3.672311	-1.056074
H	-2.152396	1.338413	-1.731380	H	-3.640834	-0.360017	-0.903411
H	-3.483170	-2.124665	-0.784869	H	-2.809750	-1.277764	-2.205009
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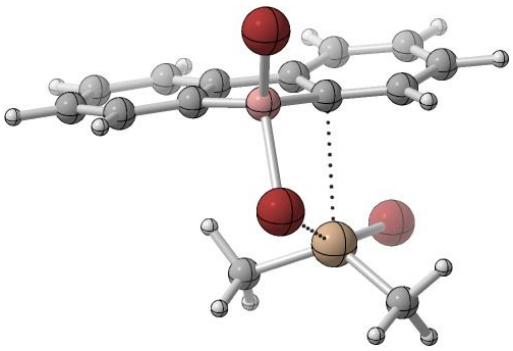

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Sum of electronic and thermal Enthalpies = -8577.036554 Hartree
Sum of electronic and thermal Free Energies = -8577.107026 Hartree

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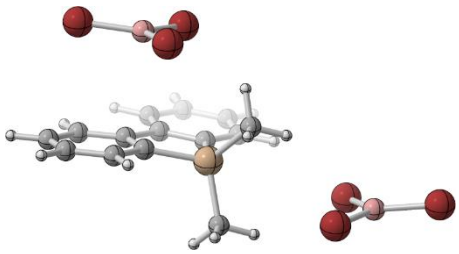
C	4.206139	-0.051625	-0.947539	C	5.091910	-0.367196	0.086515
C	5.035386	0.317738	1.304325	C	4.093099	1.327026	1.505718
C	2.109128	2.624970	0.480854	C	1.826677	3.610851	1.421919
C	0.760487	4.482857	1.185077	C	-0.023483	4.383175	0.029685
C	0.263170	3.405400	-0.919200	C	1.326633	2.512634	-0.701798
Si	-0.367936	0.463383	0.119544	C	-2.045173	0.219203	-0.661501
C	0.698662	-0.886870	0.825881	Br	-0.933433	1.681515	1.940459
B	2.121401	1.547643	-1.711176	Br	2.743258	2.395386	-3.402277
Br	0.668169	0.046314	-2.242198	H	4.260391	-0.585797	-1.899374
H	5.836732	-1.152215	-0.055000	H	5.733289	0.060908	2.102758
H	4.049476	1.857343	2.459303	H	2.430202	3.716655	2.325145
H	0.533755	5.259481	1.917992	H	-0.847188	5.080569	-0.127053
H	-0.306687	3.347581	-1.851440	H	-2.296612	1.109457	-1.256180
H	-2.801084	0.098164	0.125515	H	-2.029204	-0.650252	-1.332038
H	1.745201	-0.550076	0.884372	H	0.656930	-1.763595	0.165887
H	0.345569	-1.130256	1.836815				

DMDBS[BBr_3]



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.917128 Hartree

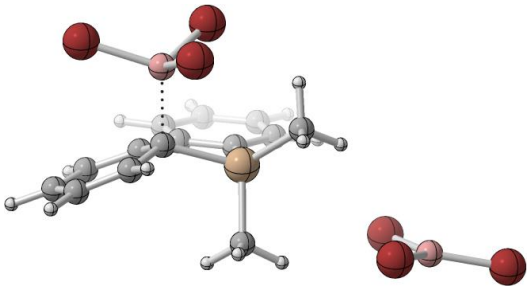
Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -16323.667058 Hartree

Sum of electronic and thermal Energies = -16323.638958 Hartree

Sum of electronic and thermal Enthalpies = -16323.638013 Hartree
Sum of electronic and thermal Free Energies = -16323.736683 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.171049	2.472281	-1.812733	C	0.107871	1.086410	-1.807560
C	1.004755	0.566755	-2.740726	C	1.619655	1.403059	-3.675362
C	1.333997	2.768712	-3.678473	C	0.441868	3.306198	-2.751216
C	-1.095655	2.937157	-0.741256	C	-1.488701	1.944029	0.186690
Si	-0.854013	0.264423	-0.408718	C	-1.580079	4.242544	-0.615856
C	-2.444096	4.564563	0.429642	C	-2.819880	3.595965	1.361874
C	-2.344506	2.289077	1.235152	C	-2.311150	-0.751919	-1.025966
C	0.206574	-0.743945	0.766118	H	1.240804	-0.500511	-2.740449
H	2.324744	0.991368	-4.399200	H	1.816580	3.423687	-4.405772
H	0.241491	4.378991	-2.755900	H	-1.292134	5.012437	-1.333757
H	-2.821400	5.584372	0.523451	H	-3.486722	3.859291	2.184352
H	-2.653033	1.534101	1.963531	H	-2.939515	-1.076852	-0.182284
H	-1.973882	-1.649440	-1.564499	H	-2.928374	-0.145537	-1.704072
H	0.567904	-1.641770	0.240710	H	1.076915	-0.174918	1.118886
H	-0.374403	-1.075640	1.640212	Br	0.600637	1.723399	3.472734
B	1.106289	3.014919	2.162848	Br	0.537455	4.814413	2.353400
Br	2.247859	2.522523	0.724614	Br	0.399230	-3.372180	-2.324773
B	-0.030611	-4.629211	-0.959596	Br	0.858689	-6.304236	-0.906502
Br	-1.348093	-4.201678	0.339573				

IM-1[BBr_3]



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

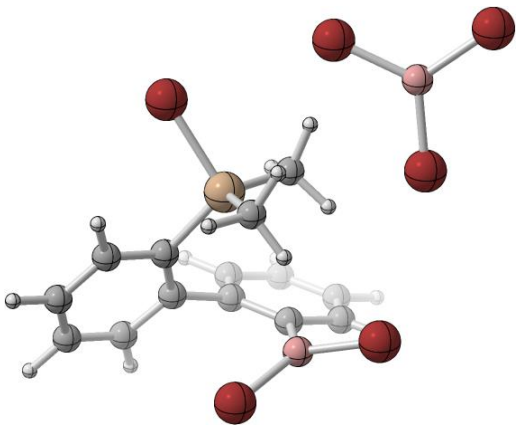
Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.897794 Hartree

Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -16323.647699 Hartree
Sum of electronic and thermal Energies = -16323.620155 Hartree
Sum of electronic and thermal Enthalpies = -16323.619211 Hartree
Sum of electronic and thermal Free Energies = -16323.713981 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.000531	2.487212	-1.718019	C	0.348655	1.123817	-1.615250
C	1.249432	0.583156	-2.534193	C	1.774859	1.381932	-3.549420
C	1.411727	2.729017	-3.652261	C	0.523137	3.288046	-2.740718
C	-0.919243	2.956644	-0.671592	C	-0.951402	2.170358	0.541586
Si	-0.492972	0.376164	-0.107282	C	-1.799990	4.023633	-0.851918
C	-2.810540	4.243545	0.077347	C	-2.988018	3.391645	1.180326
C	-2.081513	2.377132	1.399464	C	-2.171720	-0.359479	-0.525106
C	0.547238	-0.816631	0.875307	H	1.559574	-0.461495	-2.456558
H	2.480589	0.957200	-4.265148	H	1.840451	3.347818	-4.441612
H	0.271039	4.348284	-2.800374	H	-1.739541	4.641389	-1.748734
H	-3.503856	5.073290	-0.075354	H	-3.814395	3.555500	1.871660
H	-2.171634	1.760071	2.295931	H	-2.715090	-0.608630	0.399754
H	-2.067721	-1.279214	-1.117926	H	-2.771376	0.363533	-1.097110
H	0.770808	-1.670654	0.214731	H	1.488186	-0.361180	1.207058
H	0.003478	-1.191612	1.753393	Br	0.364404	1.573197	3.319890
B	0.485075	2.708420	1.667087	Br	0.210046	4.640578	2.079243
Br	2.222025	2.433309	0.731495	Br	-0.039764	-2.969839	-2.519234
B	-0.452663	-4.400944	-1.328198	Br	0.080825	-6.168522	-1.756233
Br	-1.397727	-4.044512	0.280065				

IM-2[BBr_3]



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

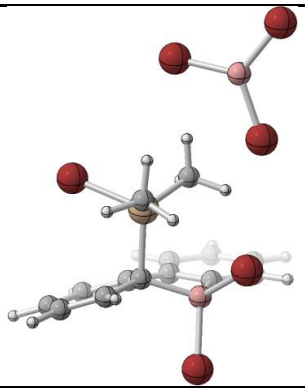
Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.939257 Hartree

Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -16323.687812 Hartree
Sum of electronic and thermal Energies = -16323.660175 Hartree
Sum of electronic and thermal Enthalpies = -16323.659231 Hartree
Sum of electronic and thermal Free Energies = -16323.755228 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.924616	1.768605	0.347217	C	2.958933	0.878241	-0.753727
C	3.870270	-0.196958	-0.710101	C	4.743440	-0.374478	0.356680
C	4.713103	0.520542	1.424827	C	3.808521	1.579180	1.415788
C	1.969161	2.912549	0.429886	C	2.509286	4.203809	0.349813
C	1.686844	5.324366	0.354557	C	0.305851	5.163573	0.458540
C	-0.230107	3.885721	0.580678	C	0.578719	2.735534	0.573370
Si	-0.344814	1.091348	0.764047	C	-1.466422	0.848501	-0.714095
C	0.681979	-0.402205	1.220902	Br	-1.740265	1.416382	2.528859
B	2.088905	1.026119	-2.037247	Br	1.599803	2.692803	-2.824759
Br	1.511947	-0.563922	-2.968166	H	3.898702	-0.904518	-1.540256
H	5.443700	-1.210504	0.355541	H	5.387605	0.389267	2.272492
H	3.763024	2.269192	2.260589	H	3.590519	4.317427	0.247318
H	2.122324	6.321276	0.271243	H	-0.352283	6.033596	0.460886
H	-1.311127	3.780901	0.707601	H	-2.029862	1.774116	-0.902135
H	-2.180314	0.034322	-0.527013	H	-0.889672	0.604579	-1.619544
H	1.434342	-0.140254	1.979104	H	1.194736	-0.828804	0.347522
H	0.011256	-1.165959	1.640223	Br	-0.876944	-2.796328	-1.119127
B	-2.163606	-3.377609	0.157008	Br	-2.779405	-5.174333	0.138507
Br	-2.823746	-2.149779	1.449233				

IM-3[BBr_3]



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.925411 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16323.673680 Hartree

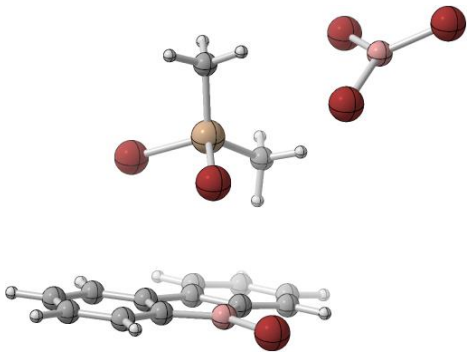
Sum of electronic and thermal Energies = -16323.646600 Hartree

Sum of electronic and thermal Enthalpies = -16323.645656 Hartree

Sum of electronic and thermal Free Energies = -16323.738695 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.141372	1.756490	0.539455	C	3.076491	0.965649	-0.625872
C	3.987294	-0.079525	-0.779160	C	4.945841	-0.306315	0.208169
C	5.008120	0.497435	1.356559	C	4.107254	1.541621	1.530704
C	2.083811	2.761554	0.524513	C	2.075842	3.980043	1.207881
C	1.096805	4.914438	0.899973	C	0.132229	4.685874	-0.105837
C	0.118339	3.480077	-0.766314	C	1.038663	2.431449	-0.420566
Si	-0.153497	1.115852	0.509904	C	-1.772374	0.972267	-0.402984
C	0.757852	-0.429233	1.004145	Br	-0.725894	2.094690	2.474116
B	1.907897	1.491303	-1.579651	Br	2.615718	2.842391	-2.920271
Br	0.906024	0.027336	-2.566727	H	3.945313	-0.711693	-1.669023
H	5.663236	-1.120334	0.088935	H	5.763210	0.296224	2.117501
H	4.137469	2.157365	2.432026	H	2.859915	4.217396	1.927791
H	1.095710	5.873414	1.422513	H	-0.585779	5.466880	-0.355135
H	-0.619128	3.287140	-1.550039	H	-2.319809	1.922056	-0.329101
H	-2.369269	0.195057	0.097416	H	-1.630438	0.694468	-1.455018
H	1.579301	-0.190670	1.693444	H	1.149848	-0.969965	0.133838
H	0.026624	-1.062296	1.530855	Br	-1.312925	-2.568354	-1.050504
B	-2.426364	-3.244460	0.328718	Br	-3.229399	-4.956876	0.174302
Br	-2.740424	-2.191511	1.890050				

Br-DBB[BBr_3]




```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.953600 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16323.702684 Hartree

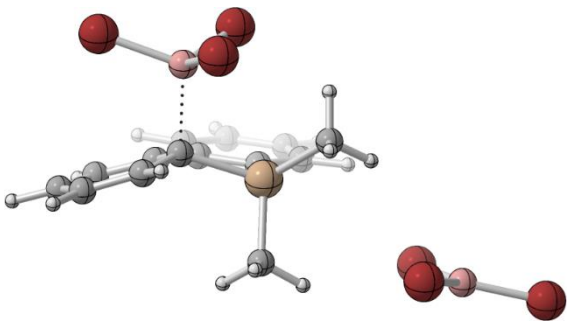
Sum of electronic and thermal Energies = -16323.674461 Hartree

Sum of electronic and thermal Enthalpies = -16323.673517 Hartree

Sum of electronic and thermal Free Energies = -16323.773157 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.889304	2.300241	0.888667	C	3.161961	1.592754	-0.307892
C	3.845237	0.382340	-0.262375	C	4.258092	-0.129695	0.974796
C	3.971611	0.566099	2.149464	C	3.279118	1.785059	2.118680
C	2.192729	3.585395	0.592891	C	1.749542	4.555564	1.480701
C	1.110055	5.692840	0.969379	C	0.919846	5.855792	-0.402340
C	1.368229	4.874982	-1.294938	C	2.004428	3.741922	-0.800755
Si	-0.777677	0.388915	1.026077	C	-2.517317	-0.253698	1.175191
C	0.595426	-0.839746	1.242099	Br	-0.528810	1.978250	2.590439
B	2.585613	2.460959	-1.472545	Br	2.622424	2.050611	-3.336295
Br	-0.576693	1.352923	-0.991188	H	4.059925	-0.160041	-1.186393
H	4.800241	-1.075057	1.023746	H	4.290580	0.155718	3.109222
H	3.059406	2.315427	3.047121	H	1.882793	4.438614	2.557946
H	0.753474	6.461635	1.657050	H	0.417966	6.749026	-0.776784
H	1.217541	4.993565	-2.370704	H	-3.229134	0.578291	1.084443
H	-2.656299	-0.734769	2.154623	H	-2.721370	-0.987169	0.382098
H	1.562247	-0.319607	1.191533	H	0.556330	-1.600722	0.449721
H	0.506008	-1.331503	2.222243	Br	-1.206190	-2.290313	-1.924509
B	-1.545540	-3.923681	-1.014529	Br	-1.848696	-5.522857	-1.988115
Br	-1.582520	-3.949190	0.890244				

TS-1[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen)
freq empiricaldispersion=gd3 nosymm
```

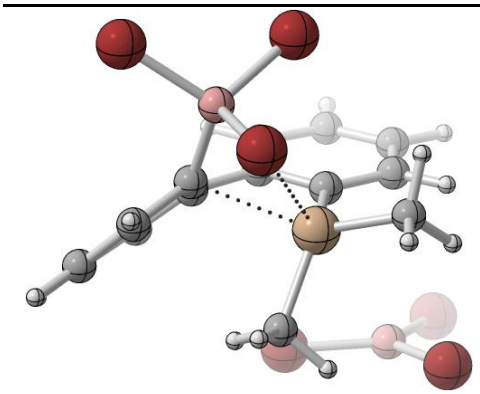
Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.897753 Hartree

Number of imaginary frequencies = 1, vi = -102.75 cm^{-1}
Sum of electronic and zero-point Energies = -16323.647999 Hartree
Sum of electronic and thermal Energies = -16323.621090 Hartree
Sum of electronic and thermal Enthalpies = -16323.620146 Hartree
Sum of electronic and thermal Free Energies = -16323.712756 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.495522	0.598643	-1.263510	C	0.839313	-0.766569	-1.166372
C	1.737867	-1.306630	-2.087655	C	2.267450	-0.506555	-3.100118
C	1.909671	0.841851	-3.196929	C	1.023310	1.400466	-2.282228
C	-0.421738	1.072219	-0.213530	C	-0.487877	0.259798	0.975567
Si	-0.003970	-1.518617	0.339681	C	-1.262501	2.175351	-0.367373
C	-2.258882	2.415687	0.572631	C	-2.460893	1.549479	1.658930
C	-1.597383	0.489895	1.846582	C	-1.667830	-2.283557	-0.087560
C	1.044183	-2.703246	1.326969	H	2.043670	-2.352929	-2.014236
H	2.971598	-0.931502	-3.817275	H	2.339906	1.462580	-3.983998
H	0.775004	2.461703	-2.339618	H	-1.180469	2.812106	-1.249056
H	-2.919297	3.275435	0.442492	H	-3.274497	1.731685	2.360886
H	-1.714033	-0.148719	2.724777	H	-2.217757	-2.528666	0.834572
H	-1.545185	-3.209209	-0.667494	H	-2.271438	-1.576190	-0.674533
H	1.277348	-3.556482	0.668759	H	1.980856	-2.242728	1.663572
H	0.499179	-3.082981	2.202477	Br	0.846523	-0.318890	3.788697
B	1.002498	0.837175	2.167774	Br	0.706512	2.754833	2.565696
Br	2.709476	0.548924	1.204019	Br	0.495628	-4.894464	-2.052722
B	0.101102	-6.318282	-0.847297	Br	0.660843	-8.082710	-1.255705
Br	-0.852486	-5.959167	0.755278				

TS-2[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.886194 Hartree

Number of imaginary frequencies = 1, vi = -143.12 cm^{-1}

Sum of electronic and zero-point Energies = -16323.635878 Hartree

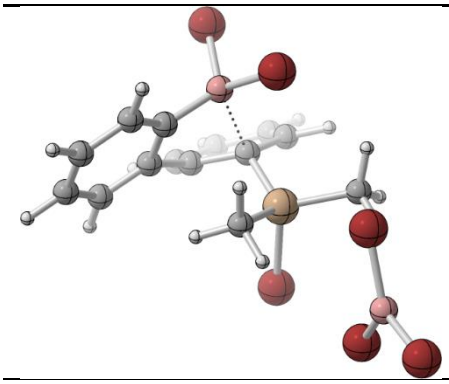
Sum of electronic and thermal Energies = -16323.609256 Hartree

