Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Unique Reactivity of B in $B[Ge_9Y_3]_3$(Y = H, CH_3, BO, CN): Formation of Lewis Base

G. Naaresh Reddy[a,e], R. Parida[a,e], R. Inostroza-Rivera[b], A. Chakraborty[c], Puru Jena[d],* and S Giri[a,*]

[a] School of Applied Sciences and Humanities, Haldia Institute of Technology, Haldia, India, 721657

[b]Facultad de Ciencias de la Salud, Universidad Arturo Prat, Casilla 121, 1110939 Iquique, Chile.

[c]Faculty of Science, Jatragachi Pranabananda High School, New Town, Kolkata, 700161, India

[d]Department of Physics, Virginia Commonwealth University, Richmond VA, USA

[e] Department of Chemistry, National Institute of Technology Rourkela, Rourkela, Odisha, 769008, India

Corresponding Authors:

E-mails: santanab.giri@gmail.com , pjena@vcu.edu

Theoretical Details:

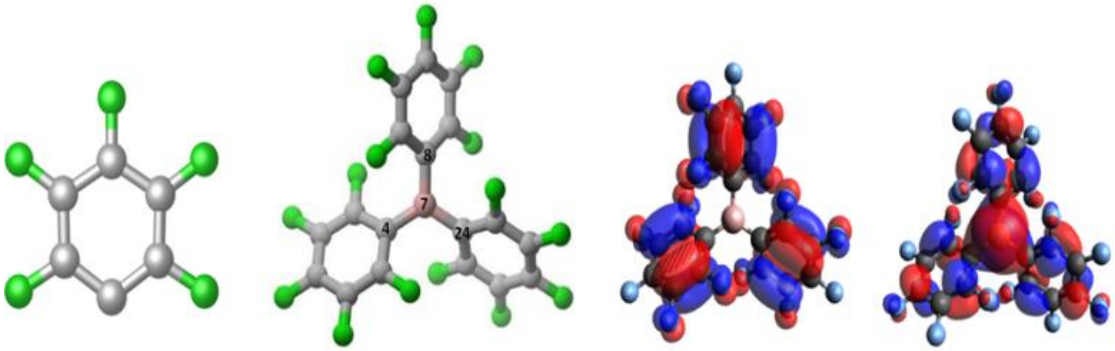
By using first principles calculations based on density functional theory we have employed B3LYP, PBE, AIM and wB97XD level of theories and SDD, 6-31+G(d,p) and Def2-TZVPP as basis sets to optimized all the ground state geometries of all the studied molecules. Also we have performed AdNDP technique in B3LYP/SDD level to know the 2c-2e bond in $B[Ge_9H_3]_3$ and $BF_3[B(Ge_9H_3)_3]$. The ADMP simulation has been performed to know the dynamical stability of $B[Ge_9H_3]_3$ and $[Ge_9H_3]^+$ molecules in B3LYP/SDD level for $B[Ge_9H_3]_3$ and wB97XD/6-31+G(d,p) level of theory for $[Ge_9H_3]^+$. The NBO analysis is performed using B3LYP/SDD level for all the studied molecules but for $B(C_6F_5)_3$ case we have used wB97XD/6-31+g(d,p) level of theory.

The dual descriptor calculation performed to know the reactivity in studied molecules. The reactivity we can understood by Fukai functions it is represented with $\Delta f(r)$ is the result of the variation of the hardness when the external potential changes. The $\Delta f(r)$ is defined as

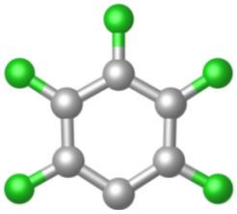
$$\Delta f(r) = [f^+(r)-f^-(r)] \sim \rho^{LUMO}(r)-\rho^{HOMO}(r)$$

If $\Delta f(r) > 0$, then the site is favored for a nucleophilic attack, whereas if $\Delta f(r) < 0$, then the site could hardly be susceptible to undertake a nucleophilic attack but it may be favored for an electrophilic attack.

S1. Optimized geometries of $[C_6F_5]$ and $[B(C_6F_5)_3]$, NBO charge on B atom, Wiberg bond index (WBI) of B-C bond and frontier MO's of $[B(C_6F_5)_3]$.

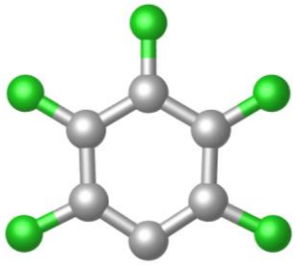


S2. Optimized geometries and cartesian coordinates of neutral, anion and cation of $[C_6F_5]$, $[C_6(BO)_5]$ and $[C_6(CN)_5]$ molecules.