Sum of electronic and thermal Enthalpies = -16323.608312 Hartree

Sum of electronic and thermal Free Energies = -16323.698371 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.581965	-1.411081	-0.324418	C	0.314300	-2.289030	0.737029
C	0.924463	-3.550137	0.756456	C	1.735571	-3.944736	-0.304024
C	1.965582	-3.075315	-1.377242	C	1.393293	-1.808595	-1.392895
C	-0.132436	-0.130214	-0.239632	C	-0.329866	0.466262	1.041401
Si	-0.820294	-1.626490	2.066628	C	-0.826212	0.332241	-1.368458
C	-1.788538	1.323183	-1.245466	C	-2.086440	1.855565	0.017062
C	-1.370164	1.437989	1.122078	C	-2.639399	-1.430573	1.708510
C	-0.511749	-2.612853	3.618785	Br	-0.216516	0.551467	4.023024
B	0.834218	0.746317	2.211191	Br	1.462460	2.645908	2.025950
Br	2.430733	-0.463963	2.286788	H	0.759684	-4.234979	1.591188
H	2.193718	-4.934919	-0.299699	H	2.612204	-3.388506	-2.198140
H	1.600790	-1.116778	-2.211238	H	-0.653297	-0.152096	-2.331713
H	-2.339675	1.658482	-2.125833	H	-2.861432	2.615130	0.123746
H	-1.564572	1.910265	2.086709	H	-3.069780	-0.720960	2.430258
H	-3.133304	-2.406746	1.832329	H	-2.811885	-1.057456	0.690134
H	-0.715623	-3.668358	3.364513	H	0.533268	-2.514220	3.941560
H	-1.176048	-2.304737	4.434933	Br	-2.167358	-3.144438	-1.706728
B	-1.719518	-4.813608	-0.920224	Br	-0.789998	-6.129132	-1.923144
Br	-2.277482	-5.203480	0.865185				

TS-3[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.920748 Hartree

Number of imaginary frequencies = 1, vi = -174.64 cm^{-1}

Sum of electronic and zero-point Energies = -16323.669999 Hartree

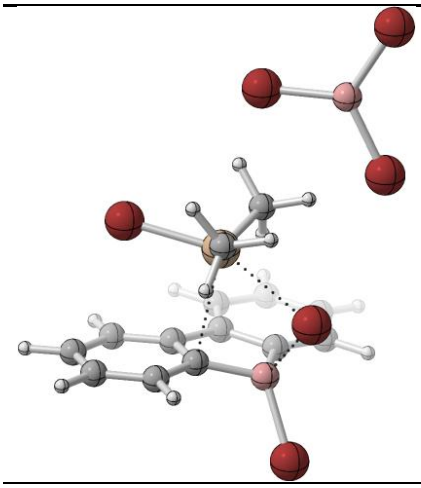
Sum of electronic and thermal Energies = -16323.643160 Hartree

Sum of electronic and thermal Enthalpies = -16323.642215 Hartree

Sum of electronic and thermal Free Energies = -16323.735081 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.793290	-0.196361	0.044496	C	1.820506	-0.888479	-1.179741
C	2.711950	-1.951544	-1.339217	C	3.573899	-2.288323	-0.296212
C	3.551944	-1.576257	0.909699	C	2.664422	-0.517983	1.088278
C	0.757298	0.844136	0.023914	C	0.955924	2.147019	0.480987
C	0.065531	3.144535	0.100544	C	-1.032155	2.862698	-0.729458
C	-1.274098	1.560035	-1.119299	C	-0.402803	0.499514	-0.743978
Si	-1.385303	-1.063670	-0.186833	C	-2.982961	-1.183295	-1.146862
C	-0.432447	-2.647323	0.052867	Br	-2.016082	-0.475161	1.921866
B	0.810688	-0.288767	-2.240650	Br	1.432575	1.319769	-3.210343
Br	-0.174723	-1.554274	-3.404918	H	2.733731	-2.510067	-2.277686
H	4.276906	-3.113833	-0.418893	H	4.227660	-1.860153	1.717731
H	2.621320	0.021995	2.036255	H	1.851136	2.391399	1.054994
H	0.244205	4.172684	0.421212	H	-1.697851	3.666813	-1.043538
H	-2.158164	1.335834	-1.721040	H	-3.620142	-0.315026	-0.929503
H	-3.519569	-2.084176	-0.818014	H	-2.806088	-1.253459	-2.228558
H	0.428535	-2.489044	0.717288	H	-0.084090	-3.064270	-0.900902
H	-1.117386	-3.361481	0.533835	Br	-2.916502	-5.005629	-1.476517
B	-3.841848	-5.292943	0.161544	Br	-4.756728	-6.928381	0.463164
Br	-3.844943	-3.935085	1.493789				

TS-4[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16323.898873 Hartree

Number of imaginary frequencies = 1, vi = -130.51 cm^{-1}

Sum of electronic and zero-point Energies = -16323.647621 Hartree

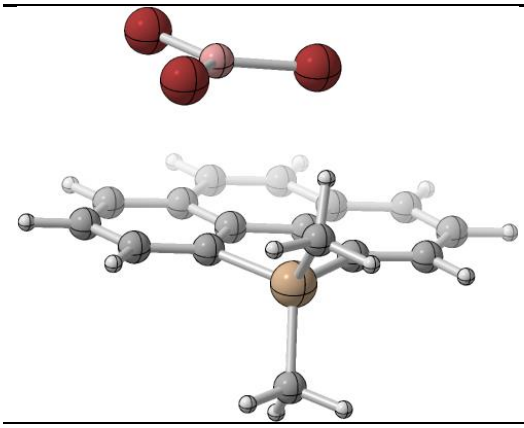
Sum of electronic and thermal Energies = -16323.620927 Hartree

Sum of electronic and thermal Enthalpies = -16323.619983 Hartree

Sum of electronic and thermal Free Energies = -16323.712327 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.211845	1.628353	0.467540	C	3.261536	0.938871	-0.764541
C	4.226745	-0.047178	-0.952428	C	5.121699	-0.348790	0.077868
C	5.061836	0.338535	1.294036	C	4.107545	1.336275	1.497199
C	2.103555	2.608827	0.477488	C	1.807932	3.584693	1.425349
C	0.730461	4.444257	1.195234	C	-0.050483	4.340300	0.038812
C	0.250354	3.372003	-0.916760	C	1.325192	2.493855	-0.706150
Si	-0.402279	0.405109	0.150936	C	-2.060846	0.320307	-0.700254
C	0.710614	-0.904869	0.862681	Br	-0.936180	1.626874	1.977321
B	2.115121	1.519450	-1.709080	Br	2.701067	2.334131	-3.428736
Br	0.679331	-0.025699	-2.195876	H	4.282590	-0.583260	-1.903156
H	5.875936	-1.124494	-0.065262	H	5.766639	0.092886	2.089982
H	4.061968	1.868703	2.449538	H	2.409675	3.690933	2.329802
H	0.492652	5.212566	1.933328	H	-0.883723	5.027105	-0.114892
H	-0.318443	3.313957	-1.849652	H	-2.168713	1.229438	-1.310510
H	-2.863312	0.294168	0.047564	H	-2.107934	-0.551284	-1.366381
H	1.742418	-0.517613	0.872098	H	0.686905	-1.800042	0.227696
H	0.401316	-1.129734	1.891330	Br	-1.151991	-3.369003	-1.488393
B	-2.181921	-3.840280	0.040772	Br	-2.933477	-5.572492	0.189559
Br	-2.457328	-2.563199	1.429321				

DMPhenS



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8653.473744 Hartree

Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -8653.217117 Hartree

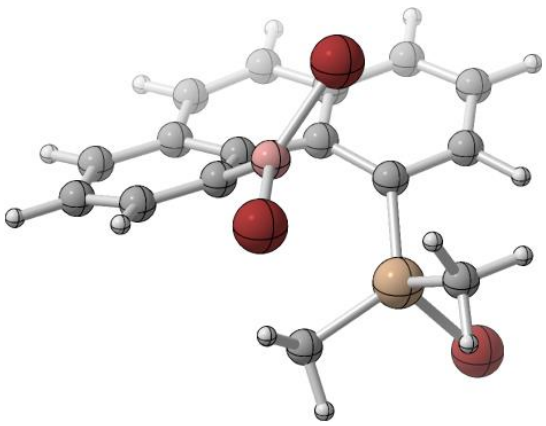
Sum of electronic and thermal Energies = -8653.195680 Hartree

Sum of electronic and thermal Enthalpies = -8653.194736 Hartree

Sum of electronic and thermal Free Energies = -8653.271473 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.205878	2.407639	-1.767450	C	0.093072	1.021692	-1.789981
C	0.980729	0.563871	-2.748969	C	1.561688	1.465469	-3.669636
C	1.255618	2.814751	-3.640729	C	0.352857	3.322478	-2.678111
C	-1.099842	2.863680	-0.729375	C	-1.564606	1.886631	0.188538
Si	-0.898913	0.205568	-0.395422	C	-1.463015	4.220987	-0.645534
C	-2.349820	4.596221	0.389118	C	-2.809655	3.654556	1.293579
C	-2.415610	2.300886	1.201809	C	-2.295754	-0.864020	-1.057361
C	0.132302	-0.775680	0.826287	C	-0.022031	4.711713	-2.562437
C	-0.890324	5.137296	-1.602280	H	1.246789	-0.494649	-2.806524
H	2.262961	1.089648	-4.416609	H	1.712145	3.498173	-4.360078
H	-2.655677	5.641034	0.479600	H	-3.483020	3.962431	2.095177
H	-2.795312	1.588993	1.939238	H	-2.953738	-1.194550	-0.239638
H	-1.898041	-1.759114	-1.558561	H	-2.899850	-0.299975	-1.781583
H	0.474321	-1.707460	0.349800	H	1.013366	-0.213106	1.162514
H	-0.464353	-1.047864	1.710137	H	0.407368	5.426445	-3.267792
H	-1.160657	6.193457	-1.537280	Br	0.582148	1.786131	3.470985
B	1.117549	3.041626	2.138817	Br	0.599824	4.859474	2.300086
Br	2.232130	2.494337	0.699885				

IM-2*



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

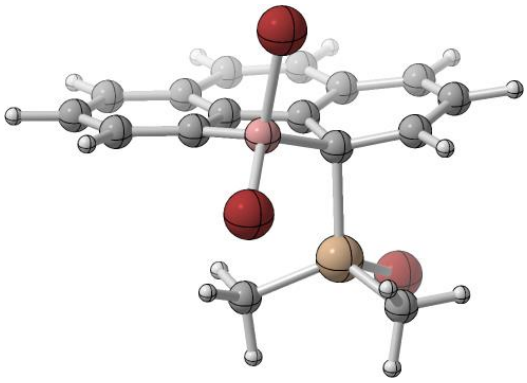
Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8653.475367 Hartree

Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -8653.217515 Hartree
Sum of electronic and thermal Energies = -8653.196663 Hartree
Sum of electronic and thermal Enthalpies = -8653.195719 Hartree
Sum of electronic and thermal Free Energies = -8653.268898 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.033978	1.833783	0.347710	C	2.882828	0.737975	-0.562106
C	3.816658	-0.303501	-0.514448	C	4.940321	-0.251839	0.323423
C	5.182704	0.892367	1.054061	C	4.261536	1.962753	1.049754
C	2.022657	2.864256	0.529038	C	2.467241	4.141477	0.974406
C	1.593732	5.246766	0.915715	C	0.288336	5.082502	0.503377
C	-0.197993	3.786115	0.272589	C	0.624458	2.661945	0.318917
Si	-0.365930	1.049035	0.501151	C	-1.512382	0.783159	-0.954756
C	0.534946	-0.486974	1.075269	Br	-1.771161	1.497393	2.237478
B	2.016264	0.764204	-1.852131	Br	1.712715	2.363946	-2.857325
Br	1.394950	-0.877115	-2.659033	C	4.599537	3.212836	1.676953
C	3.778825	4.283630	1.549667	H	3.703445	-1.154395	-1.187600
H	5.648293	-1.080961	0.337403	H	6.101528	0.996067	1.635132
H	1.964639	6.227737	1.219491	H	-0.386517	5.937081	0.442582
H	-1.274316	3.662976	0.124901	H	-2.193543	1.640730	-1.050060
H	-2.120914	-0.117038	-0.785083	H	-0.968339	0.666781	-1.902239
H	1.314713	-0.228636	1.806601	H	0.994028	-1.046737	0.251107
H	-0.206219	-1.130401	1.570812	H	5.560601	3.295803	2.187433
H	4.069230	5.262449	1.935940				

IM-3*



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

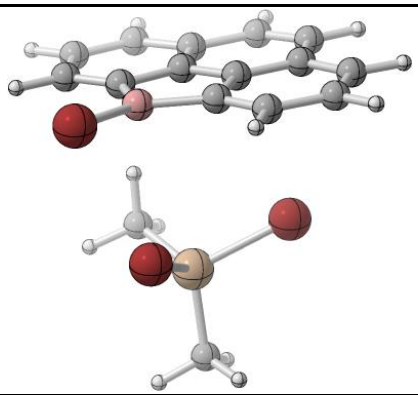
Electronic Energy = -8653.471048 Hartree

Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -8653.213243 Hartree

Sum of electronic and thermal Energies = -8653.192588 Hartree
Sum of electronic and thermal Enthalpies = -8653.191643 Hartree
Sum of electronic and thermal Free Energies = -8653.263383 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.128889	1.722684	0.480583	C	3.090832	0.872028	-0.644009
C	4.084225	-0.090677	-0.723144	C	5.081604	-0.142567	0.277731
C	5.133385	0.758394	1.338155	C	4.139864	1.751365	1.455783
C	2.059619	2.646705	0.501637	C	2.078054	3.751451	1.369259
C	1.098545	4.730786	1.135362	C	0.179273	4.611928	0.080255
C	0.145475	3.475414	-0.718995	C	1.037589	2.382494	-0.480462
Si	-0.214802	1.081100	0.408981	C	-1.791147	0.927728	-0.573390
C	0.657073	-0.482745	0.917057	Br	-0.847300	2.017931	2.372226
B	1.915023	1.386905	-1.618675	Br	2.661541	2.720756	-2.955698
Br	0.923480	-0.074589	-2.607052	C	4.080942	2.821089	2.429233
C	3.121820	3.791627	2.369842	H	4.119520	-0.789120	-1.562110
H	5.863617	-0.900282	0.199033	H	5.947662	0.706569	2.063225
H	1.067664	5.620294	1.769969	H	-0.536055	5.415790	-0.093520
H	-0.608729	3.388757	-1.505872	H	-2.407417	1.826368	-0.434937
H	-2.351604	0.065457	-0.182054	H	-1.591599	0.763029	-1.639382
H	1.478735	-0.263271	1.612202	H	1.039086	-1.042632	0.055235
H	-0.093263	-1.089689	1.447139	H	4.851940	2.869580	3.200852
H	3.132878	4.618412	3.082141				

Br-PhenB



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8653.501050 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -8653.243512 Hartree

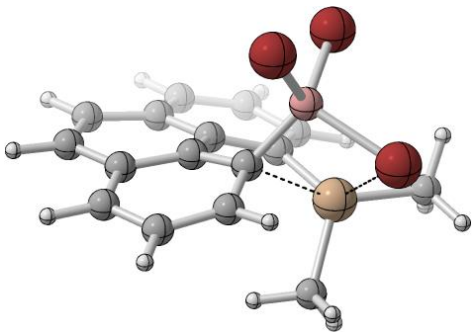
Sum of electronic and thermal Energies = -8653.222015 Hartree

Sum of electronic and thermal Enthalpies = -8653.221071 Hartree

Sum of electronic and thermal Free Energies = -8653.297987 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.885818	2.292928	0.747237	C	3.086068	1.575517	-0.456985
C	3.737262	0.358919	-0.367030	C	4.160181	-0.107324	0.906682
C	3.941018	0.616910	2.069281	C	3.279045	1.873167	2.017565
C	2.233631	3.547746	0.540007	C	1.957977	4.410794	1.598337
C	1.286445	5.611753	1.250178	C	0.949425	5.865836	-0.070633
C	1.260724	4.960820	-1.118783	C	1.916440	3.781004	-0.818600
B	2.471510	2.512058	-1.575398	Br	2.532632	2.233003	-3.461850
C	2.984537	2.768130	3.115713	C	2.362016	3.971091	2.915725
H	3.932239	-0.244921	-1.256348	H	4.674251	-1.067597	0.972520
H	4.283054	0.221414	3.028381	H	1.029155	6.336416	2.025966
H	0.428976	6.793612	-0.313242	H	0.978912	5.204687	-2.145632
H	3.272997	2.471719	4.126366	H	2.157431	4.619194	3.770696
Si	-0.881400	0.468650	0.712229	C	-2.607549	-0.221056	0.795538
C	0.458771	-0.692505	1.260344	Br	-0.794541	2.310893	1.971390
Br	-0.491227	1.055943	-1.418429	H	-3.333388	0.528223	0.452024
H	-2.850440	-0.499134	1.831508	H	-2.688503	-1.111719	0.155523
H	1.438577	-0.200043	1.187152	H	0.465121	-1.590248	0.624927
H	0.290155	-0.989419	2.306043				

TS-2*



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8653.426023 Hartree

Number of imaginary frequencies = 1, vi = -141.14 cm^{-1}

Sum of electronic and zero-point Energies = -8653.169585 Hartree

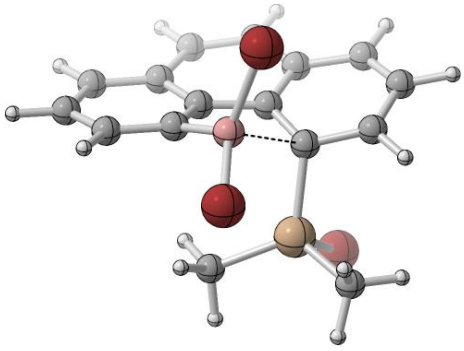
Sum of electronic and thermal Energies = -8653.149507 Hartree

Sum of electronic and thermal Enthalpies = -8653.148563 Hartree

Sum of electronic and thermal Free Energies = -8653.218278 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.465263	-1.414039	-0.294792	C	0.353798	-2.249757	0.837197
C	0.958835	-3.501113	0.802867	C	1.607764	-3.937440	-0.366269
C	1.614500	-3.156318	-1.512241	C	1.010088	-1.884070	-1.512128
C	-0.122079	-0.110570	-0.211558	C	-0.463143	0.439754	1.068371
Si	-0.758368	-1.622773	2.214515	C	-0.479994	0.535203	-1.418926
C	-1.403472	1.594163	-1.355512	C	-1.962216	1.968670	-0.138872
C	-1.482041	1.418411	1.050536	C	-2.585295	-1.621736	1.816114
C	-0.388810	-2.661769	3.726830	Br	-0.508629	0.490559	4.047160
B	0.632209	0.796918	2.287757	Br	1.152915	2.731224	2.188813
Br	2.294641	-0.308457	2.423946	C	0.838002	-1.078620	-2.695431
C	0.072125	0.044058	-2.659474	H	0.914686	-4.168174	1.665967
H	2.071331	-4.924929	-0.384780	H	2.067491	-3.532459	-2.431701
H	-1.707286	2.092650	-2.278854	H	-2.717550	2.754120	-0.103338
H	-1.816789	1.848265	1.997455	H	-3.107292	-0.906731	2.467188
H	-2.989951	-2.628287	2.004187	H	-2.758402	-1.344214	0.768156
H	-0.497364	-3.721372	3.439592	H	0.637834	-2.488830	4.076600
H	-1.089184	-2.441109	4.542040	H	1.269006	-1.427510	-3.635606
H	-0.140881	0.600485	-3.574228				

TS-3*



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8653.464239 Hartree

Number of imaginary frequencies = 1, vi = -180.82 cm^{-1}

Sum of electronic and zero-point Energies = -8653.207177 Hartree

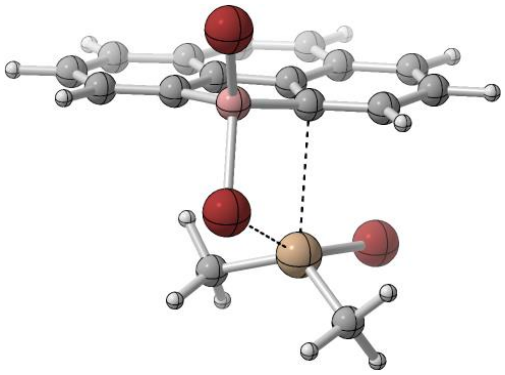
Sum of electronic and thermal Energies = -8653.186901 Hartree

Sum of electronic and thermal Enthalpies = -8653.185957 Hartree

Sum of electronic and thermal Free Energies = -8653.257252 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.809556	-0.231201	-0.118514	C	1.752078	-1.141252	-1.196167
C	2.698283	-2.156247	-1.237177	C	3.713832	-2.205092	-0.260247
C	3.828721	-1.227967	0.719899	C	2.881081	-0.186096	0.794402
C	0.763033	0.735044	-0.071034	C	0.958497	1.927067	0.653228
C	0.048737	2.976831	0.419554	C	-0.996978	2.826921	-0.487854
C	-1.259542	1.581515	-1.066961	C	-0.426653	0.470013	-0.823695
Si	-1.503204	-0.988333	-0.186846	C	-3.060290	-1.174476	-1.202756
C	-0.627093	-2.565682	0.284106	Br	-2.209665	-0.186333	1.826424
B	0.735778	-0.726596	-2.330621	Br	1.283257	0.757669	-3.494201
Br	-0.284769	-2.122935	-3.262053	C	2.965774	0.961201	1.667474
C	2.084424	1.994818	1.556250	H	2.688858	-2.887608	-2.048443
H	4.459816	-2.999986	-0.309076	H	4.664993	-1.248931	1.421468
H	0.182522	3.926328	0.943158	H	-1.666530	3.665229	-0.682476
H	-2.178814	1.454621	-1.644902	H	-3.734503	-0.326345	-1.022386
H	-3.579329	-2.089305	-0.880915	H	-2.845288	-1.254215	-2.276306
H	0.205503	-2.352291	0.968941	H	-0.250841	-3.122410	-0.582476
H	-1.363405	-3.182433	0.821668	H	3.791370	1.017932	2.379518
H	2.209009	2.893077	2.163886				

TS-4*



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8653.445432 Hartree

Number of imaginary frequencies = 1, vi = -128.00 cm^{-1}

Sum of electronic and zero-point Energies = -8653.188156 Hartree

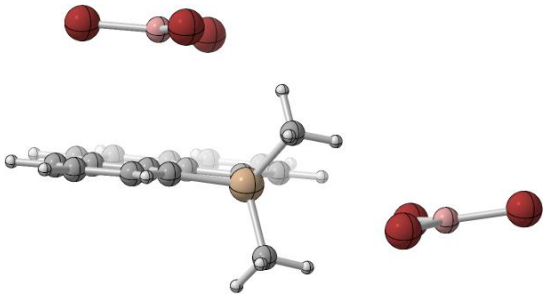
Sum of electronic and thermal Energies = -8653.167833 Hartree

Sum of electronic and thermal Enthalpies = -8653.166889 Hartree

Sum of electronic and thermal Free Energies = -8653.238590 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.177981	1.624236	0.371142	C	3.247328	0.867496	-0.821582
C	4.255820	-0.076674	-0.893267	C	5.143267	-0.237881	0.201527
C	5.059732	0.535391	1.351472	C	4.049816	1.520783	1.462057
C	2.101199	2.555177	0.375903	C	1.912559	3.467014	1.417328
C	0.843955	4.380201	1.246509	C	0.042108	4.333958	0.109715
C	0.253005	3.385667	-0.912682	C	1.298921	2.465495	-0.790841
B	2.094053	1.456998	-1.786157	Br	2.734676	2.273050	-3.485740
C	3.825551	2.436685	2.559556	C	2.822767	3.368863	2.535144
H	4.386363	-0.695460	-1.784169	H	5.930960	-0.990341	0.131316
H	5.774367	0.388917	2.163974	H	0.641700	5.126663	2.018300
H	-0.773817	5.051196	0.010235	H	-0.373611	3.399137	-1.809116
H	4.489738	2.385861	3.425128	H	2.699063	4.052962	3.377075
Si	-0.397588	0.418474	0.088574	C	-2.082463	0.189562	-0.678460
C	0.677227	-0.934657	0.777629	Br	-0.907483	1.631660	1.924555
H	-2.323417	1.073431	-1.286574	H	-2.836222	0.090373	0.113588
H	-2.081264	-0.690477	-1.335448	H	1.723814	-0.595224	0.820296
H	0.628459	-1.812408	0.119758	H	0.340968	-1.175781	1.794757
Br	0.622586	-0.023786	-2.287704				

DMPhenS[BBr_3]



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

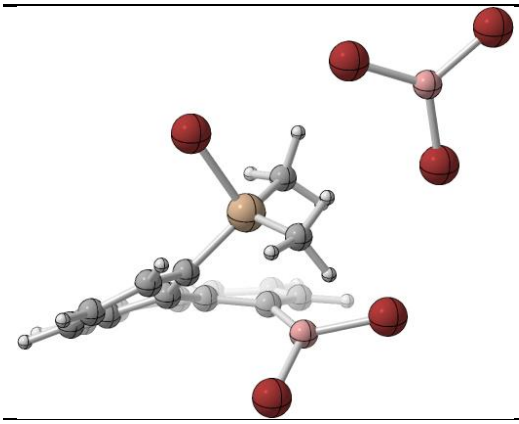
Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16400.068216 Hartree

Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -16399.805154 Hartree
Sum of electronic and thermal Energies = -16399.776279 Hartree
Sum of electronic and thermal Enthalpies = -16399.775335 Hartree
Sum of electronic and thermal Free Energies = -16399.876708 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.206917	2.396893	-1.771539	C	0.094465	1.010918	-1.795772
C	0.993799	0.561135	-2.747871	C	1.577922	1.465974	-3.663097
C	1.264847	2.813441	-3.635540	C	0.354533	3.315372	-2.677236
C	-1.101283	2.850864	-0.732961	C	-1.562355	1.872195	0.184594
Si	-0.902014	0.189535	-0.404770	C	-1.465121	4.207876	-0.646023
C	-2.350328	4.580897	0.390763	C	-2.807532	3.637324	1.294504
C	-2.412196	2.284161	1.199696	C	-2.329262	-0.845485	-1.056473
C	0.139024	-0.774703	0.822128	C	-0.022347	4.703879	-2.559687
C	-0.892888	5.126711	-1.600445	H	1.270041	-0.494669	-2.801525
H	2.287708	1.093849	-4.403808	H	1.723310	3.500104	-4.350561
H	-2.656366	5.625440	0.483763	H	-3.479520	3.943327	2.098006
H	-2.789754	1.570656	1.936743	H	-2.975410	-1.174211	-0.228004
H	-1.967982	-1.739987	-1.583961	H	-2.935376	-0.247730	-1.752091
H	0.538914	-1.676776	0.334420	H	0.983325	-0.174663	1.187381
H	-0.463719	-1.094356	1.685932	H	0.408437	5.420375	-3.262421
H	-1.164083	6.182545	-1.533419	Br	0.585935	1.819733	3.473277
B	1.120989	3.063463	2.130047	Br	0.608342	4.884021	2.279325
Br	2.230640	2.502910	0.692546	Br	0.487693	-3.340954	-2.271130
B	0.040886	-4.644269	-0.955483	Br	0.941013	-6.314031	-0.938701
Br	-1.302917	-4.266295	0.332066				

IM-2*[BBr_3]



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16400.072939 Hartree

Number of imaginary frequencies = 0
Sum of electronic and zero-point Energies = -16399.808281 Hartree

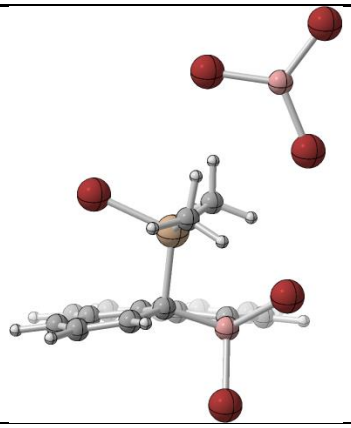
Sum of electronic and thermal Energies = -16399.780244 Hartree

Sum of electronic and thermal Enthalpies = -16399.779300 Hartree

Sum of electronic and thermal Free Energies = -16399.874120 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.032160	1.830356	0.344477	C	2.885270	0.736139	-0.568388
C	3.822642	-0.302556	-0.522079	C	4.944959	-0.250349	0.317104
C	5.183072	0.892635	1.050980	C	4.259028	1.960377	1.048079
C	2.018287	2.858117	0.528671	C	2.460803	4.135121	0.977577
C	1.586140	5.239538	0.921562	C	0.281360	5.074460	0.507938
C	-0.202670	3.777943	0.273630	C	0.620365	2.654119	0.318042
Si	-0.370855	1.039037	0.498741	C	-1.519228	0.794225	-0.958202
C	0.549043	-0.481539	1.083309	Br	-1.766915	1.506699	2.242664
B	2.017977	0.760629	-1.857478	Br	1.687033	2.358597	-2.854953
Br	1.426771	-0.886783	-2.680499	C	4.594124	3.209065	1.679477
C	3.771529	4.278515	1.554339	H	3.712812	-1.152371	-1.196935
H	5.655028	-1.077678	0.329764	H	6.100735	0.997551	1.633673
H	1.955655	6.220050	1.228485	H	-0.394889	5.928085	0.449052
H	-1.278864	3.654204	0.125726	H	-2.086050	1.719557	-1.136397
H	-2.234199	-0.010771	-0.736383	H	-0.976418	0.538021	-1.879141
H	1.324769	-0.198433	1.810428	H	1.017199	-1.040437	0.263243
H	-0.179721	-1.134946	1.584774	H	5.554497	3.292118	2.191227
H	4.059403	5.256884	1.943633	Br	-1.201811	-2.985871	-1.048764
B	-2.530477	-3.352311	0.263545	Br	-3.280251	-5.091854	0.402461
Br	-3.093184	-1.964414	1.432287				

IM-3[BBr_3]



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16400.068415 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16399.803628 Hartree

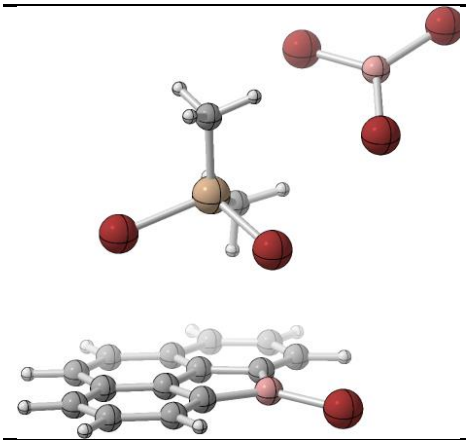
Sum of electronic and thermal Energies = -16399.775871 Hartree

Sum of electronic and thermal Enthalpies = -16399.774927 Hartree

Sum of electronic and thermal Free Energies = -16399.868709 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.130154	1.715893	0.474923	C	3.095287	0.868631	-0.652154
C	4.095155	-0.086848	-0.736977	C	5.094572	-0.136328	0.261913
C	5.141119	0.759537	1.326788	C	4.141054	1.745203	1.450223
C	2.055290	2.633616	0.501009	C	2.065329	3.731319	1.377587
C	1.081553	4.707790	1.148842	C	0.170343	4.594828	0.086558
C	0.147366	3.465542	-0.723762	C	1.037938	2.371849	-0.486167
Si	-0.228376	1.068026	0.405786	C	-1.799537	0.962381	-0.591007
C	0.687234	-0.461322	0.942873	Br	-0.886258	2.003371	2.362258
B	1.908886	1.373606	-1.619255	Br	2.635404	2.690924	-2.981655
Br	0.920770	-0.112321	-2.587848	C	4.074222	2.807069	2.431719
C	3.107605	3.770495	2.379840	H	4.132928	-0.782485	-1.578199
H	5.881493	-0.888470	0.178790	H	5.955962	0.709235	2.051342
H	1.043078	5.591186	1.791489	H	-0.546358	5.397756	-0.085918
H	-0.597283	3.385544	-1.520071	H	-2.337825	1.917261	-0.514378
H	-2.431886	0.180057	-0.147403	H	-1.605185	0.716203	-1.642319
H	1.480052	-0.188066	1.653103	H	1.116433	-1.015376	0.099839
H	-0.046384	-1.093549	1.465789	H	4.844522	2.855098	3.204067
H	3.111787	4.591422	3.098978	Br	-1.448229	-2.631301	-0.996510
B	-2.604631	-3.119341	0.427142	Br	-3.519487	-4.781536	0.405695
Br	-2.852731	-1.924259	1.895410				

Br-PhenB[BBr_3]



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16400.097300 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16399.833157 Hartree

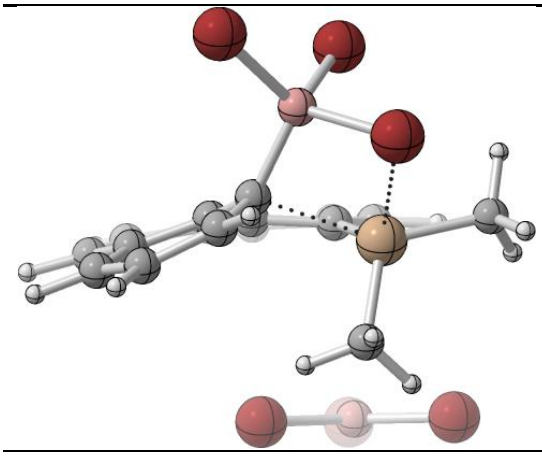
Sum of electronic and thermal Energies = -16399.804339 Hartree

Sum of electronic and thermal Enthalpies = -16399.803395 Hartree

Sum of electronic and thermal Free Energies = -16399.903843 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.887712	2.289815	0.747183	C	3.084844	1.569905	-0.456088
C	3.734444	0.352574	-0.365052	C	4.160625	-0.111130	0.908442
C	3.945850	0.616112	2.069934	C	3.283875	1.872378	2.017391
C	2.233225	3.543300	0.539380	C	1.956627	4.406631	1.597217
C	1.282232	5.605853	1.248632	C	0.943740	5.858231	-0.072102
C	1.255900	4.952928	-1.119748	C	1.914040	3.774632	-0.819098
B	2.468831	2.504997	-1.574795	Br	2.531305	2.224886	-3.461605
C	2.989115	2.767998	3.114903	C	2.363184	3.969096	2.914527
H	3.925769	-0.253836	-1.253439	H	4.673502	-1.071984	0.975050
H	4.290460	0.222667	3.028949	H	1.023896	6.330474	2.024107
H	0.421112	6.784698	-0.315036	H	0.972398	5.195206	-2.146510
H	3.279348	2.473236	4.125526	H	2.157823	4.617363	3.769178
Si	-0.884210	0.452766	0.708142	C	-2.619189	-0.214514	0.788717
C	0.476484	-0.679818	1.265506	Br	-0.802751	2.296432	1.971963
Br	-0.492023	1.066911	-1.419347	H	-3.330983	0.567589	0.490906
H	-2.850279	-0.531957	1.816334	H	-2.729491	-1.074937	0.113453
H	1.434510	-0.141307	1.242385	H	0.543275	-1.557727	0.607376
H	0.282122	-1.013009	2.296032	Br	-0.942139	-2.692039	-1.778216
B	-1.357530	-4.167774	-0.654967	Br	-1.520541	-5.912322	-1.381157
Br	-1.609581	-3.886123	1.212079				