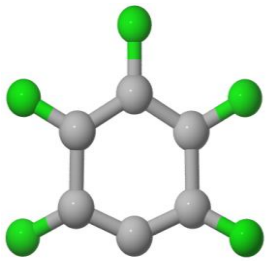
$[C_6F_5]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.196350	-0.992810	0.000105
2	6	0	1.237011	0.376590	-0.000479
3	6	0	0.000105	1.064785	-0.000400
4	6	0	-1.236853	0.376683	-0.000060
5	6	0	-1.196550	-0.992685	0.000167
6	6	0	-0.000154	-1.758726	0.000520
7	9	0	-2.353431	1.095502	-0.000069
8	9	0	-2.361667	-1.640135	0.000156
9	9	0	0.000075	2.373926	-0.000366
10	9	0	2.353741	1.095253	-0.000149
11	9	0	2.361342	-1.640437	0.000526



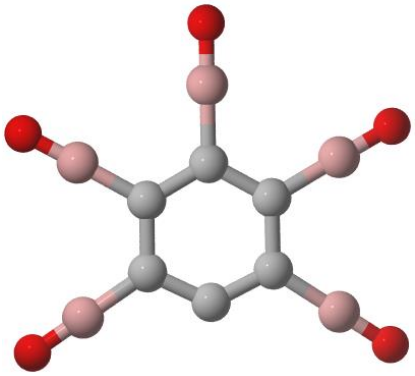
$[C_6F_5]^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.149291	-1.016110	-0.000002
2	6	0	-1.198581	0.374484	0.000015
3	6	0	-0.000001	1.077006	0.000015
4	6	0	1.198577	0.374485	0.000040
5	6	0	1.149296	-1.016112	0.000088
6	6	0	0.000002	-1.766003	0.000031
7	9	0	-2.363363	1.073972	-0.000005
8	9	0	-0.000003	2.430103	-0.000027
9	9	0	2.363363	1.073973	-0.000005
10	9	0	2.387917	-1.631605	-0.000063
11	9	0	-2.387916	-1.631610	-0.000025



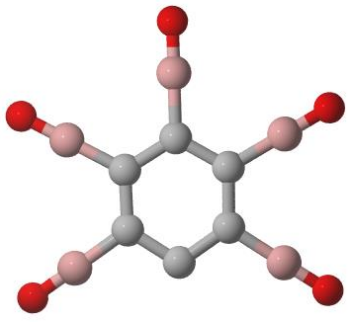
$[C_6F_5]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.222305	-1.061216	0.109027
2	6	0	-1.195233	0.398490	0.210103
3	6	0	0.000621	1.093343	0.000226
4	6	0	1.195830	0.397988	-0.210236
5	6	0	1.221365	-1.061767	-0.109086
6	6	0	-0.000696	-1.582808	-0.000835
7	9	0	2.321910	1.018186	-0.117205
8	9	0	2.345448	-1.615401	0.225245
9	9	0	0.000825	2.401980	0.000467
10	9	0	-2.320694	1.019643	0.116455
11	9	0	-2.347210	-1.613762	-0.224427



$[C_6(BO)_5]$

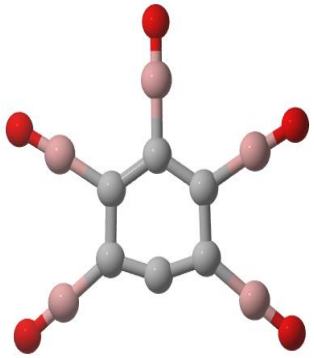
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.234888	1.152624	-0.000000
2	6	0	-1.227804	-0.263931	0.000000
3	6	0	-0.000003	-0.959994	-0.000000
4	6	0	1.227802	-0.263937	-0.000000
5	6	0	1.234892	1.152618	0.000000
6	6	0	0.000004	1.760341	0.000000
7	5	0	-0.000006	-2.499422	-0.000001
8	5	0	-2.565646	-1.029980	-0.000001
9	5	0	2.565640	-1.029993	0.000001
10	5	0	2.516576	2.003616	-0.000000
11	5	0	-2.516566	2.003628	0.000000
12	8	0	-0.000020	-3.701577	0.000000
13	8	0	-3.616167	-1.614015	-0.000001
14	8	0	-3.517037	2.670721	0.000001
15	8	0	3.517056	2.670693	-0.000001
16	8	0	3.616167	-1.614018	0.000001



$[C_6(BO)_5]^-$

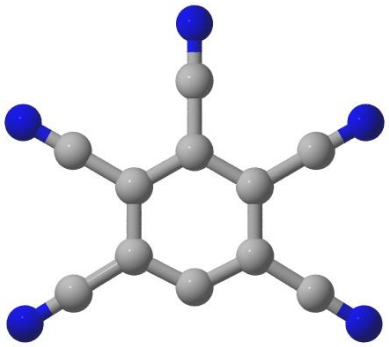
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.187382	1.132926	-0.000039
2	6	0	-1.215420	-0.278295	-0.000000
3	6	0	-0.000000	-0.999587	-0.000007
4	6	0	1.215428	-0.278308	0.000001
5	6	0	1.187403	1.132914	0.000035
6	6	0	0.000015	1.922771	-0.000003

7	5	0	-0.000007	-2.524626	-0.000003
8	5	0	-2.555376	-1.021190	0.000033
9	5	0	2.555376	-1.021217	-0.000029
10	5	0	2.454820	1.994516	0.000136
11	5	0	-2.454789	1.994544	-0.000136
12	8	0	-0.000019	-3.734847	-0.000001
13	8	0	-3.613594	-1.606715	0.000085
14	8	0	-3.464680	2.667600	-0.000027
15	8	0	3.464665	2.667642	0.000030
16	8	0	3.613582	-1.606763	-0.000077



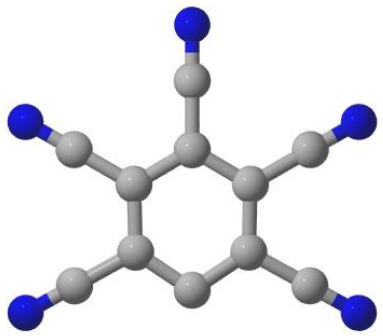
$[C_6(BO)_5]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.278313	-1.160184	-0.000011
2	6	0	-1.230095	0.291484	0.000016
3	6	0	0.000000	0.979358	0.000001
4	6	0	1.230095	0.291484	-0.000015
5	6	0	1.278313	-1.160184	0.000012
6	6	0	-0.000000	-1.496083	0.000000
7	5	0	0.000000	2.529955	-0.000000
8	5	0	-2.598330	1.024425	0.000027
9	5	0	2.598330	1.024425	-0.000027
10	5	0	2.545718	-2.042737	0.000012
11	5	0	-2.545719	-2.042737	-0.000013
12	8	0	0.000000	3.725874	-0.000000
13	8	0	-3.670437	1.554023	0.000034
14	8	0	-3.524870	-2.725829	-0.000014
15	8	0	3.524870	-2.725830	0.000013
16	8	0	3.670438	1.554023	-0.000035



$[C_6(CN)_5]$

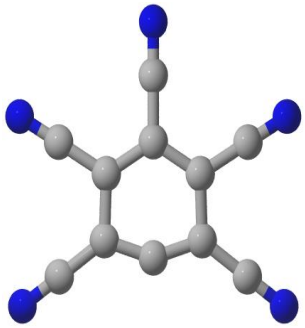
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.227209	-1.142128	-0.000032
2	6	0	-1.223252	0.270422	-0.000008
3	6	0	-0.000000	0.965775	-0.000000
4	6	0	1.223252	0.270423	0.000008
5	6	0	1.227209	-1.142128	0.000032
6	6	0	0.000000	-1.764545	-0.000000
7	6	0	-0.000001	2.399854	0.000000
8	6	0	-2.462351	0.989666	-0.000001
9	6	0	2.462351	0.989666	0.000001
10	6	0	2.448740	-1.893388	-0.000008
11	6	0	-2.448739	-1.893389	0.000008
12	7	0	-0.000001	3.557532	0.000000
13	7	0	3.469371	1.561246	0.000008
14	7	0	-3.469371	1.561246	-0.000008
15	7	0	-3.431883	-2.504397	0.000016
16	7	0	3.431884	-2.504395	-0.000016



$[C_6(CN)_5]^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.173977	-1.155431	0.000006
2	6	0	-1.208408	0.254246	0.000010
3	6	0	0.000000	0.971089	0.000004
4	6	0	1.208408	0.254246	-0.000009

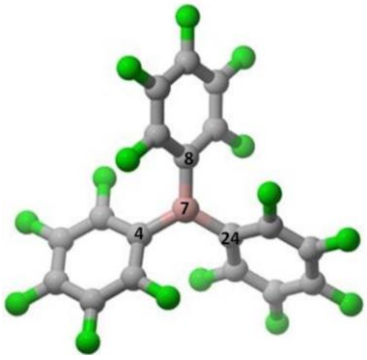
5	6	0	1.173977	-1.155431	-0.000016
6	6	0	0.000000	-1.945250	-0.000009
7	6	0	0.000000	2.404060	0.000011
8	6	0	2.451801	0.974373	-0.000013
9	6	0	-2.451801	0.974373	0.000020
10	6	0	-2.441535	-1.853316	0.000011
11	6	0	2.441535	-1.853316	-0.000022
12	7	0	-0.000000	3.563692	0.000014
13	7	0	-3.459494	1.547940	0.000033
14	7	0	3.459494	1.547940	-0.000019
15	7	0	-3.455679	-2.416776	0.000022
16	7	0	3.455679	-2.416776	-0.000044