TS-2*[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen)
freq empiricaldispersion=gd3 nosymm
```

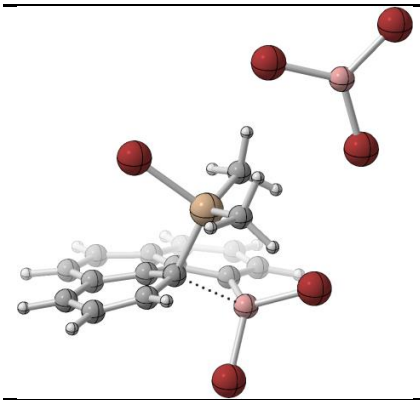
Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16400.030328 Hartree

Number of imaginary frequencies = 1, vi = -140.09 cm^{-1}
Sum of electronic and zero-point Energies = -16399.767205 Hartree
Sum of electronic and thermal Energies = -16399.739923 Hartree
Sum of electronic and thermal Enthalpies = -16399.738979 Hartree
Sum of electronic and thermal Free Energies = -16399.829924 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.495953	-1.407729	-0.289166	C	0.371892	-2.251029	0.834355
C	0.978586	-3.502505	0.798241	C	1.631907	-3.933523	-0.370504
C	1.640701	-3.147257	-1.514637	C	1.041558	-1.873601	-1.508179
C	-0.109158	-0.112574	-0.203846	C	-0.449370	0.434020	1.077547
Si	-0.767522	-1.634617	2.193758	C	-0.490041	0.519630	-1.411477
C	-1.424895	1.568035	-1.344466	C	-1.970152	1.947435	-0.123113
C	-1.473728	1.407216	1.063915	C	-2.594979	-1.575807	1.805180
C	-0.415741	-2.668349	3.711285	Br	-0.487934	0.498746	4.060847
B	0.645282	0.787147	2.302766	Br	1.175766	2.719005	2.183437
Br	2.304498	-0.325107	2.440214	C	0.845269	-1.077266	-2.693743
C	0.056449	0.029289	-2.655647	H	0.923748	-4.176465	1.655710
H	2.090663	-4.923433	-0.393356	H	2.085228	-3.525402	-2.437471
H	-1.745653	2.056475	-2.267446	H	-2.731234	2.727139	-0.083735
H	-1.805297	1.836158	2.012341	H	-3.074259	-0.835499	2.461654
H	-3.038779	-2.564108	1.998739	H	-2.767824	-1.293342	0.758514
H	-0.535162	-3.726177	3.419176	H	0.611126	-2.506699	4.065629
H	-1.118928	-2.440691	4.521960	H	1.271306	-1.424535	-3.636722
H	-0.177250	0.575882	-3.571317	Br	-2.148599	-3.292213	-1.613892
B	-1.676402	-4.953652	-0.829596	Br	-0.810524	-6.290351	-1.866315
Br	-2.141186	-5.325385	0.985460				

TS-3*[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16400.060981 Hartree

Number of imaginary frequencies = 1, vi = -184.01 cm^{-1}

Sum of electronic and zero-point Energies = -16399.796799 Hartree

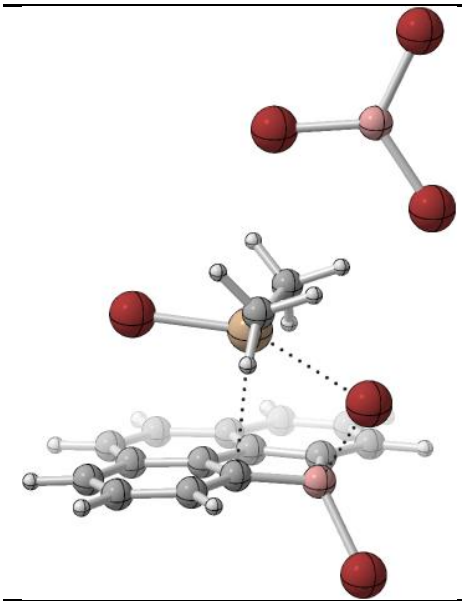
Sum of electronic and thermal Energies = -16399.769448 Hartree

Sum of electronic and thermal Enthalpies = -16399.768503 Hartree

Sum of electronic and thermal Free Energies = -16399.861576 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.801330	-0.242625	-0.122759	C	1.742080	-1.145515	-1.205985
C	2.688921	-2.159649	-1.257246	C	3.707365	-2.215782	-0.284267
C	3.822948	-1.247003	0.703889	C	2.874761	-0.206699	0.789024
C	0.754629	0.723436	-0.064095	C	0.953710	1.907616	0.673190
C	0.050081	2.964586	0.449906	C	-0.991436	2.830547	-0.464233
C	-1.256818	1.593334	-1.059084	C	-0.435145	0.472113	-0.821644
Si	-1.531677	-0.990298	-0.214141	C	-3.072812	-1.129513	-1.260831
C	-0.616292	-2.533207	0.297494	Br	-2.303301	-0.209112	1.786242
B	0.716616	-0.737109	-2.333117	Br	1.243577	0.740283	-3.512671
Br	-0.291496	-2.156754	-3.251059	C	2.961358	0.930229	1.675007
C	2.079931	1.964651	1.576523	H	2.675917	-2.885840	-2.073113
H	4.453722	-3.009753	-0.341516	H	4.660107	-1.273209	1.404227
H	0.187202	3.907047	0.985196	H	-1.655478	3.674379	-0.653763
H	-2.171117	1.481000	-1.646954	H	-3.660320	-0.205586	-1.168832
H	-3.687688	-1.951983	-0.870068	H	-2.848977	-1.323451	-2.317615
H	0.192563	-2.261850	0.991181	H	-0.199097	-3.095716	-0.545880
H	-1.334951	-3.164610	0.840259	H	3.788132	0.978495	2.386301
H	2.205069	2.856357	2.193642	Br	-2.710569	-4.769308	-1.620439
B	-3.799683	-5.239724	-0.134361	Br	-4.541127	-6.982447	-0.006169
Br	-4.145433	-3.956759	1.230167				

TS-4*[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16400.043155 Hartree

Number of imaginary frequencies = 1, vi = -127.94 cm^{-1}

Sum of electronic and zero-point Energies = -16399.778676 Hartree

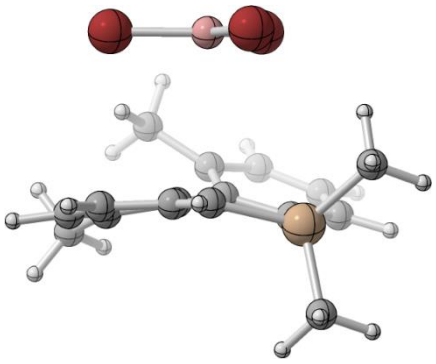
Sum of electronic and thermal Energies = -16399.751368 Hartree

Sum of electronic and thermal Enthalpies = -16399.750424 Hartree

Sum of electronic and thermal Free Energies = -16399.843835 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.175682	1.612481	0.365297	C	3.250049	0.864609	-0.832316
C	4.261460	-0.076153	-0.909255	C	5.147407	-0.243041	0.185666
C	5.057532	0.520031	1.341934	C	4.043820	1.500864	1.458235
C	2.094895	2.539852	0.374072	C	1.897208	3.437959	1.426136
C	0.824660	4.347806	1.263838	C	0.028783	4.310140	0.123331
C	0.249765	3.375150	-0.910522	C	1.299425	2.460727	-0.797323
B	2.088284	1.446280	-1.791017	Br	2.700441	2.237869	-3.511974
C	3.811129	2.403634	2.564874	C	2.803547	3.330532	2.546607
H	4.394211	-0.688486	-1.804346	H	5.937849	-0.992244	0.111302
H	5.769818	0.368640	2.155655	H	0.615314	5.083220	2.044236
H	-0.790869	5.023852	0.028201	H	-0.373633	3.397831	-1.809017
H	4.471962	2.346278	3.432639	H	2.672594	4.004084	3.395999
Si	-0.440457	0.377319	0.101626	C	-2.101813	0.312195	-0.744239
C	0.676436	-0.938590	0.796717	Br	-0.929907	1.592241	1.940503
H	-2.195433	1.215147	-1.365648	H	-2.903007	0.306910	0.005372
H	-2.163892	-0.566645	-1.399696	H	1.708699	-0.552413	0.793886
H	0.644686	-1.833891	0.162493	H	0.380430	-1.161058	1.829727
Br	0.631490	-0.071366	-2.259798	Br	-1.237261	-3.390017	-1.513018
B	-2.246590	-3.842766	0.035580	Br	-2.995909	-5.572934	0.214481
Br	-2.504494	-2.549092	1.412214				

Me_2-DMDBS



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8655.844502 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -8655.545304 Hartree

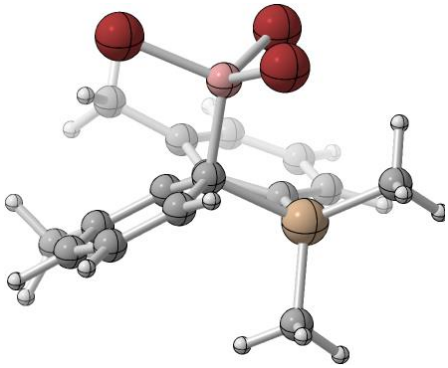
Sum of electronic and thermal Energies = -8655.521752 Hartree

Sum of electronic and thermal Enthalpies = -8655.520807 Hartree

Sum of electronic and thermal Free Energies = -8655.600214 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.140785	2.587861	-1.899023	C	-0.037981	1.174238	-1.981438
C	0.784175	0.577984	-2.931851	C	1.540636	1.374689	-3.794472
C	1.541147	2.752980	-3.618396	C	0.742778	3.386602	-2.652034
C	-1.095438	3.064695	-0.843420	C	-1.346176	2.105203	0.175388
Si	-0.837302	0.405479	-0.462386	C	-1.823343	4.272104	-0.842384
C	-2.606669	4.568069	0.284753	C	-2.737154	3.687604	1.352661
C	-2.145827	2.425849	1.269557	C	-2.382702	-0.613209	-0.792773
C	0.379643	-0.607188	0.547183	C	1.015081	4.843867	-2.366480
C	-1.922989	5.202245	-2.026617	H	0.863880	-0.510779	-2.989820
H	2.178381	0.920414	-4.554538	H	2.217460	3.369496	-4.216138
H	-3.155516	5.513341	0.299529	H	-3.347698	3.959546	2.215146
H	-2.329437	1.687164	2.054559	H	-2.876094	-0.887020	0.152244
H	-2.133814	-1.542099	-1.327446	H	-3.096086	-0.040695	-1.401715
H	0.620085	-1.539012	0.011910	H	1.314303	-0.058344	0.725553
H	-0.054744	-0.880770	1.520774	H	0.658051	5.130518	-1.368669
H	0.558851	5.517300	-3.106075	H	2.100832	5.014639	-2.393673
H	-1.348430	6.128478	-1.883127	H	-2.974431	5.489096	-2.169302
H	-1.574665	4.721004	-2.948190	Br	0.988326	1.957264	3.212660
B	1.336766	3.190229	1.800857	Br	0.640327	4.954438	1.888859
Br	2.464768	2.681731	0.356185				

IM-1**



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8655.833241 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -8655.533860 Hartree

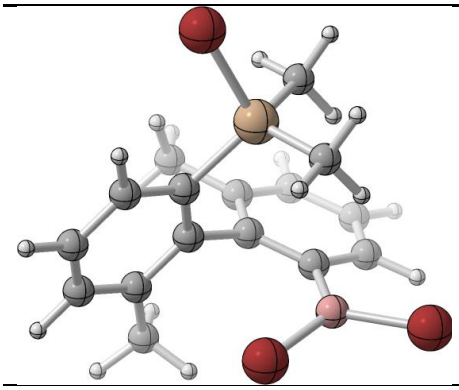
Sum of electronic and thermal Energies = -8655.510725 Hartree

Sum of electronic and thermal Enthalpies = -8655.509781 Hartree

Sum of electronic and thermal Free Energies = -8655.586059 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.100838	2.582317	-1.718855	C	0.342264	1.191098	-1.675599
C	1.222567	0.609128	-2.583885	C	1.868850	1.416923	-3.519715
C	1.690571	2.799295	-3.494705	C	0.825149	3.418736	-2.585911
C	-0.889714	3.005392	-0.702647	C	-0.770874	2.314781	0.571589
Si	-0.452293	0.478581	-0.134001	C	-1.995875	3.823699	-0.986505
C	-2.996807	3.921045	-0.011064	C	-2.966658	3.215756	1.196548
C	-1.879599	2.416970	1.473443	C	-2.164102	-0.229135	-0.434664
C	0.603910	-0.709277	0.832817	C	0.821351	4.920343	-2.463188
C	-2.216979	4.508057	-2.309877	H	1.429682	-0.462918	-2.554146
H	2.557157	0.975166	-4.242124	H	2.274610	3.426991	-4.171882
H	-3.867843	4.543869	-0.233457	H	-3.790777	3.305002	1.904063
H	-1.820993	1.888741	2.426911	H	-2.648479	-0.497720	0.516029
H	-2.095844	-1.137952	-1.051380	H	-2.800654	0.497866	-0.959596
H	0.724359	-1.619749	0.222877	H	1.591756	-0.283769	1.049969
H	0.123342	-0.986811	1.780918	H	1.858203	5.284380	-2.462831
H	0.361944	5.245804	-1.520379	H	0.300293	5.403359	-3.303127
H	-3.289278	4.540463	-2.543852	H	-1.698711	3.985371	-3.123285
H	-1.850589	5.544330	-2.287773	Br	0.711375	1.785582	3.237731
B	0.672211	2.807924	1.494145	Br	0.406599	4.786377	1.825294
Br	2.404618	2.519753	0.525523				

IM-2**



#p m062x/def2svp opt freq empiricaldispersion=gd3 nosymm

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8655.879948 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -8655.579606 Hartree

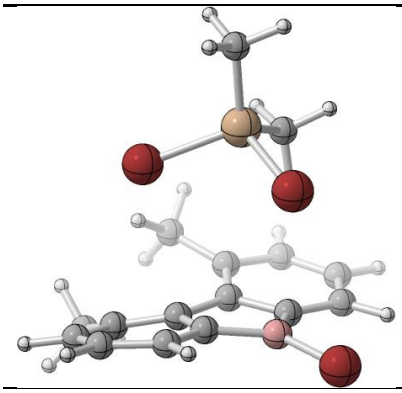
Sum of electronic and thermal Energies = -8655.556187 Hartree

Sum of electronic and thermal Enthalpies = -8655.555243 Hartree

Sum of electronic and thermal Free Energies = -8655.634252 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.582845	1.655355	0.244291	C	2.535349	0.889106	-0.949529
C	3.161694	-0.376582	-0.947229	C	3.830554	-0.854633	0.170478
C	3.873442	-0.082503	1.328517	C	3.250472	1.166010	1.386423
C	1.894346	2.976493	0.387742	C	2.656660	4.149832	0.226521
C	2.022528	5.384332	0.366737	C	0.663255	5.461345	0.661857
C	-0.076468	4.296519	0.834263	C	0.524620	3.033346	0.707849
Si	-0.559295	1.486557	0.855119	C	-1.331745	1.042516	-0.790888
C	0.207121	-0.015546	1.666809	Br	-2.287977	2.063630	2.208011
B	1.865762	1.347669	-2.285939	Br	1.491118	3.156108	-2.779082
Br	1.404775	0.038445	-3.629593	C	3.259652	1.955182	2.670533
C	4.109116	4.072361	-0.164447	H	3.128947	-0.991475	-1.846313
H	4.314468	-1.831617	0.142573	H	4.386758	-0.460828	2.215387
H	2.603573	6.299072	0.229804	H	0.180005	6.434240	0.763289
H	-1.137063	4.369342	1.082094	H	-1.698655	1.942506	-1.304471
H	-2.176978	0.357447	-0.632187	H	-0.605927	0.536376	-1.445689
H	0.691999	0.239287	2.619697	H	0.946323	-0.497002	1.009321
H	-0.599449	-0.733972	1.875523	H	3.719180	2.944896	2.533771
H	3.810901	1.419888	3.453938	H	2.234595	2.140040	3.025591
H	4.561023	5.071872	-0.198302	H	4.212183	3.614466	-1.161020
H	4.690831	3.450352	0.531773				

Me_2-Br-DBB



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8655.881008 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -8655.580744 Hartree

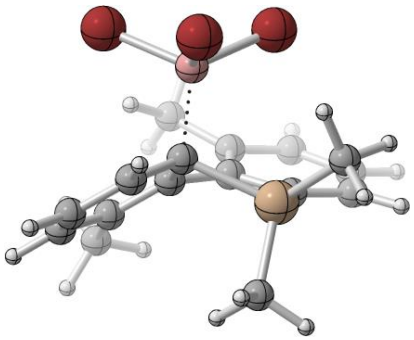
Sum of electronic and thermal Energies = -8655.556972 Hartree

Sum of electronic and thermal Enthalpies = -8655.556028 Hartree

Sum of electronic and thermal Free Energies = -8655.637168 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.993416	2.353046	0.936221	C	3.267656	1.764804	-0.331960
C	3.956856	0.566757	-0.443439	C	4.369006	-0.089131	0.723123
C	4.000078	0.427394	1.958033	C	3.271058	1.628373	2.103162
C	2.277840	3.664048	0.737233	C	2.100855	4.751740	1.599992
C	1.270290	5.799245	1.149985	C	0.706234	5.824352	-0.119061
C	1.033861	4.816666	-1.032295	C	1.825114	3.759799	-0.608786
B	2.522664	2.620624	-1.396640	Br	2.585527	2.398956	-3.294443
C	2.728636	1.958516	3.471394	C	2.821256	4.936925	2.912177
H	4.153957	0.140121	-1.429719	H	4.926307	-1.025316	0.668601
H	4.244958	-0.134526	2.863174	H	1.093539	6.639475	1.826683
H	0.065959	6.656795	-0.413920	H	0.688777	4.859994	-2.067936
H	3.441300	2.517482	4.094125	H	2.494909	1.024435	4.001657
H	1.802742	2.541216	3.393508	H	2.205905	4.661774	3.780665
H	3.095627	5.994672	3.027319	H	3.743833	4.345390	2.943104
Si	-0.846205	0.561289	0.633434	C	-2.557389	-0.151575	0.795039
C	0.522467	-0.540926	1.234797	Br	-0.804290	2.500275	1.752362
Br	-0.476470	1.002211	-1.530513	H	-3.302906	0.558430	0.412361
H	-2.778998	-0.360117	1.851951	H	-2.631530	-1.086526	0.220633
H	1.500244	-0.105749	0.983050	H	0.440303	-1.523820	0.747217
H	0.458593	-0.672978	2.325082				

TS-1**



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8655.830956 Hartree

Number of imaginary frequencies = 1, vi = -129.55 cm^{-1}

Sum of electronic and zero-point Energies = -8655.531807 Hartree

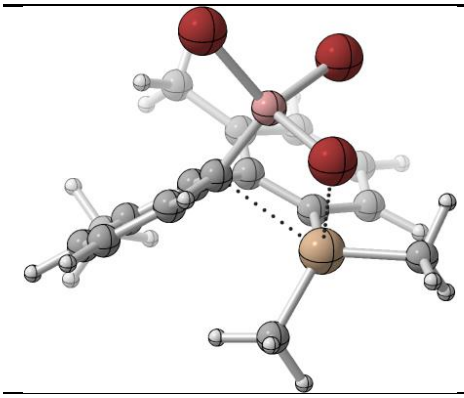
Sum of electronic and thermal Energies = -8655.509342 Hartree

Sum of electronic and thermal Enthalpies = -8655.508397 Hartree

Sum of electronic and thermal Free Energies = -8655.583385 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.009216	2.565110	-1.757627	C	0.208781	1.167421	-1.744425
C	1.058635	0.576576	-2.675744	C	1.719323	1.382667	-3.602581
C	1.584586	2.769203	-3.547429	C	0.747647	3.396814	-2.617767
C	-0.961224	2.993138	-0.725193	C	-0.846206	2.281309	0.538886
Si	-0.577074	0.443991	-0.202951	C	-2.048037	3.843816	-0.987529
C	-3.033184	3.959555	0.001168	C	-3.007937	3.239749	1.200539
C	-1.942900	2.404275	1.453375	C	-2.313503	-0.209760	-0.482766
C	0.484073	-0.785315	0.718595	C	0.781479	4.896326	-2.476167
C	-2.264283	4.550234	-2.300102	H	1.231624	-0.502098	-2.670292
H	2.384561	0.934703	-4.342562	H	2.179322	3.392228	-4.219573
H	-3.888432	4.609948	-0.202936	H	-3.820814	3.343452	1.919023
H	-1.894032	1.859530	2.397565	H	-2.785705	-0.479758	0.473793
H	-2.278988	-1.112334	-1.111611	H	-2.940848	0.540372	-0.985486
H	1.361586	-1.032021	0.103301	H	0.854578	-0.370029	1.665384
H	-0.083720	-1.702825	0.927495	H	1.826544	5.236058	-2.482582
H	0.339576	5.220913	-1.524908	H	0.263783	5.400638	-3.305679
H	-3.337572	4.610708	-2.523888	H	-1.765613	4.026467	-3.124931
H	-1.873439	5.577273	-2.267790	Br	0.609286	1.854441	3.257907
B	0.623774	2.739270	1.436602	Br	0.488985	4.748507	1.642539
Br	2.328914	2.258624	0.497989				

TS-2**



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8655.814855 Hartree

Number of imaginary frequencies = 1, vi = -142.90 cm^{-1}

Sum of electronic and zero-point Energies = -8655.515671 Hartree

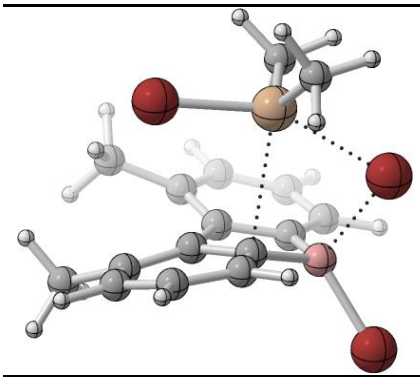
Sum of electronic and thermal Energies = -8655.493082 Hartree

Sum of electronic and thermal Enthalpies = -8655.492138 Hartree

Sum of electronic and thermal Free Energies = -8655.567129 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.648004	-1.451651	-0.361493	C	0.313774	-2.349218	0.668649
C	0.969799	-3.579860	0.765957	C	1.937656	-3.913177	-0.177265
C	2.288699	-2.997853	-1.169222	C	1.665324	-1.750573	-1.280273
C	-0.157087	-0.208216	-0.317983	C	-0.272785	0.447292	0.945973
Si	-0.812701	-1.663796	1.988264	C	-1.005465	0.124202	-1.400453
C	-1.985281	1.097077	-1.199486	C	-2.157677	1.724536	0.036997
C	-1.321308	1.399092	1.085386	C	-2.635201	-1.460277	1.669915
C	-0.486940	-2.610010	3.561765	Br	-0.038716	0.538927	3.911868
B	0.940480	0.723414	2.053868	Br	1.569046	2.621723	1.832274
Br	2.537947	-0.490204	2.091584	C	2.164118	-0.749284	-2.288555
C	-0.950395	-0.581090	-2.732185	H	0.745588	-4.272065	1.579853
H	2.449394	-4.874966	-0.121260	H	3.096831	-3.243253	-1.862567
H	-2.661430	1.337222	-2.023740	H	-2.944338	2.467988	0.169816
H	-1.433830	1.916950	2.038826	H	-3.065737	-0.781905	2.420262
H	-3.113896	-2.446672	1.776408	H	-2.832846	-1.060686	0.666676
H	-0.721734	-3.668363	3.350353	H	0.569014	-2.525777	3.851174
H	-1.118993	-2.258866	4.386042	H	1.921687	-1.057496	-3.316677
H	3.257582	-0.664280	-2.217593	H	1.740334	0.247762	-2.112412
H	-1.939946	-0.573580	-3.207398	H	-0.620670	-1.623127	-2.630849
H	-0.253242	-0.077592	-3.418058				

TS-4**



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#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -8655.827213 Hartree

Number of imaginary frequencies = 1, vi = -142.87 cm^{-1}

Sum of electronic and zero-point Energies = -8655.527201 Hartree

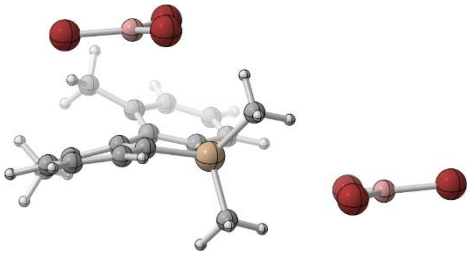
Sum of electronic and thermal Energies = -8655.504641 Hartree

Sum of electronic and thermal Enthalpies = -8655.503697 Hartree

Sum of electronic and thermal Free Energies = -8655.579457 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.167274	1.689352	0.521874	C	3.275847	1.100989	-0.765266
C	4.196299	0.089294	-1.003977	C	4.979994	-0.384032	0.051353
C	4.781799	0.111428	1.337496	C	3.859122	1.134053	1.614573
C	2.119124	2.754233	0.502201	C	1.922445	3.869822	1.327841
C	0.778583	4.654947	1.087176	C	-0.105300	4.417711	0.036838