$[C_6(CN)_5]^+$

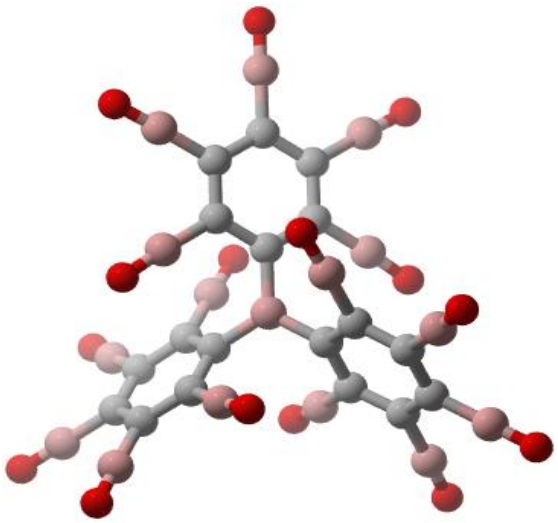
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.282023	-1.150485	-0.000043
2	6	0	1.229827	0.295997	-0.000063
3	6	0	0.000000	0.986911	0.000000
4	6	0	-1.229827	0.295997	0.000063
5	6	0	-1.282023	-1.150485	0.000043
6	6	0	-0.000000	-1.523488	0.000000
7	6	0	0.000000	2.416010	0.000000
8	6	0	2.479508	0.977989	-0.000039
9	6	0	-2.479508	0.977989	0.000039
10	6	0	-2.464666	-1.933574	-0.000027
11	6	0	2.464666	-1.933574	0.000027
12	7	0	0.000000	3.573788	0.000000
13	7	0	-3.498865	1.530239	0.000026
14	7	0	3.498865	1.530239	-0.000026
15	7	0	3.431049	-2.571112	0.000073
16	7	0	-3.431049	-2.571112	-0.000073

S3. Optimized geometry and cartesian coordinates of $B(C_6F_5)_3$, $B(C_6(BO)_5)_3$ and $B(C_6(CN)_5)_3$ molecules.



$B(C_6F_5)_3$

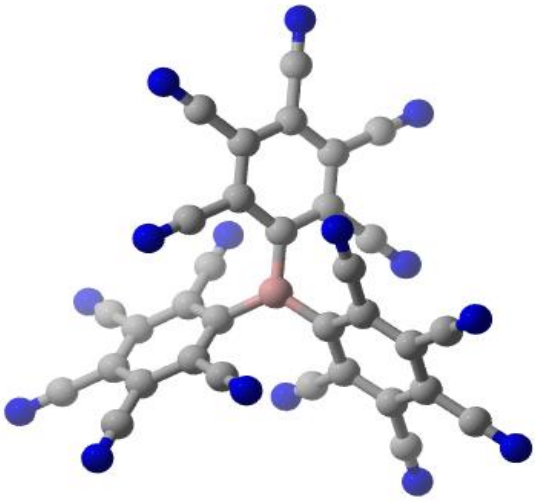
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.437085	-2.716002	0.001009
2	6	0	-2.332706	-2.995457	0.792541
3	6	0	-1.250922	-2.132967	0.771036
4	6	0	-1.227464	-0.972095	-0.000576
5	6	0	-2.362607	-0.726203	-0.771321
6	6	0	-3.452724	-1.577720	-0.791597
7	5	0	0.000238	-0.000378	0.000382
8	6	0	1.455411	-0.578453	0.000359
9	6	0	2.471680	-0.019894	0.774020
10	6	0	3.760091	-0.523693	0.794637
11	6	0	4.072187	-1.616625	-0.000527
12	6	0	3.094940	-2.198263	-0.794910
13	6	0	1.811623	-1.681756	-0.773640
14	9	0	4.694171	0.024753	1.559350
15	9	0	2.215668	1.026291	1.561368
16	9	0	5.299889	-2.103565	-0.001474
17	9	0	3.398757	-3.236484	-1.561530
18	9	0	0.907751	-2.266774	-1.561418
19	9	0	-0.215412	-2.436598	1.555545
20	9	0	-2.418242	0.350825	-1.556608
21	9	0	-2.324936	-4.079234	1.556327
22	9	0	-4.506028	-1.318562	-1.554095
23	9	0	-4.473765	-3.534305	0.001990
24	6	0	-0.227342	1.548226	0.000186
25	6	0	0.560769	2.409871	-0.761521
26	6	0	0.367107	3.779564	-0.782601
27	6	0	-0.635733	4.333355	-0.000421
28	6	0	-1.437431	3.515569	0.782256
29	6	0	-1.229633	2.147833	0.761670
30	9	0	-0.827211	5.640104	-0.000936
31	9	0	1.125420	4.563558	-1.536411
32	9	0	-2.388664	4.049195	1.536143
33	9	0	1.530245	1.921591	-1.536857
34	9	0	-2.017883	1.402556	1.537992



$B(C_6(BO)_5)_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.010219	4.399728	-0.000110
2	6	0	-0.835243	3.696332	0.877662
3	6	0	-0.852091	2.290492	0.860212
4	6	0	0.003560	1.569873	-0.000273
5	6	0	0.862559	2.286568	-0.860692
6	6	0	0.852338	3.692468	-0.877975
7	5	0	-0.000012	-0.007535	-0.000238
8	6	0	-1.367373	-0.793840	-0.013850
9	6	0	-1.586053	-1.861045	0.882499
10	6	0	-2.817745	-2.539255	0.903608
11	6	0	-3.828422	-2.187184	-0.009571
12	6	0	-3.611036	-1.143377	-0.928034
13	6	0	-2.395629	-0.437032	-0.911952
14	6	0	1.363688	-0.800097	0.013473
15	6	0	1.577401	-1.868809	-0.882263
16	6	0	2.805916	-2.552786	-0.902969
17	6	0	3.818244	-2.204879	0.009970
18	6	0	3.605755	-1.159509	0.927798
19	6	0	2.393634	-0.447553	0.911345
20	5	0	-1.757169	4.455914	1.852024
21	5	0	0.013697	5.941700	0.000025
22	5	0	1.777870	4.448070	-1.852010
23	5	0	1.778169	1.505267	-1.821559
24	5	0	-1.771524	1.513551	1.820966
25	5	0	-2.136491	0.704869	-1.912261
26	5	0	-4.698335	-0.750647	-1.947552
27	5	0	-5.171562	-2.944421	-0.005794
28	5	0	-3.041933	-3.670330	1.926523
29	5	0	-0.473195	-2.237054	1.878213
30	5	0	0.462768	-2.240385	-1.877670
31	5	0	2.140100	0.696087	1.911122

32	5	0	4.695000	-0.771228	1.946951
33	5	0	5.157780	-2.968478	0.006566
34	5	0	3.024731	-3.685507	-1.925230
35	8	0	0.016242	7.142918	0.000107
36	8	0	-2.499478	5.013615	2.614380
37	8	0	2.522838	5.002833	-2.613912
38	8	0	2.477488	0.821441	-2.524922
39	8	0	-2.474321	0.833256	2.524296
40	8	0	-1.846894	1.623357	-2.635869
41	8	0	5.521354	-0.425589	2.747609
42	8	0	1.855256	1.616317	2.634397
43	8	0	-0.469000	-2.475363	-2.604026
44	8	0	3.151702	-4.570439	-2.727899
45	8	0	6.200827	-3.564390	0.005454
46	8	0	0.457582	-2.475709	2.604645
47	8	0	-3.173127	-4.554201	2.729683
48	8	0	-6.217448	-3.535333	-0.004480
49	8	0	-5.522748	-0.401455	-2.748669

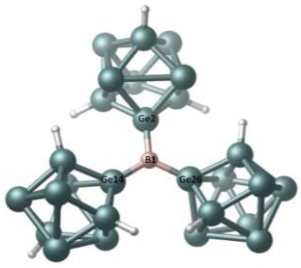


$B(C_6(CN)_5)_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.816379	3.449771	-0.000272
2	6	0	3.013469	2.367455	-0.894983
3	6	0	2.118981	1.265481	-0.878328
4	6	0	0.999555	1.225207	-0.000736
5	6	0	0.814988	2.330093	0.876770
6	6	0	1.716191	3.426637	0.894023
7	5	0	-0.000183	0.000357	-0.000315
8	6	0	0.560456	-1.477918	0.000320
9	6	0	0.036012	-2.467716	-0.877224
10	6	0	0.544099	-3.793017	-0.894210
11	6	0	1.580208	-4.162936	0.000416
12	6	0	2.109367	-3.198494	0.895192
13	6	0	1.609396	-1.870165	0.878268
14	6	0	-1.560820	0.253697	-0.000121
15	6	0	-2.424304	-0.456498	0.880125

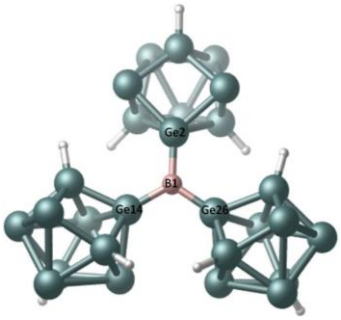
16	6	0	-3.824652	-0.225272	0.897358
17	6	0	-4.395894	0.712842	0.000478
18	6	0	-3.558104	1.422704	-0.896763
19	6	0	-2.156354	1.200004	-0.880176
20	6	0	1.509802	4.514538	1.808066
21	6	0	3.724127	4.561139	-0.000036
22	6	0	-0.288182	2.341265	1.802293
23	6	0	4.120640	2.382895	-1.809074
24	6	0	2.349730	0.187177	-1.804433
25	6	0	2.169038	-0.920140	1.804516
26	6	0	3.154577	-3.563288	1.809563
27	6	0	2.089902	-5.504342	0.000255
28	6	0	0.004500	-4.759827	-1.808372
29	6	0	-1.013636	-2.129226	-1.803139
30	6	0	-4.662601	-0.945822	1.814013
31	6	0	-1.880670	-1.413872	1.808349
32	6	0	-5.812426	0.942160	0.000686
33	6	0	-4.126153	2.370781	-1.813309
34	6	0	-1.338587	1.936195	-1.809128
35	7	0	-6.978148	1.130796	0.000850
36	7	0	-5.347039	-1.543453	2.568360
37	7	0	-4.587387	3.153713	-2.567588
38	7	0	-0.658578	2.537606	-2.564830
39	7	0	-1.425065	-2.199669	2.563420
40	7	0	-1.198260	2.343097	2.555237
41	7	0	1.333431	5.407779	2.560176
42	7	0	4.471134	5.475730	0.000153
43	7	0	5.031009	2.388786	-2.561301
44	7	0	2.532605	-0.704161	-2.557598
45	7	0	2.624109	-0.132237	2.557713
46	7	0	4.016138	-3.856787	2.562041
47	7	0	2.509434	-6.608194	0.000150
48	7	0	-0.445035	-5.551483	-2.560606
49	7	0	-1.877386	-1.843070	-2.556283

S4. Optimized geometries and Cartesian coordinates of $[B(Ge_9H_3)_3]$ and $[B(Ge_9H_3)_3]^-$ molecules.