C	0.189884	3.410775	-0.879480	C	1.301579	2.590833	-0.656329
B	2.129477	1.694210	-1.689124	Br	2.636891	2.548596	-3.405859
C	3.559428	1.456793	3.057637	C	2.904354	4.341773	2.368511
H	4.281302	-0.348299	-2.001486	H	5.708825	-1.179119	-0.114987
H	5.331949	-0.330905	2.171641	H	0.597498	5.508680	1.745718
H	-0.975998	5.060680	-0.097248	H	-0.400389	3.285786	-1.792111
H	3.669801	0.547501	3.664452	H	2.528800	1.817425	3.173621
H	4.237799	2.212843	3.477676	H	2.951699	5.439335	2.352652
H	3.909837	3.955193	2.163623	H	2.618816	4.038725	3.386050
Si	-0.228450	0.426662	0.191985	C	-1.963952	0.203693	-0.453018
C	0.843490	-0.964383	0.810624	Br	-0.625100	1.626404	2.080759
H	-2.273136	1.119156	-0.977902	H	-2.648447	0.036139	0.389268
H	-2.001541	-0.633281	-1.163098	H	1.904497	-0.671607	0.780049
H	0.709894	-1.831820	0.149253	H	0.567067	-1.207919	1.845103
Br	0.690390	0.105604	-2.180799				

Me$_2$-Br-DBB[BBr_3]



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#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.438960 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16402.133228 Hartree

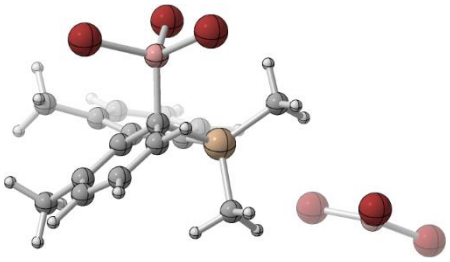
Sum of electronic and thermal Energies = -16402.103244 Hartree

Sum of electronic and thermal Enthalpies = -16402.102300 Hartree

Sum of electronic and thermal Free Energies = -16402.202009 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.139710	2.581646	-1.901489	C	-0.032664	1.167950	-1.982834
C	0.799296	0.575991	-2.927380	C	1.556650	1.374559	-3.787334
C	1.548361	2.753088	-3.614816	C	0.742856	3.383560	-2.652456
C	-1.093851	3.057038	-0.845226	C	-1.337370	2.098424	0.175845
Si	-0.837236	0.395888	-0.466424	C	-1.825601	4.262053	-0.844359
C	-2.605807	4.558058	0.284913	C	-2.729439	3.679084	1.354878
C	-2.134553	2.418912	1.271883	C	-2.409665	-0.583316	-0.788405
C	0.385968	-0.610275	0.542297	C	1.007473	4.842453	-2.367725
C	-1.932459	5.188857	-2.030610	H	0.888095	-0.512057	-2.979565
H	2.201766	0.921519	-4.541863	H	2.224145	3.372148	-4.210524
H	-3.157616	5.501614	0.299742	H	-3.337584	3.950704	2.219194
H	-2.313844	1.680896	2.058568	H	-2.893111	-0.859834	0.161454
H	-2.200029	-1.508259	-1.345150	H	-3.115095	0.026557	-1.370589
H	0.659488	-1.522190	-0.011017	H	1.302572	-0.038575	0.742651
H	-0.053534	-0.916913	1.503855	H	0.648399	5.127882	-1.370253
H	0.548033	5.512995	-3.107994	H	2.092304	5.018995	-2.394591
H	-1.363144	6.118783	-1.890002	H	-2.985792	5.469192	-2.172484
H	-1.582610	4.707577	-2.951592	Br	0.998819	1.961058	3.210612
B	1.342237	3.191609	1.795289	Br	0.643149	4.954921	1.881180
Br	2.469292	2.682405	0.350183	Br	-0.025488	-3.341024	-2.435056
B	-0.305156	-4.546329	-0.986903	Br	0.434611	-6.292126	-1.057399
Br	-1.326635	-3.998119	0.517114				

IM-1**[BBr_3]



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#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
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Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.428873 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16402.122618 Hartree

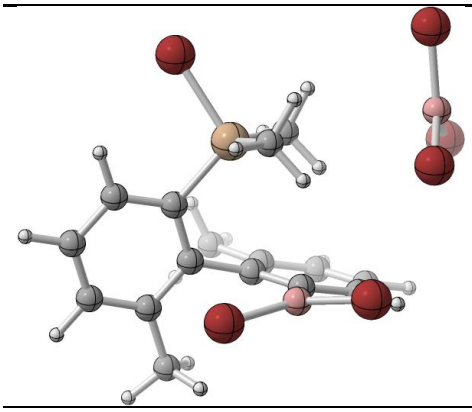
Sum of electronic and thermal Energies = -16402.092288 Hartree

Sum of electronic and thermal Enthalpies = -16402.091344 Hartree

Sum of electronic and thermal Free Energies = -16402.190909 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.103254	2.576942	-1.724642	C	0.350691	1.186652	-1.680997
C	1.260133	0.617016	-2.568934	C	1.914576	1.431169	-3.493141
C	1.714786	2.810557	-3.478339	C	0.828305	3.420467	-2.583839
C	-0.885911	2.996467	-0.705639	C	-0.748163	2.319749	0.573440
Si	-0.465370	0.469374	-0.151252	C	-2.004904	3.795762	-0.991926
C	-3.002999	3.887764	-0.013118	C	-2.954219	3.195750	1.201240
C	-1.851932	2.418397	1.481217	C	-2.213180	-0.155990	-0.428376
C	0.583159	-0.720844	0.819910	C	0.801093	4.922273	-2.466682
C	-2.238402	4.465384	-2.320648	H	1.490589	-0.449680	-2.525365
H	2.626209	0.996949	-4.197255	H	2.301245	3.444095	-4.147929
H	-3.885027	4.494197	-0.237497	H	-3.775384	3.279387	1.912933
H	-1.778976	1.903672	2.441002	H	-2.678654	-0.431024	0.530356
H	-2.214397	-1.043738	-1.076560	H	-2.825376	0.625008	-0.903594
H	0.732068	-1.615969	0.193980	H	1.558443	-0.279321	1.061873
H	0.088390	-1.025092	1.752590	H	1.831532	5.303850	-2.469445
H	0.337095	5.243957	-1.524774	H	0.270592	5.392964	-3.307811
H	-3.311191	4.478940	-2.554362	H	-1.711928	3.944818	-3.130175
H	-1.888527	5.507554	-2.306637	Br	0.749077	1.774206	3.223949
B	0.701892	2.790302	1.474433	Br	0.456687	4.774868	1.804851
Br	2.430307	2.488925	0.500574	Br	-0.308641	-2.788357	-2.552873
B	-0.862089	-4.214325	-1.413687	Br	-0.740210	-6.006297	-2.017334
Br	-1.537242	-3.826529	0.318945				

IM-2**[BBr_3]



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.480013 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16402.172949 Hartree

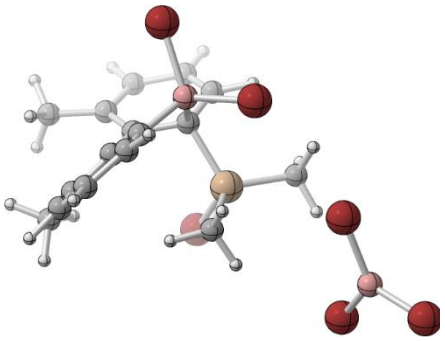
Sum of electronic and thermal Energies = -16402.142337 Hartree

Sum of electronic and thermal Enthalpies = -16402.141393 Hartree

Sum of electronic and thermal Free Energies = -16402.241687 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.580044	1.657105	0.237611	C	2.532897	0.895554	-0.959986
C	3.151395	-0.374029	-0.959603	C	3.806092	-0.864152	0.161323
C	3.849912	-0.095941	1.321895	C	3.241361	1.159992	1.379822
C	1.894193	2.979385	0.384125	C	2.657622	4.152261	0.227194
C	2.023898	5.387015	0.368583	C	0.664025	5.464558	0.660416
C	-0.077089	4.299914	0.829381	C	0.523577	3.036901	0.701925
Si	-0.554888	1.487475	0.854575	C	-1.318050	1.014960	-0.786726
C	0.222738	0.007637	1.698160	Br	-2.298380	2.062919	2.187863
B	1.873464	1.364343	-2.296545	Br	1.488172	3.173157	-2.778438
Br	1.432825	0.067291	-3.663169	C	3.255372	1.946729	2.665457
C	4.110665	4.074364	-0.161439	H	3.121037	-0.985025	-1.861501
H	4.275871	-1.847960	0.133329	H	4.352347	-0.483283	2.211234
H	2.605967	6.301614	0.235052	H	0.181359	6.437674	0.762421
H	-1.138051	4.372840	1.075586	H	-1.762360	1.895779	-1.272080
H	-2.104695	0.262368	-0.628508	H	-0.570456	0.579035	-1.466953
H	0.690557	0.280352	2.654925	H	0.982131	-0.464242	1.056511
H	-0.579692	-0.716802	1.908379	H	3.731194	2.929358	2.532886
H	3.794556	1.401829	3.450655	H	2.231760	2.147138	3.016010
H	4.564720	5.073113	-0.188314	H	4.214688	3.622469	-1.160668
H	4.689766	3.446737	0.531850	Br	0.259977	-2.468697	-1.236395
B	0.069477	-3.211536	0.501804	Br	1.613466	-3.608281	1.539329
Br	-1.662537	-3.557437	1.204559				

IM-3**[BBr_3]



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.456788 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16402.149370 Hartree

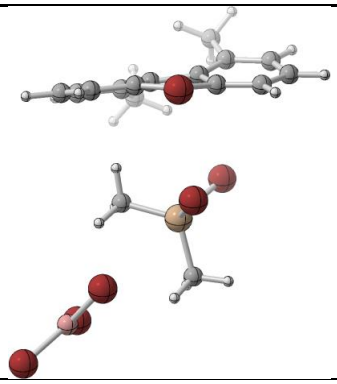
Sum of electronic and thermal Energies = -16402.119231 Hartree

Sum of electronic and thermal Enthalpies = -16402.118286 Hartree

Sum of electronic and thermal Free Energies = -16402.217877 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.071026	1.784412	0.725151	C	3.039844	1.073779	-0.495317
C	3.891105	-0.010687	-0.684317	C	4.750563	-0.383327	0.349247
C	4.725015	0.287171	1.574670	C	3.879722	1.379434	1.802311
C	2.070637	2.866114	0.658645	C	2.249910	4.204077	1.046492
C	1.271159	5.118711	0.645628	C	0.160246	4.780787	-0.144719
C	0.009127	3.478322	-0.557150	C	0.938645	2.469599	-0.152100
Si	-0.076602	1.030290	0.695357	C	-1.768381	0.889850	-0.077827
C	0.831982	-0.566849	0.992246	Br	-0.455205	1.874822	2.777359
B	1.911768	1.668948	-1.448316	Br	2.594436	3.150656	-2.636987
Br	0.875070	0.323320	-2.538376	C	3.777508	1.977108	3.182372
C	3.489348	4.706702	1.736091	H	3.865824	-0.569883	-1.622038
H	5.426824	-1.230055	0.218448	H	5.355349	-0.068399	2.393080
H	1.413323	6.168478	0.917228	H	-0.542962	5.554558	-0.452126
H	-0.822307	3.197252	-1.208593	H	-2.348065	1.804561	0.107620
H	-2.293890	0.048153	0.397810	H	-1.701489	0.699339	-1.157791
H	1.712035	-0.412416	1.631305	H	1.142590	-1.034474	0.049220
H	0.126650	-1.233475	1.513667	H	3.852922	1.184485	3.939382
H	2.815684	2.487853	3.325687	H	4.586350	2.696096	3.379681
H	3.700551	5.738716	1.427374	H	4.355948	4.084589	1.477758
H	3.378727	4.700051	2.829718	Br	-1.224269	-2.501490	-1.305028
B	-2.258978	-3.447257	-0.026767	Br	-2.979096	-5.154882	-0.437276
Br	-2.577634	-2.676450	1.689417				

Me_2-Br-DBB[BBr_3]



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#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm
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Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.477168 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -16402.170240 Hartree

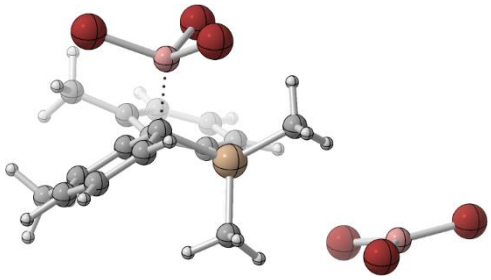
Sum of electronic and thermal Energies = -16402.139160 Hartree

Sum of electronic and thermal Enthalpies = -16402.138215 Hartree

Sum of electronic and thermal Free Energies = -16402.242818 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.997623	2.353610	0.936085	C	3.270337	1.764045	-0.331788
C	3.959644	0.566061	-0.442999	C	4.374330	-0.088099	0.723544
C	4.007729	0.430028	1.958462	C	3.277927	1.630558	2.103383
C	2.278909	3.662822	0.736908	C	2.099891	4.750398	1.599382
C	1.266612	5.795791	1.149558	C	0.701852	5.819238	-0.119189
C	1.031028	4.811856	-1.032175	C	1.824807	3.756867	-0.608763
B	2.522920	2.617909	-1.396188	Br	2.585420	2.395056	-3.294317
C	2.734537	1.959999	3.471402	C	2.820821	4.937789	2.910992
H	4.154762	0.138146	-1.429129	H	4.931698	-1.024262	0.669236
H	4.254190	-0.130779	2.863855	H	1.088206	6.635743	1.826173
H	0.059424	6.650064	-0.413921	H	0.684823	4.853813	-2.067496
H	3.446010	2.519773	4.094782	H	2.501326	1.025383	4.000960
H	1.807741	2.541163	3.392689	H	2.206572	4.661933	3.780026
H	3.093241	5.996143	3.025299	H	3.744524	4.347992	2.941671
Si	-0.851310	0.536937	0.630529	C	-2.575828	-0.143549	0.787848
C	0.529469	-0.544513	1.240791	Br	-0.800781	2.478076	1.752168
Br	-0.471661	0.999957	-1.531688	H	-3.302318	0.601660	0.435801
H	-2.790547	-0.377228	1.841210	H	-2.681769	-1.059079	0.188413
H	1.496468	-0.066993	1.026161	H	0.494758	-1.518350	0.731594
H	0.438596	-0.701834	2.326135	Br	-0.934087	-2.778844	-1.626527
B	-1.286694	-4.189378	-0.402859	Br	-1.360270	-5.987461	-1.001723
Br	-1.564849	-3.788116	1.439068				

TS-1**[BBr_3]



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#p m062x/def2svp opt=(calcfc,ts,noeigen)
freq empiricaldispersion=gd3 nosymm
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Charge = 0, Multiplicity = 1, Point group = C1

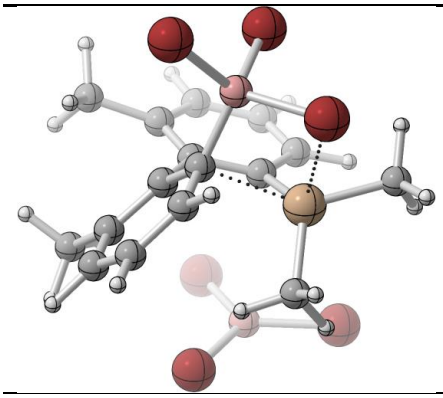
Electronic Energy = -16402.428683 Hartree

Number of imaginary frequencies = 1, vi = -7.70 cm^{-1}
Sum of electronic and zero-point Energies = -16402.122493 Hartree

Sum of electronic and thermal Energies = -16402.093070 Hartree
Sum of electronic and thermal Enthalpies = -16402.092125 Hartree
Sum of electronic and thermal Free Energies = -16402.187824 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.017981	2.565111	-1.763866	C	0.234476	1.169047	-1.745988
C	1.121054	0.593220	-2.652832	C	1.786852	1.408382	-3.568095
C	1.621714	2.791827	-3.525620	C	0.757031	3.406560	-2.613226
C	-0.958232	2.988367	-0.734091	C	-0.834088	2.283481	0.531377
Si	-0.583520	0.443524	-0.221684	C	-2.057965	3.820633	-1.000766
C	-3.050580	3.917751	-0.016861	C	-3.016221	3.200404	1.183331
C	-1.933305	2.390157	1.444064	C	-2.338448	-0.159347	-0.499220
C	0.460222	-0.776695	0.720469	C	0.767806	4.906151	-2.468083
C	-2.279397	4.522099	-2.315036	H	1.321673	-0.480240	-2.633807
H	2.480498	0.969972	-4.287402	H	2.218275	3.423209	-4.188302
H	-3.917721	4.550493	-0.226131	H	-3.833321	3.290168	1.898925
H	-1.870974	1.853854	2.392727	H	-2.805093	-0.437892	0.457953
H	-2.352764	-1.041134	-1.155780	H	-2.941982	0.633910	-0.965186
H	0.641795	-1.637523	0.055918	H	1.425130	-0.335435	1.000901
H	-0.048094	-1.132341	1.627192	H	1.807471	5.261851	-2.469935
H	0.317369	5.221514	-1.517458	H	0.244634	5.405722	-3.297023
H	-3.352403	4.567484	-2.543600	H	-1.769616	4.004309	-3.136925
H	-1.902931	5.554521	-2.282225	Br	0.657648	1.668916	3.170054
B	0.625879	2.716856	1.439306	Br	0.416358	4.698578	1.804193
Br	2.345528	2.401721	0.454393	Br	-0.486035	-2.857641	-2.625762
B	-0.564707	-4.117984	-1.195660	Br	0.591012	-5.619234	-1.195611
Br	-1.798126	-3.852506	0.224392				

TS-2**[BBr_3]



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#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
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Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.420245 Hartree

Number of imaginary frequencies = 1, vi = -139.49 cm^{-1}

Sum of electronic and zero-point Energies = -16402.114020 Hartree

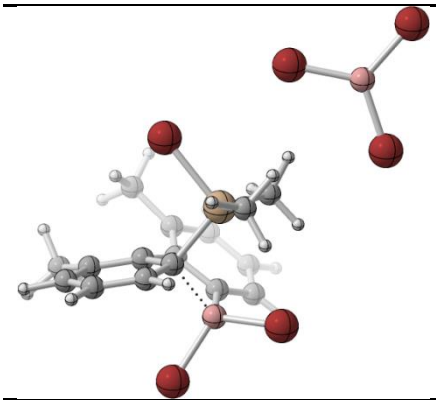
Sum of electronic and thermal Energies = -16402.084550 Hartree

Sum of electronic and thermal Enthalpies = -16402.083605 Hartree

Sum of electronic and thermal Free Energies = -16402.177675 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.611971	-1.481407	-0.388292	C	0.274632	-2.376723	0.644192
C	0.972180	-3.583357	0.779076	C	1.978090	-3.897164	-0.127513
C	2.321107	-2.988574	-1.129638	C	1.660200	-1.765842	-1.279321
C	-0.188242	-0.234494	-0.347860	C	-0.302920	0.413043	0.921184
Si	-0.839617	-1.691243	1.980747	C	-1.013618	0.126327	-1.437778
C	-1.995090	1.096675	-1.228991	C	-2.175943	1.706994	0.014794
C	-1.343923	1.371046	1.064054	C	-2.668511	-1.416415	1.778452
C	-0.470617	-2.645114	3.539573	Br	-0.029034	0.519130	3.890438
B	0.921459	0.689540	2.020447	Br	1.553442	2.585314	1.777151
Br	2.519872	-0.525289	2.043444	C	2.161841	-0.763670	-2.285120
C	-0.919576	-0.528906	-2.792341	H	0.745834	-4.272146	1.595239
H	2.522129	-4.838522	-0.038329	H	3.156967	-3.216601	-1.795617
H	-2.659558	1.354959	-2.057397	H	-2.961402	2.451135	0.151010
H	-1.455711	1.883568	2.020639	H	-3.005989	-0.767591	2.600336
H	-3.182267	-2.388082	1.860287	H	-2.918965	-0.945547	0.820710
H	-0.721865	-3.700244	3.328558	H	0.594076	-2.572395	3.798825
H	-1.076549	-2.292425	4.382538	H	1.897260	-1.056162	-3.312363
H	3.257256	-0.698662	-2.229990	H	1.756960	0.238155	-2.092312
H	-1.897495	-0.517423	-3.291344	H	-0.581043	-1.571973	-2.724890
H	-0.212292	0.012422	-3.438160	Br	-3.295976	-2.763066	-1.473720
B	-2.089684	-4.175147	-1.061049	Br	-0.742782	-4.661597	-2.299418
Br	-2.301431	-5.140760	0.572810				

TS-3**[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.456159 Hartree

Number of imaginary frequencies = 1, vi = -32.01 cm^{-1}

Sum of electronic and zero-point Energies = -16402.149572 Hartree

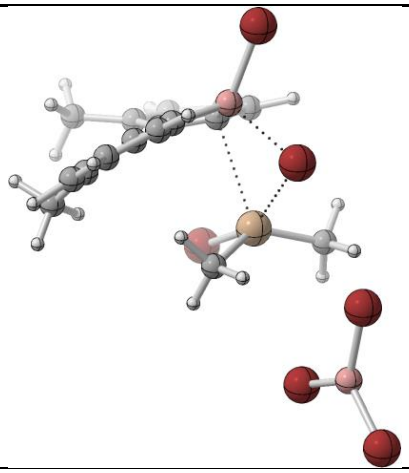
Sum of electronic and thermal Energies = -16402.119835 Hartree

Sum of electronic and thermal Enthalpies = -16402.118891 Hartree

Sum of electronic and thermal Free Energies = -16402.217289 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.808646	-0.171558	0.053442	C	1.893499	-0.789730	-1.212052
C	2.770533	-1.853828	-1.403070	C	3.543807	-2.292984	-0.328043
C	3.411535	-1.705372	0.932200	C	2.537011	-0.635634	1.160725
C	0.793744	0.899397	-0.017766	C	0.971198	2.229369	0.394650
C	0.033536	3.166108	-0.051814	C	-1.044829	2.843790	-0.888745
C	-1.213482	1.538032	-1.291948	C	-0.307786	0.521555	-0.868747
Si	-1.277114	-1.047183	-0.269249	C	-2.909690	-1.172481	-1.165159
C	-0.346081	-2.650763	-0.098745	Br	-1.795829	-0.450082	1.872152
B	0.861665	-0.136039	-2.229008	Br	1.568652	1.472304	-3.189250
Br	-0.083011	-1.375141	-3.487186	C	2.330845	-0.107732	2.557000
C	2.177959	2.695279	1.163142	H	2.833421	-2.345586	-2.376099
H	4.238060	-3.124861	-0.459258	H	3.981126	-2.107249	1.773433
H	0.183532	4.213050	0.225496	H	-1.722350	3.627413	-1.227722
H	-2.039900	1.271793	-1.955394	H	-3.550096	-0.311835	-0.928364
H	-3.422528	-2.084557	-0.827118	H	-2.758772	-1.237465	-2.251756
H	0.540747	-2.540044	0.539919	H	-0.043232	-3.039292	-1.080031
H	-1.036833	-3.362924	0.377663	H	2.342805	-0.935943	3.278787
H	1.364210	0.405583	2.650275	H	3.127046	0.593495	2.848519
H	2.008001	2.651284	2.248548	H	2.415924	3.734897	0.903565
H	3.051365	2.071482	0.931745	Br	-3.110092	-5.128994	-1.245235
B	-3.858219	-5.237182	0.501512	Br	-4.753050	-6.815830	1.058058
Br	-3.697794	-3.755966	1.682680				

TS-4**[BBr_3]



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
```