$[B(Ge_9H_3)_3]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000033	-0.017502	-0.055092
2	32	0	-1.792933	-1.037800	-0.022909
3	32	0	-2.395449	-3.229337	-1.252526
4	32	0	-4.089860	-0.215498	-0.862632
5	32	0	-4.617399	-2.323000	-2.435008
6	32	0	-2.136953	-3.333168	1.491409
7	32	0	-4.642938	-4.363883	-0.356382
8	1	0	-1.275227	-4.147232	-1.815073
9	32	0	-6.139418	-1.723386	-0.044892
10	32	0	-3.743748	-0.453450	1.857418
11	1	0	-4.333843	1.293889	-1.142470
12	32	0	-4.696288	-2.894521	1.860871
13	1	0	-5.424669	-3.474494	3.095233
14	32	0	1.792067	-1.039404	-0.023397
15	32	0	4.089796	-0.219487	-0.863098
16	32	0	2.392448	-3.231782	-1.252305
17	32	0	4.615269	-2.327862	-2.434894
18	32	0	3.743506	-0.456866	1.857080
19	32	0	6.137497	-1.729218	-0.044308
20	1	0	4.335692	1.289696	-1.142425
21	32	0	4.639014	-4.368370	-0.356307
22	32	0	2.133158	-3.334933	1.491462
23	1	0	1.271551	-4.148323	-1.815678
24	32	0	4.692928	-2.899302	1.861125
25	1	0	5.421037	-3.479392	3.095595
26	32	0	0.000935	2.043189	-0.098647
27	32	0	1.743805	3.603931	1.005983
28	32	0	-1.740146	3.605660	1.006222
29	32	0	0.002625	5.034884	2.452446
30	32	0	1.671601	3.521235	-1.738226
31	32	0	1.526248	6.155168	0.247972
32	1	0	3.133248	3.048884	1.426500
33	32	0	-1.520062	6.156620	0.248218
34	32	0	-1.668343	3.522807	-1.738053
35	1	0	-3.130113	3.052188	1.427087
36	32	0	0.002619	5.542293	-1.850219
37	1	0	0.002863	6.507577	-3.058234

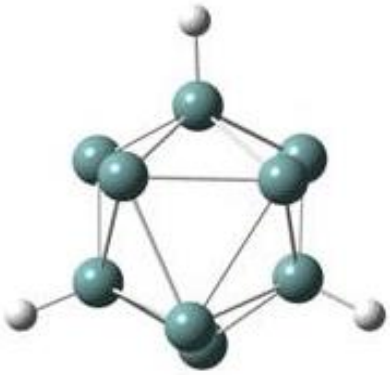


$[B(Ge_9H_3)_3]^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000048	0.066297	0.436121
2	32	0	1.770419	-0.971911	0.140582
3	32	0	2.408131	-3.229561	1.232861
4	32	0	4.142029	-0.197987	0.757699
5	32	0	4.647353	-2.285819	2.364965
6	32	0	2.028000	-3.212286	-1.498969
7	32	0	4.645323	-4.369584	0.382241
8	1	0	1.346194	-4.138013	1.913795
9	32	0	6.130378	-1.767177	-0.040393
10	32	0	3.587831	-0.546275	-1.931419
11	1	0	4.483793	1.295127	1.022473
12	32	0	4.621403	-2.964851	-1.875014
13	1	0	5.317317	-3.564036	-3.126080
14	32	0	-1.770659	-0.971542	0.141269
15	32	0	-4.142239	-0.197113	0.757549
16	32	0	-2.409231	-3.228760	1.233743
17	32	0	-4.648886	-2.284726	2.364710
18	32	0	-3.587212	-0.545890	-1.931539
19	32	0	-6.130713	-1.765851	-0.041281
20	1	0	-4.483979	1.296113	1.021750
21	32	0	-4.646025	-4.368691	0.381954
22	32	0	-2.028406	-3.212005	-1.498246
23	1	0	-1.347670	-4.137732	1.914596
24	32	0	-4.621644	-2.964088	-1.875297
25	1	0	-5.317087	-3.563396	-3.126556
26	32	0	0.000337	1.974563	1.178110
27	32	0	-1.734072	3.536022	-0.806973
28	32	0	1.734100	3.535312	-0.807966
29	32	0	-0.000266	4.575662	-2.496908
30	32	0	-1.973566	3.725394	1.725817
31	32	0	-1.351536	6.270977	-0.637273
32	1	0	-2.809665	2.687835	-1.566346
33	32	0	1.352746	6.270458	-0.638085
34	32	0	1.975248	3.724596	1.724655
35	1	0	2.808801	2.686608	-1.568032
36	32	0	0.001170	5.484608	1.651446
37	1	0	0.001659	6.674787	2.670173