Charge = 0, Multiplicity = 1, Point group = C1

Electronic Energy = -16402.424420 Hartree

Number of imaginary frequencies = 1, vi = -141.69 cm^{-1}

Sum of electronic and zero-point Energies = -16402.117672 Hartree

Sum of electronic and thermal Energies = -16402.087876 Hartree

Sum of electronic and thermal Enthalpies = -16402.086932 Hartree

Sum of electronic and thermal Free Energies = -16402.185563 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	3.170782	1.683910	0.517734	C	3.280947	1.094399	-0.768681
C	4.211517	0.092444	-1.009291	C	5.004891	-0.370455	0.043344
C	4.805115	0.123929	1.329573	C	3.871612	1.136152	1.608680
C	2.112343	2.739036	0.499728	C	1.905982	3.850755	1.329025
C	0.755516	4.626544	1.091886	C	-0.125418	4.384319	0.040425
C	0.179051	3.382552	-0.878989	C	1.296863	2.571658	-0.658951
B	2.121580	1.669254	-1.688315	Br	2.604347	2.504695	-3.422153
C	3.570621	1.453303	3.052817	C	2.884934	4.329555	2.369591
H	4.296730	-0.345953	-2.006462	H	5.742212	-1.157333	-0.124710
H	5.362535	-0.311563	2.162534	H	0.567188	5.476912	1.752708
H	-1.001506	5.020222	-0.092771	H	-0.409550	3.256567	-1.792586
H	3.691290	0.543918	3.657610	H	2.536330	1.802651	3.170716
H	4.241262	2.215665	3.473819	H	2.921862	5.427559	2.355890
H	3.893821	3.953104	2.162582	H	2.603920	4.021888	3.387007
Si	-0.249755	0.385797	0.219749	C	-1.976230	0.293646	-0.479058
C	0.857132	-0.975915	0.842742	Br	-0.620804	1.588885	2.111182
H	-2.168617	1.227290	-1.028136	H	-2.704284	0.205981	0.337573
H	-2.063456	-0.548003	-1.179104	H	1.903727	-0.634091	0.798281
H	0.755444	-1.853420	0.189754	H	0.598869	-1.217796	1.881866
Br	0.702670	0.049187	-2.150306	Br	-1.076687	-3.326085	-1.623941
B	-1.980733	-3.956562	-0.072926	Br	-2.643443	-5.730344	-0.008244
Br	-2.215861	-2.799089	1.422670				

3. Results of IRC Analysis of Transition States

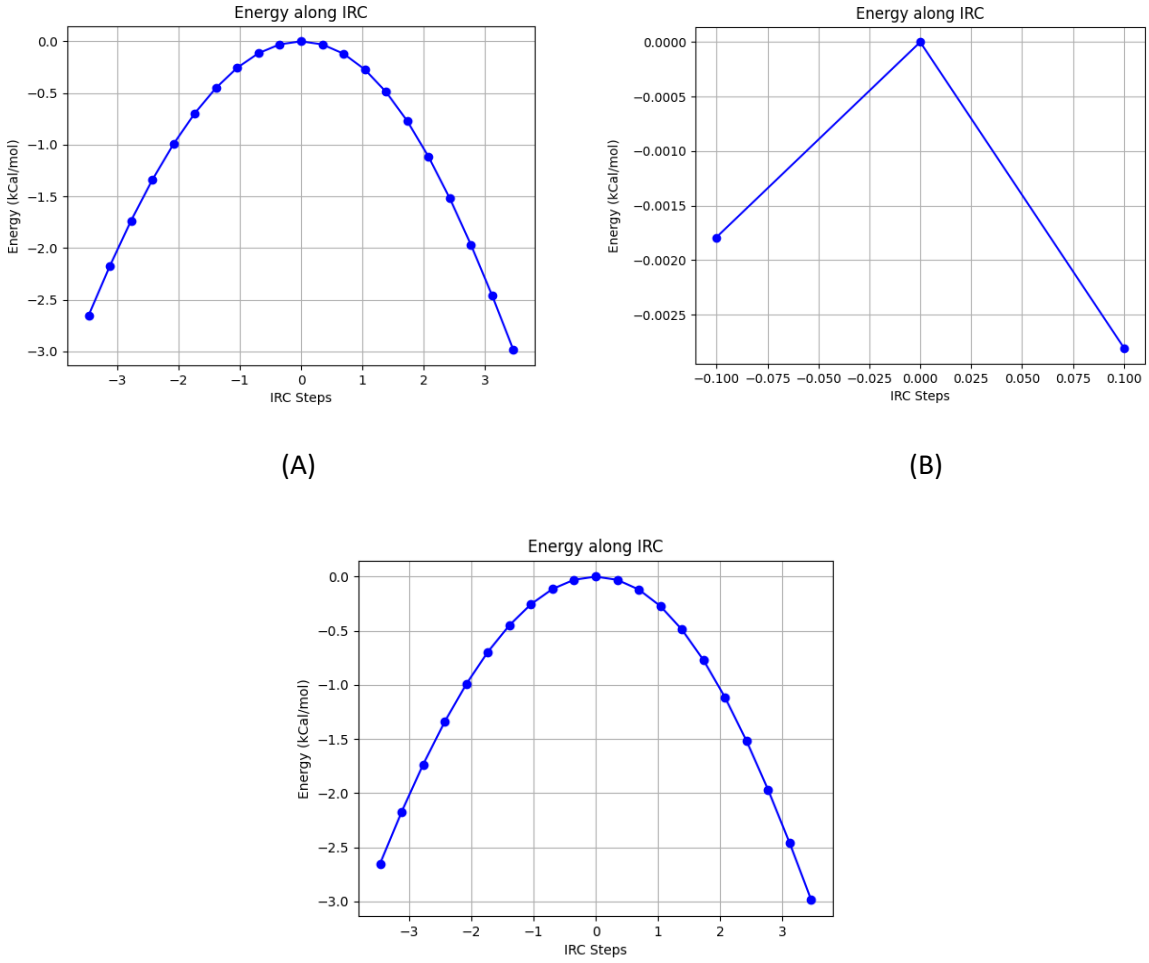
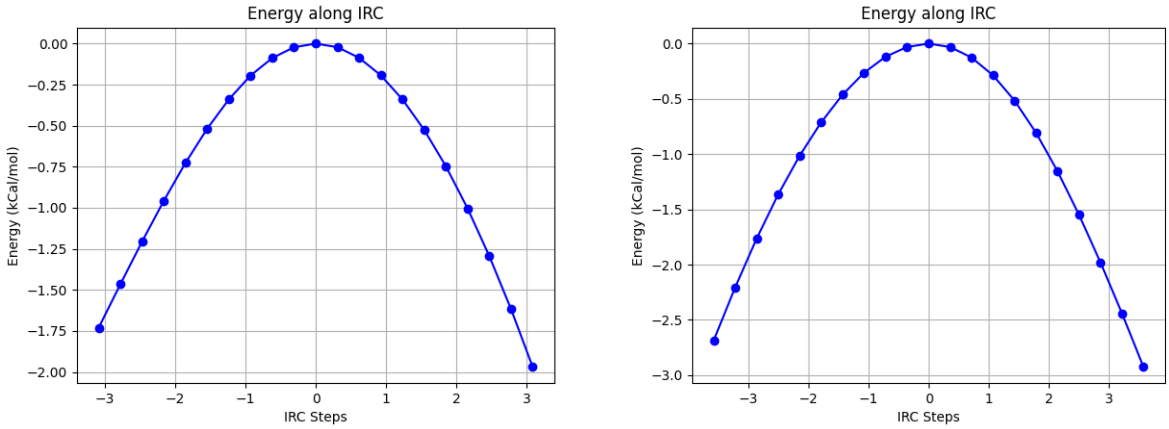
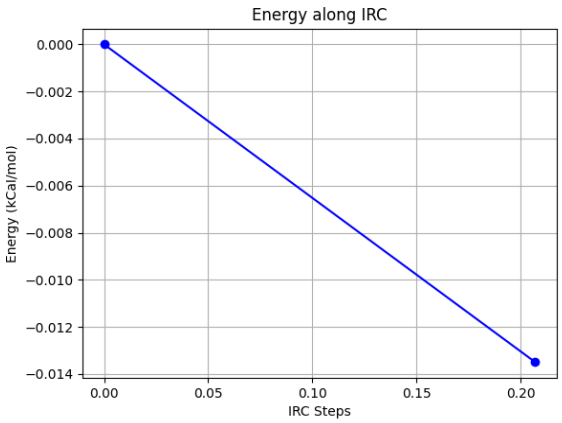


Figure S-1: IRC scan profiles for (A) **TS-2****, (B) **TS-3****, and (C) **TS-4****.

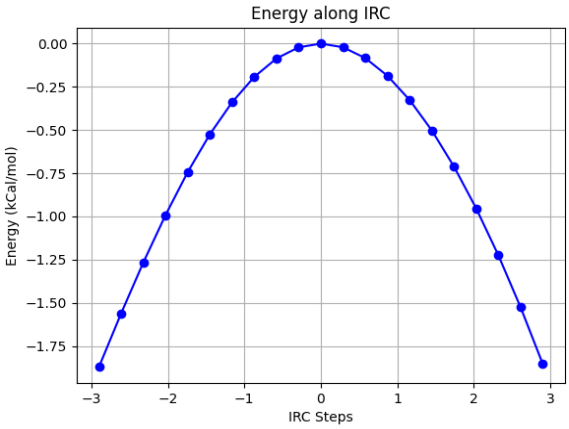


(A) (B)

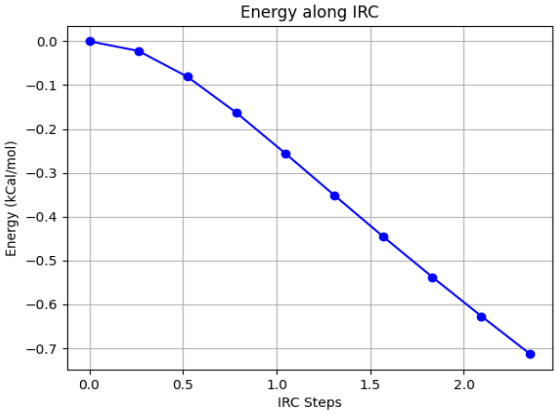
Figure S-2: IRC scan profiles for (A) **TS-2****[BBr_3] and (B) **TS-4****[BBr_3]



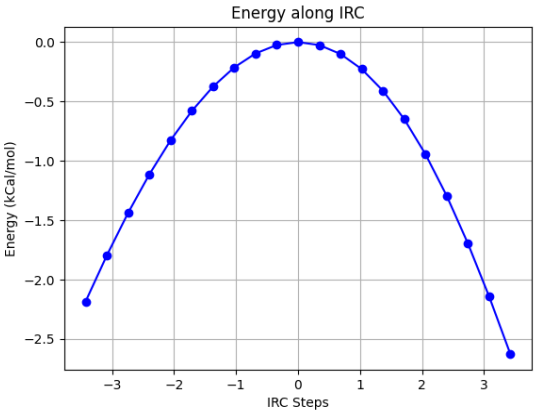
(A)



(B)



(C)



(D)

Figure S-3: IRC scan profiles for (A) **TS-1**, (B) **TS-2**, (D) **TS-3** , and (D) **TS-4**.

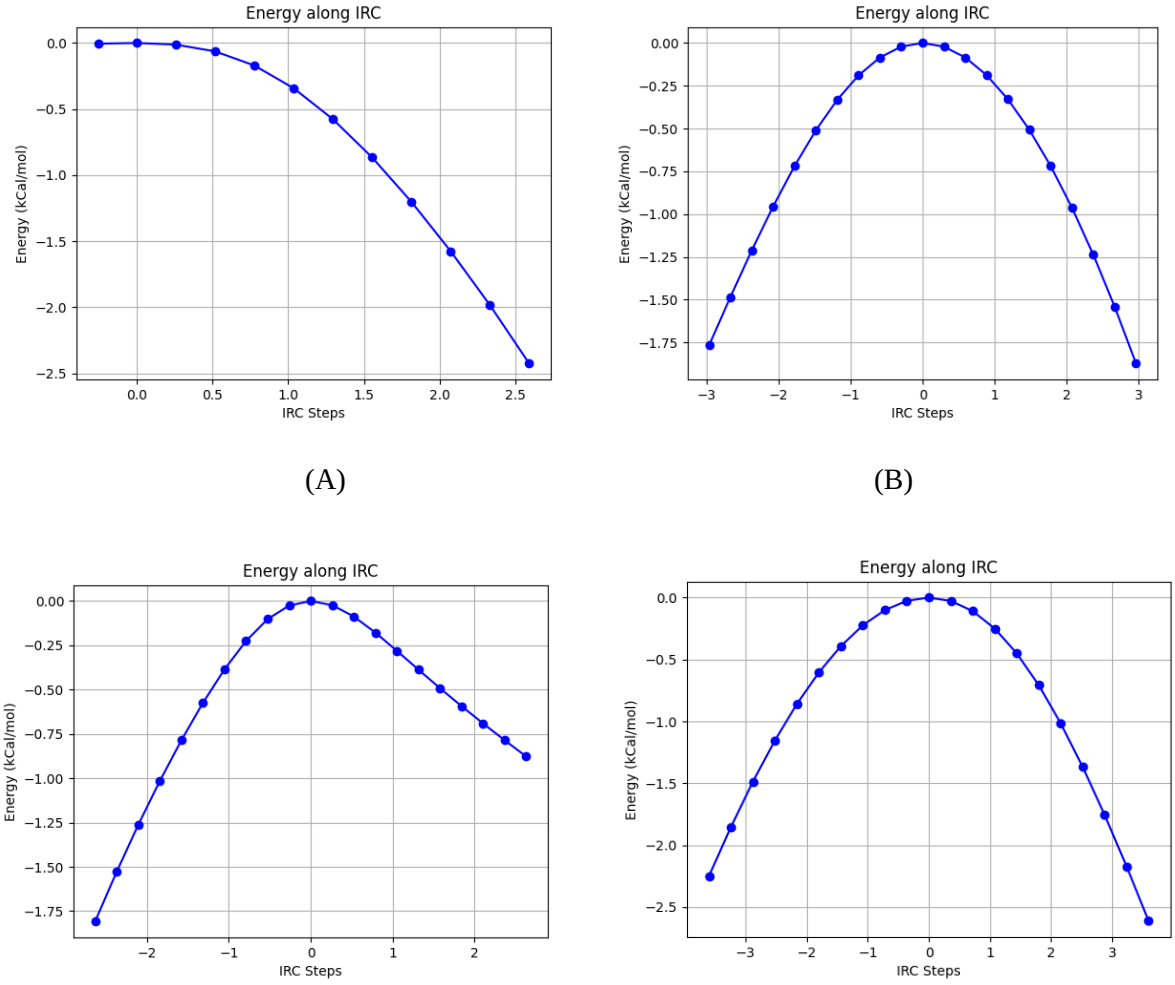
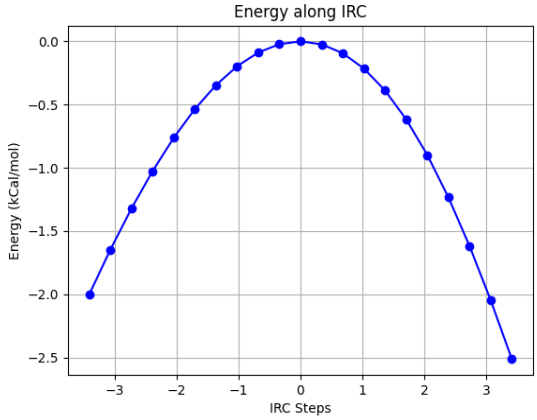
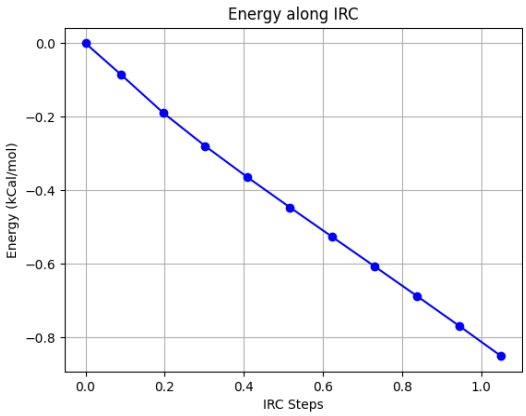


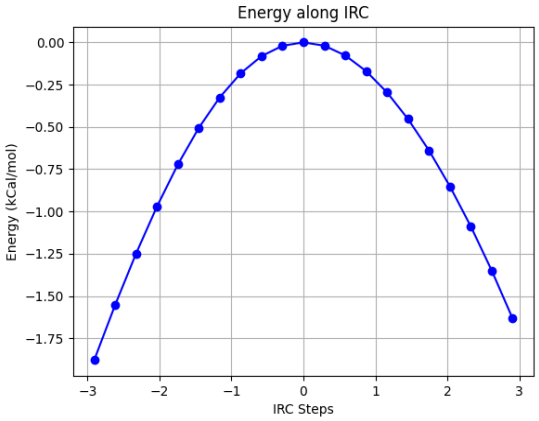
Figure S-4: IRC scan profiles for (A) **TS-1**[BBr_3], (B) **TS-2**[BBr_3], (C) **TS-3**[BBr_3], and (D) **TS-4**[BBr_3].



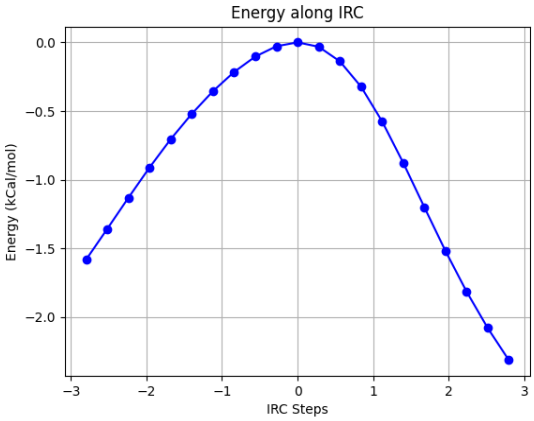
(A)



(B)

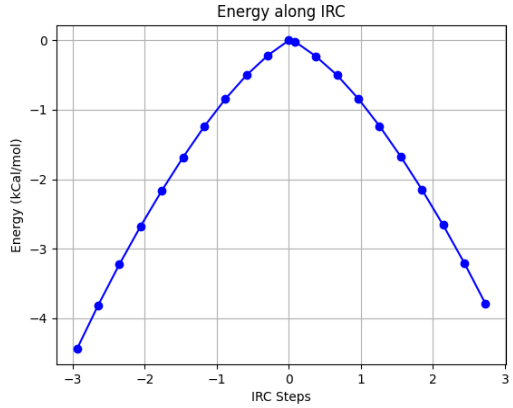


(C)

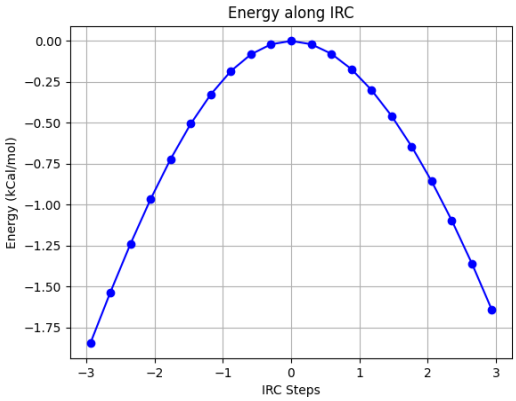


(D)

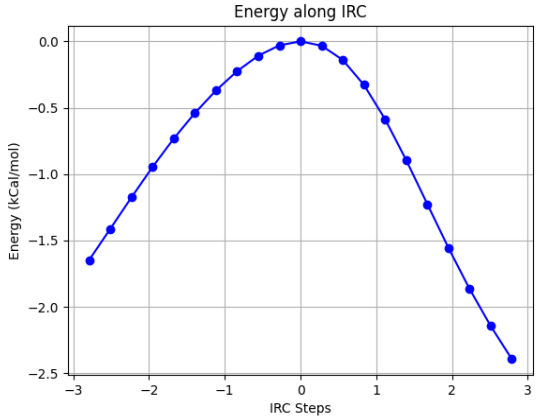
Figure S-5: IRC scan profiles for (A) **TS-1***, (B) **TS-2***, (C) **TS-3***, and (D) **TS-4***.



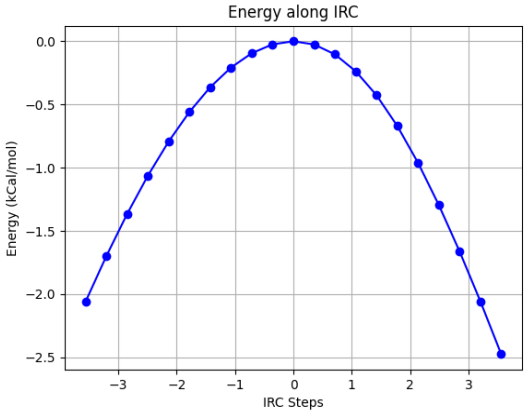
(A)



(B)



(C)

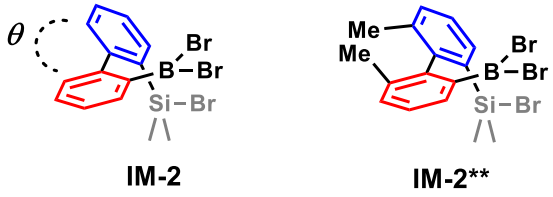


(D)

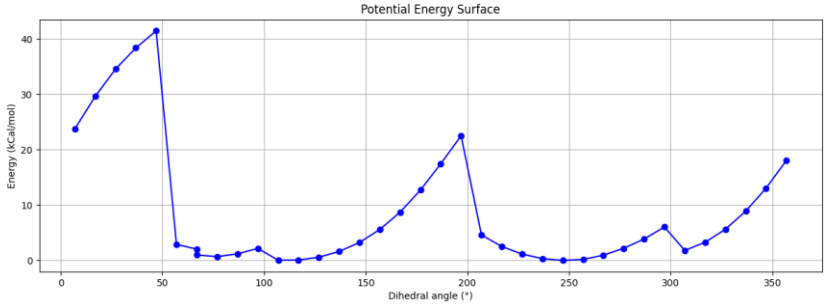
Figure S-6: IRC scan profiles for (A) **TS-1*[**BBr_3], (B) **TS-2*[**BBr_3], (C) **TS-3***[BBr_3], and (D) **TS-4***[BBr_3].

4. Rotational Potential Energy Surfaces of IM-2 and IM-2**

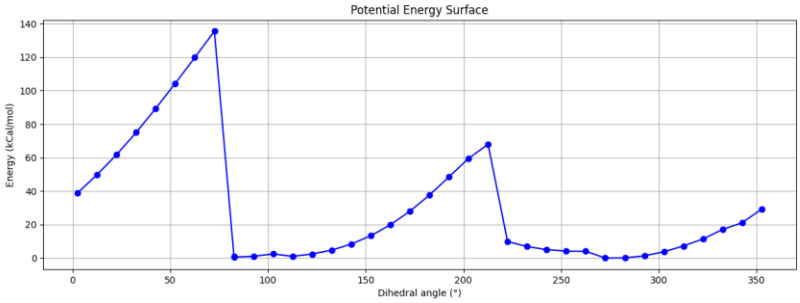
Relaxed scans were performed on **IM-2** and **IM-2**** using the method implemented in *Gaussian 16* program at the M06-2X-GD3/Def2-SVP level of theory to obtain the correlation between total energy and the dihedral angle (θ) of the biphenyl unit.



IM-2 IM-2**



(A)



(B)

Figure S-7: Results of relax scans showing the energy profiles of (A) **IM-2** and (B) **IM-2**** in relation to the biphenyl dihedral angle.

5. Results of NMR Analysis

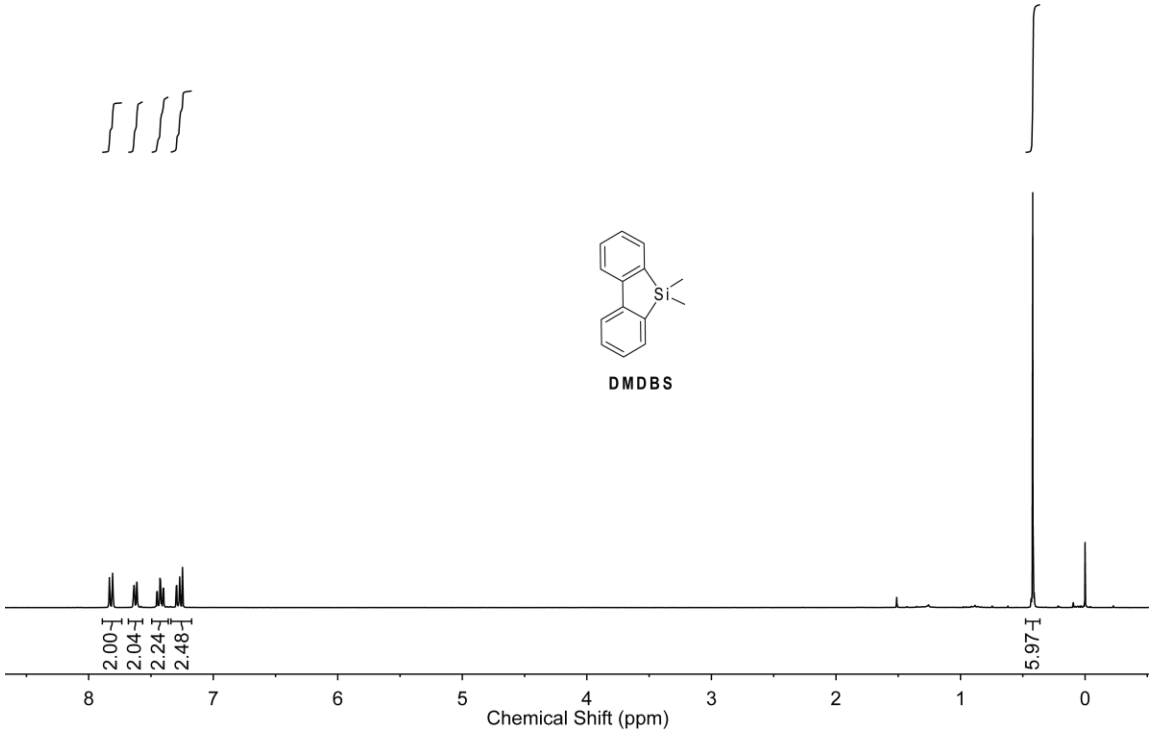


Figure S-8: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **DMDBS**.

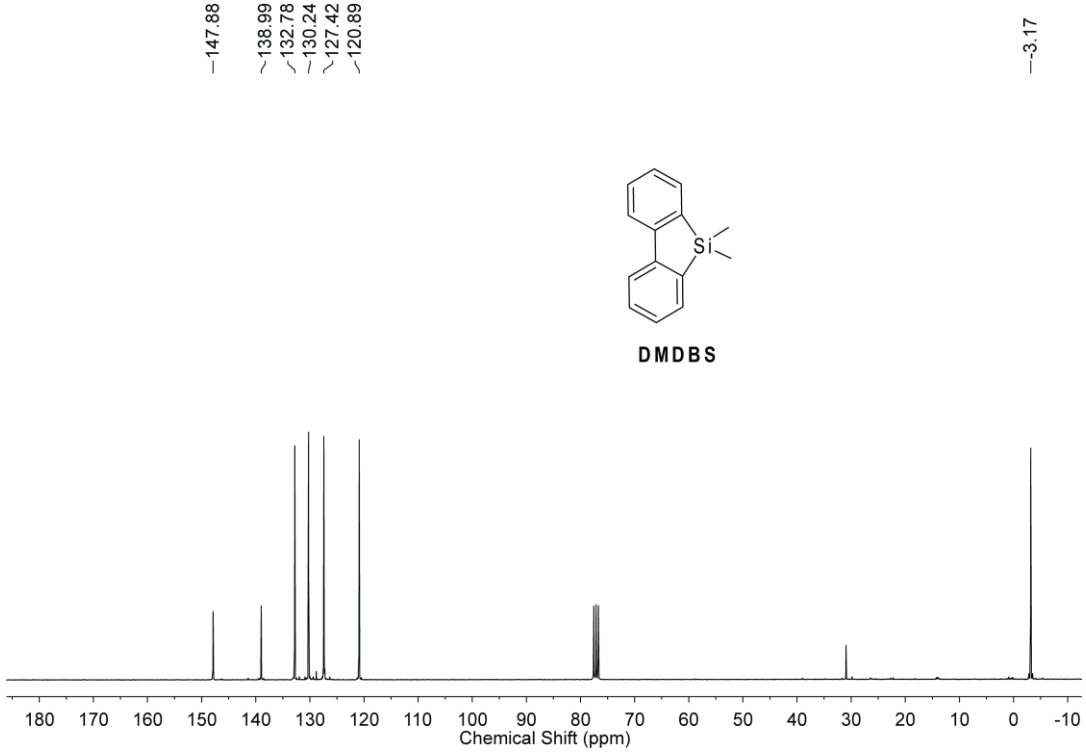


Figure S-9: ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **DMDBS**.

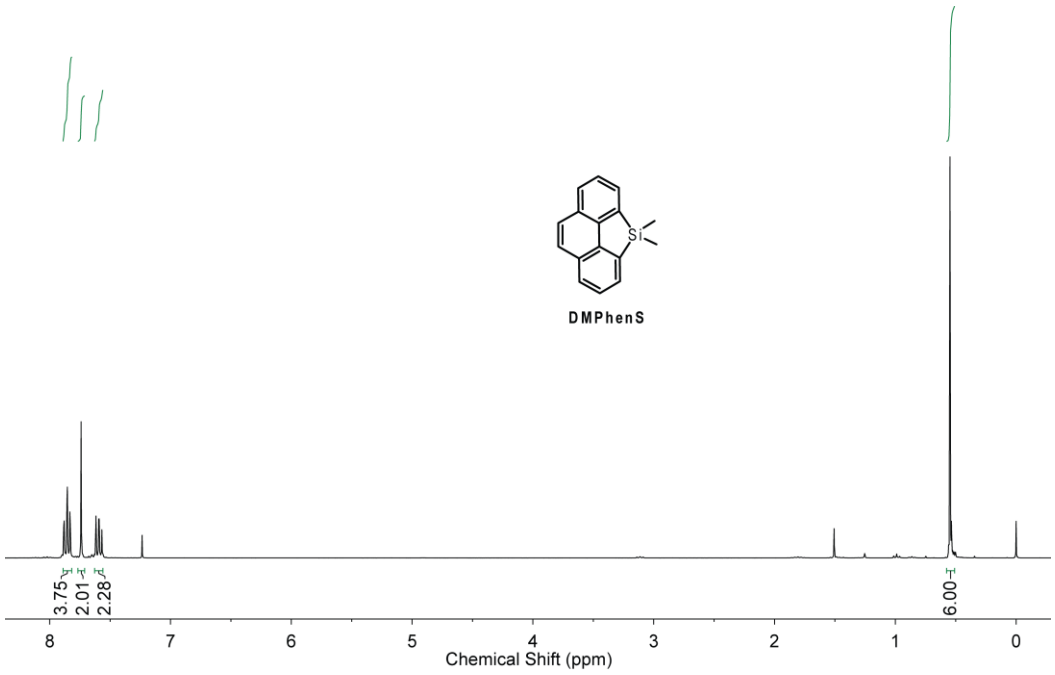


Figure S-10: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **DMPhenS**.