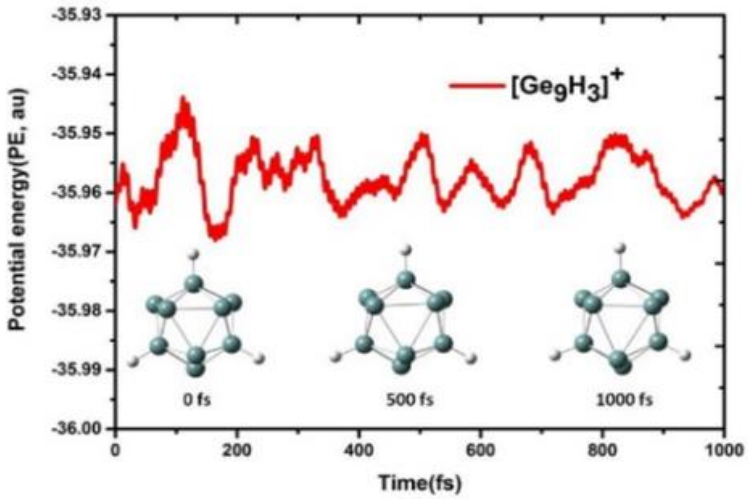
S5. Optimized geometry and Cartesian coordinates of $[Ge_9H_3]^+$ cluster and ADMP molecular dynamics simulation on Ge_9H_3 cation.

.



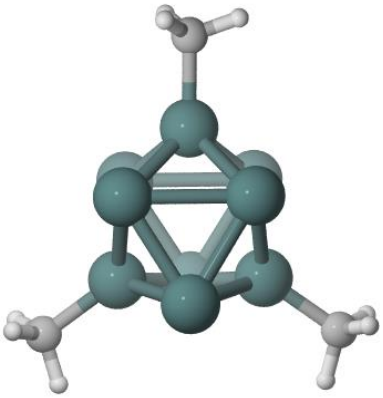
$[Ge_9H_3]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	-1.079658	1.279986	1.704575
2	32	0	-1.512477	1.798184	-1.474776
3	32	0	1.396288	-1.657503	-0.226627
4	32	0	-0.799344	-2.208413	-1.475853
5	32	0	0.738194	2.037483	-0.225067
6	32	0	1.648702	0.292719	1.705164
7	32	0	2.313237	0.412637	-1.475083
8	32	0	-0.571086	-1.575626	1.703086
9	32	0	-2.133872	-0.379483	-0.227745
10	1	0	1.262866	3.486063	-0.080000
11	1	0	-3.650871	-0.649294	-0.083257
12	1	0	2.388522	-2.836235	-0.082303



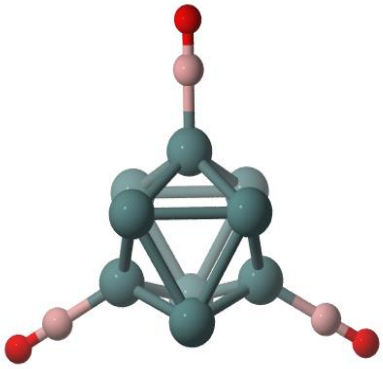
ADMP Results of Ge_9H_3 cation

S6. Optimized geometries and Cartesian coordinates of $[Ge_9(CH_3)_3]$, $[Ge_9(BO)_3]$, $[Ge_9(CN)_3]$, $B[Ge_9(CH_3)_3]_3$, $B[Ge_9(BO)_3]_3$ and $B[Ge_9(CN)_3]_3$ clusters.



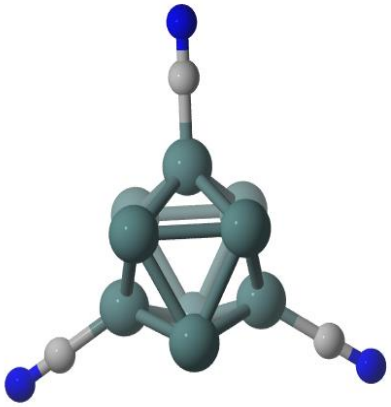
$[Ge_9(CH_3)_3]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.741477	1.677341	-1.388184
2	32	0	0.820109	1.688866	1.333946
3	32	0	-1.385935	2.004014	0.040161
4	32	0	0.741033	-1.677433	-1.388247
5	32	0	0.819653	-1.689179	1.333785
6	32	0	-1.386538	-2.003611	0.039996
7	32	0	-1.063263	0.000063	1.558447
8	32	0	2.024315	-0.000217	-0.050946
9	32	0	-1.159292	0.000210	-1.496902
10	6	0	-2.129707	0.000098	3.158207
11	1	0	-1.917583	-0.891946	3.752246
12	1	0	-1.915066	0.890438	3.753904
13	1	0	-3.191062	0.001838	2.897061
14	6	0	-2.326845	0.000381	-3.024413
15	1	0	-2.154074	-0.891119	-3.631683
16	1	0	-2.153311	0.891443	-3.632109
17	1	0	-3.368285	0.000901	-2.692556
18	6	0	3.940546	-0.000641	-0.074562
19	1	0	4.311289	-0.889030	-0.590098
20	1	0	4.322396	-0.002471	0.949244
21	1	0	4.311833	0.889209	-0.587174