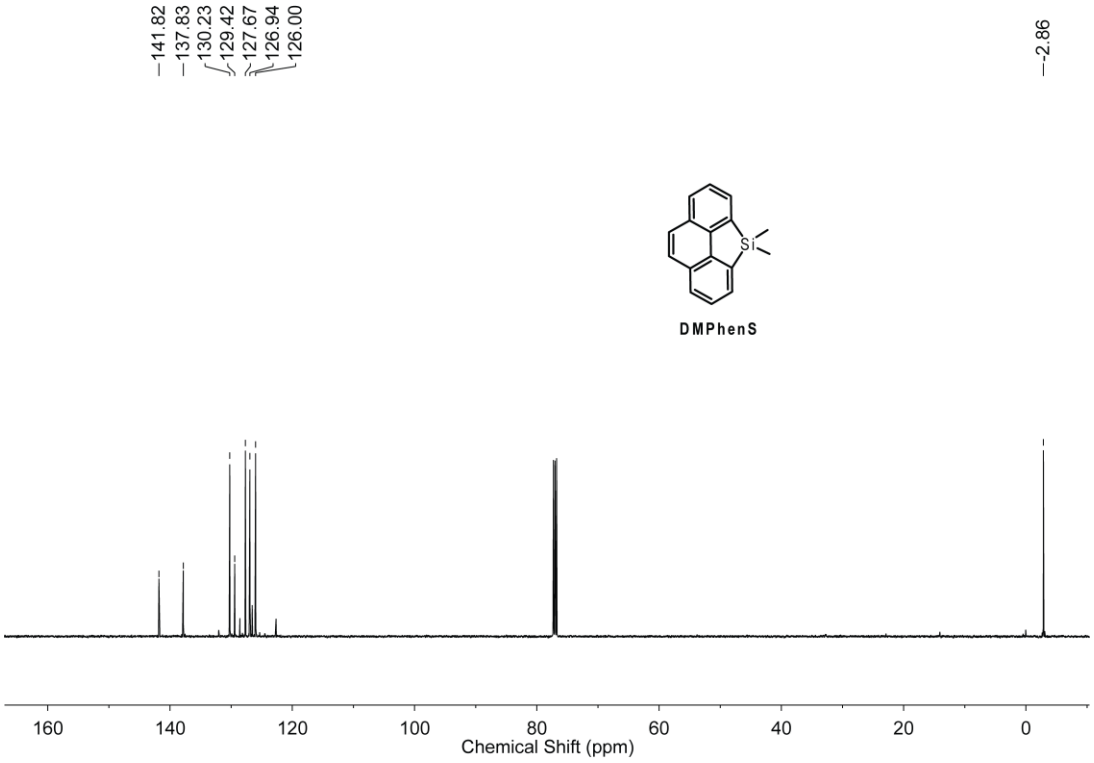


Figure S-11: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **DMPhenS**.

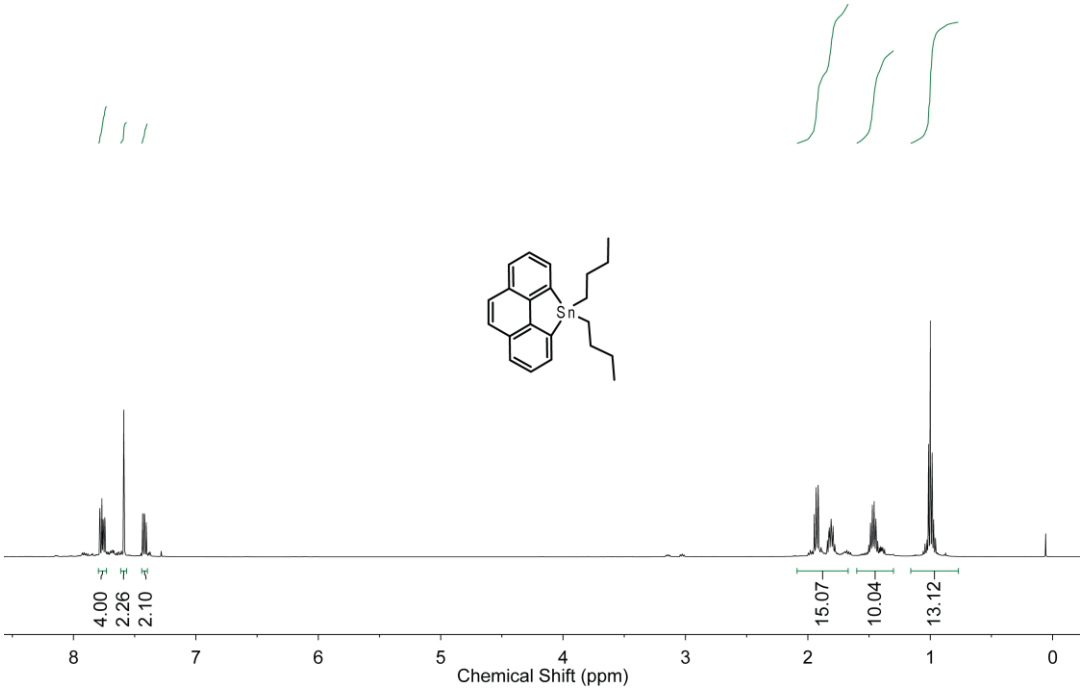


Figure S-12: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of 4,4-dibutyl-4*H*-phenanthro[4,5-*bcd*]stannole.

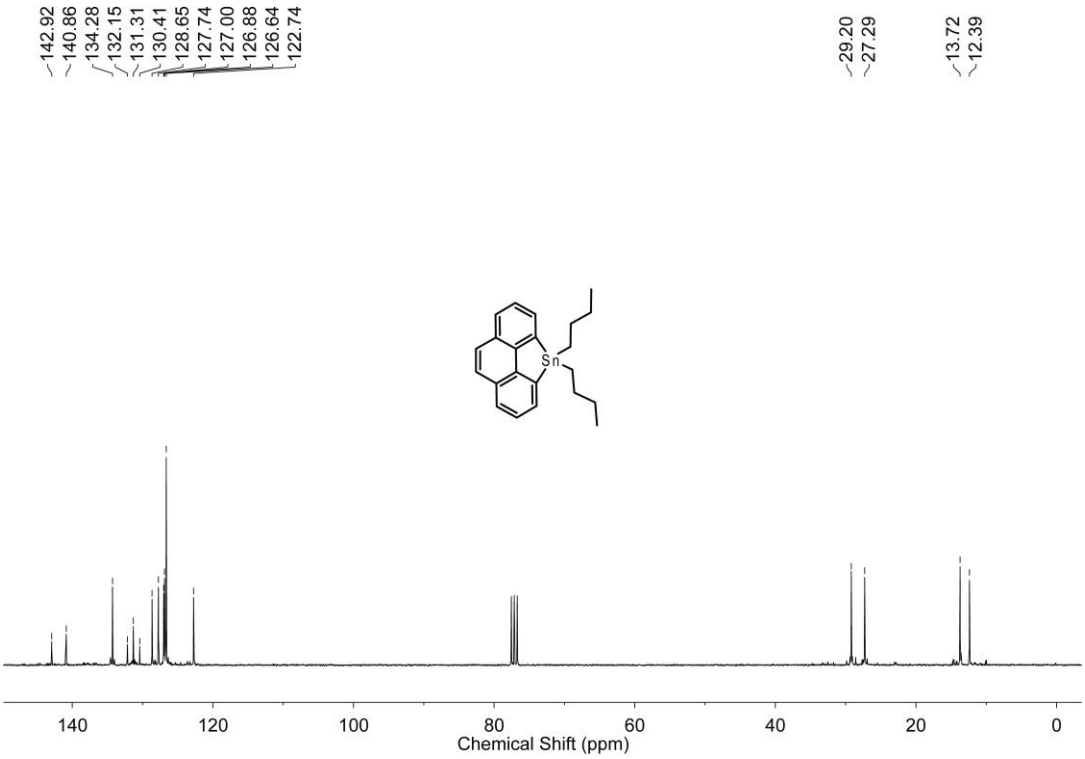


Figure S-13: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of 4,4-dibutyl-4*H*-phenanthro[4,5-*bcd*]stannole.

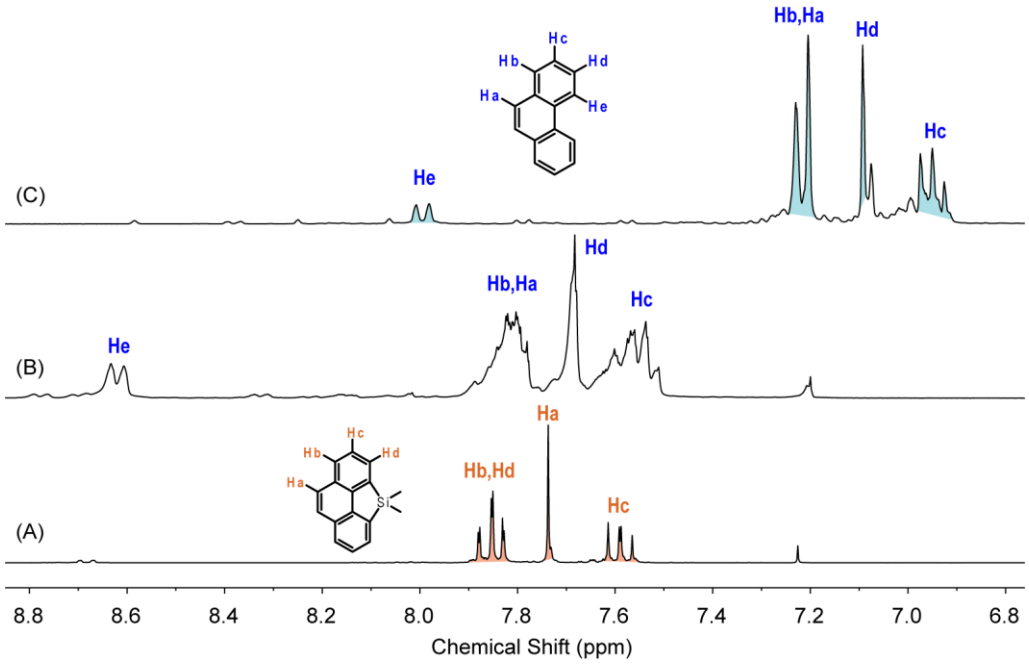


Figure S-14: ^{1}H NMR (500 MHz) spectra of (A) pure **DMPhenS** in $CDCl_3$, (B) **DMPhenS** reacted with excess BBr_3 in $CDCl_3$ at 50 °C for 12 hours, and (C) **DMPhenS** reacted with excess BBr_3 (neat) at 50 °C for 12 hours.

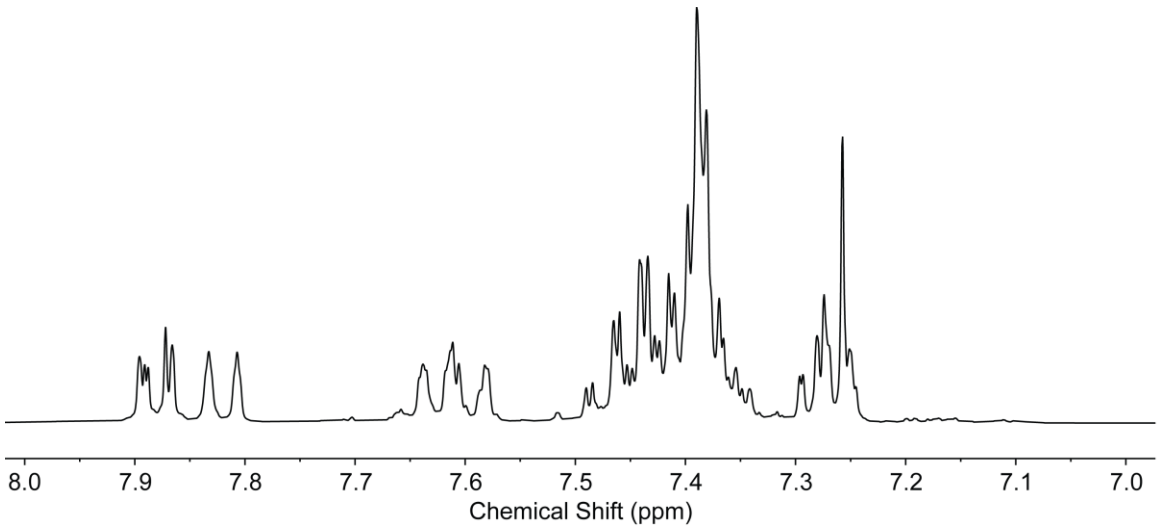


Figure S-15: ^{1}H NMR (300 MHz, $CDCl_3$) spectrum measured after the 1:1 (mole ratio) mixture of **DMDBS** and BBr_3 was heated at 50 °C for 48 hours.

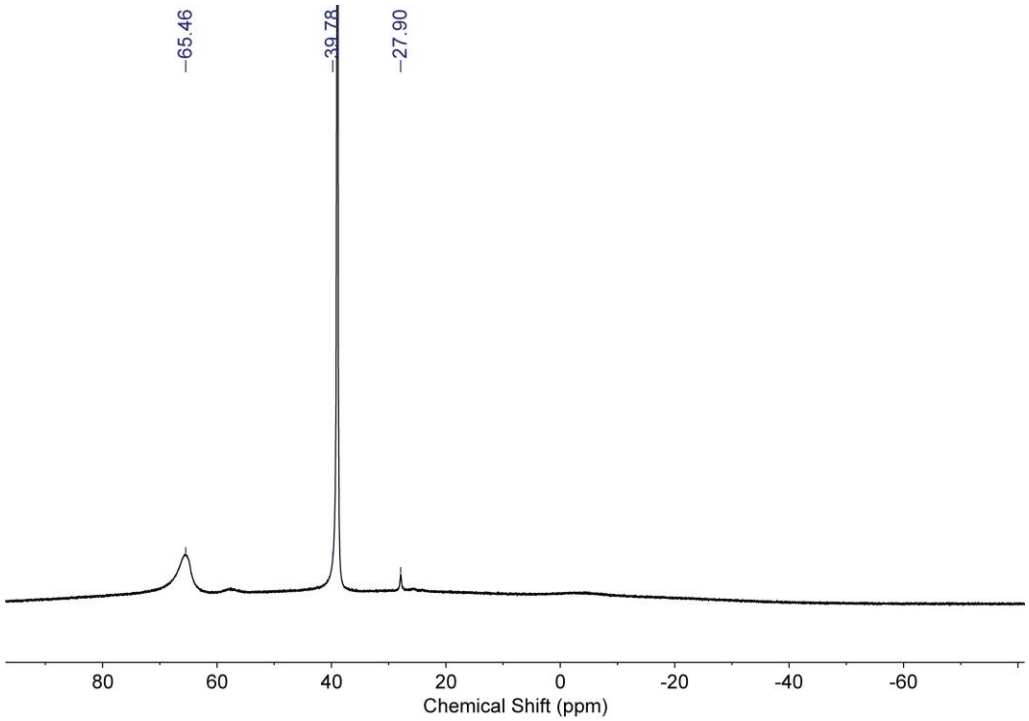


Figure S-16: ^{11}B NMR (160 MHz, $CDCl_3$) of the reaction mixture after mixing 4,4-dibutyl-4*H*-phenanthro[4,5-*bcd*]stannole with BBr_3 at room temperature for 20 min. The signal at 65.46 ppm is due to **Br-PhenB**. The signal at 39.78 ppm is due to BBr_3 and the small peak at 27.90 ppm is likely due to a boronic / boronate byproduct(s).

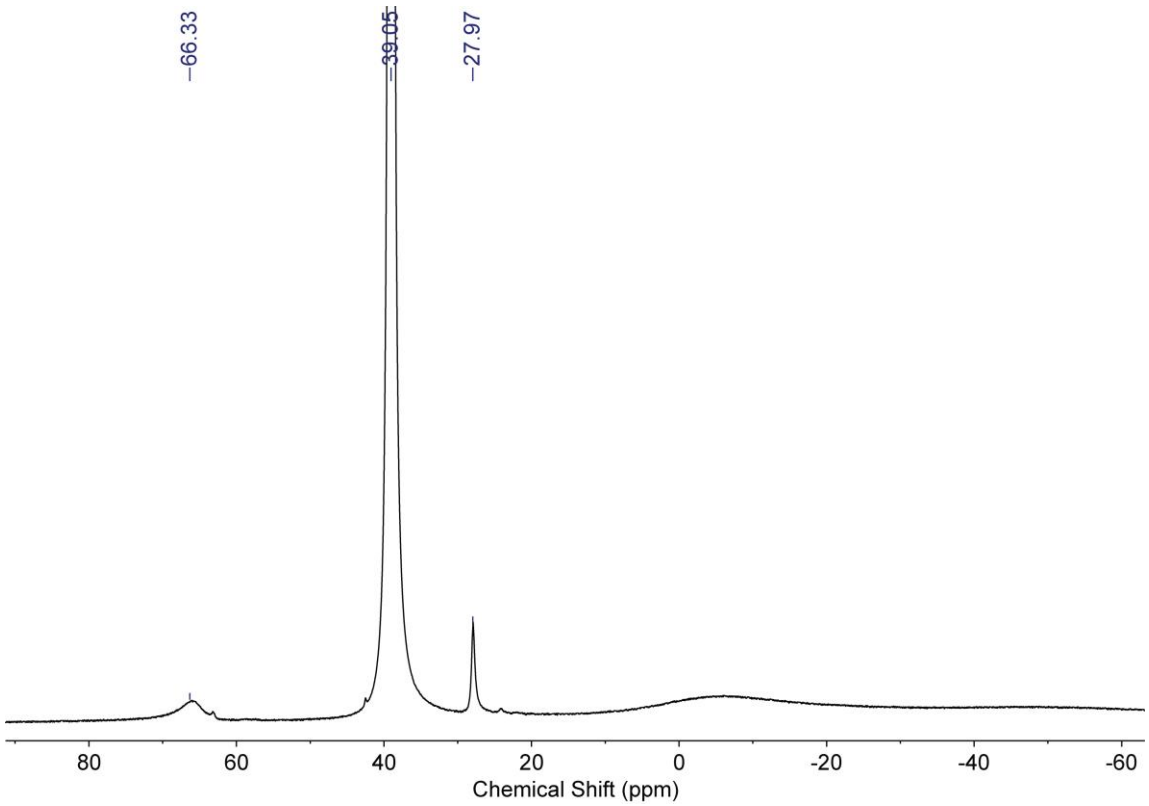


Figure S-17: ^{11}B NMR (96 MHz, $CDCl_3$) of the reaction mixture after mixing **DMDBS** with BBr_3 (1: 50 mole ratio) at 50 °C for 48 h. The signal at 66.33 ppm is due to **Br-DBB**. The signal at 39.05 ppm is due to excess BBr_3 and the peak at 27.97 ppm is likely due to a boronic / boronate byproduct(s).