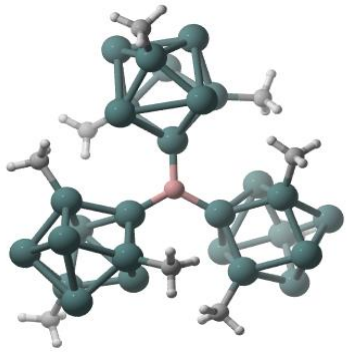
$[Ge_9(BO)_3]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	1.431277	-1.071945	1.746460
2	32	0	1.431096	-1.072090	-1.746510
3	32	0	-1.725642	1.292528	0.000038
4	32	0	0.212680	1.775304	-1.747568
5	32	0	-0.257526	-2.140713	0.000132
6	32	0	-1.644009	-0.703376	1.747699
7	32	0	-1.644053	-0.703479	-1.747539
8	32	0	0.212852	1.775309	1.747482
9	32	0	1.982437	0.848924	-0.000158
10	5	0	-3.344275	2.506235	0.000075
11	5	0	3.843323	1.642618	-0.000057
12	5	0	-0.497665	-4.149514	-0.000003
13	8	0	-4.331589	3.246963	-0.000074
14	8	0	-0.644471	-5.375041	-0.000121
15	8	0	4.978753	2.126640	0.000037



$[Ge_9(CN)_3]$

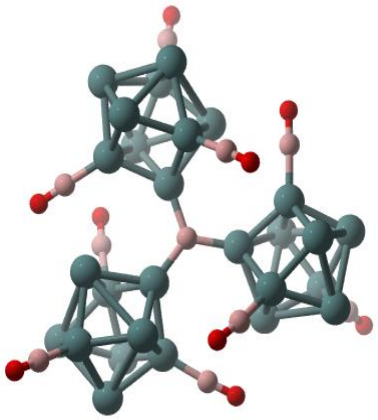
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.813712	1.417083	-1.721857
2	32	0	2.008642	-0.000957	-0.000019
3	32	0	0.813758	1.417804	1.721240
4	32	0	-1.383628	0.000353	-2.096018
5	32	0	-1.105831	-1.486584	0.000316
6	32	0	-1.383541	0.001213	2.096060
7	32	0	0.812317	-1.417645	1.721835
8	32	0	0.812264	-1.418326	-1.721289
9	32	0	-1.104312	1.487100	-0.000296
10	6	0	-2.224116	3.006638	-0.000535
11	6	0	3.888789	-0.001695	-0.000079
12	6	0	-2.227028	-3.005067	0.000689
13	7	0	-2.931556	3.932279	-0.000528
14	7	0	5.053084	-0.002032	-0.000006
15	7	0	-2.934969	-3.930327	0.000598



$B[Ge_9(CH_3)_3]_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.037388	0.020263	-0.047080
2	32	0	-1.378262	1.522223	-0.316198
3	32	0	-3.921185	1.739699	-0.813908
4	32	0	-1.173514	3.800899	-1.536707
5	32	0	-3.712792	3.924072	-2.352017
6	32	0	-3.110050	1.899436	1.856806
7	32	0	-4.992605	3.981276	0.227311
8	32	0	-2.606599	5.780876	-0.412804
9	32	0	-0.610098	3.782678	1.175497
10	32	0	-3.011161	4.532762	1.896456
11	32	0	-0.582162	-1.965476	-0.010214
12	32	0	0.533724	-4.300017	-0.088319
13	32	0	-2.174658	-2.907764	-1.838835
14	32	0	-0.885506	-5.225600	-2.178749
15	32	0	-0.831384	-3.584139	2.247977
16	32	0	-1.218811	-6.266559	0.471262
17	32	0	-3.547541	-5.077380	-1.060994
18	32	0	-3.274959	-2.271973	0.619877
19	32	0	-3.097935	-4.709751	1.535940
20	32	0	2.055669	0.485083	0.131498
21	32	0	3.744313	-0.664956	1.733198
22	32	0	3.519728	2.595585	0.444426
23	32	0	5.108636	1.554571	2.340073
24	32	0	3.666279	-1.564073	-0.887489
25	32	0	6.274839	-0.637814	0.845602
26	32	0	6.079574	2.185553	-0.286972
27	32	0	3.500700	1.403511	-2.085585
28	32	0	5.650922	-0.045249	-1.666353
29	6	0	6.871612	-0.573996	-3.166152
30	1	0	7.550955	-1.360627	-2.823571
31	1	0	6.272148	-0.946489	-4.003183
32	1	0	7.449697	0.297361	-3.489231
33	6	0	3.002603	4.539377	0.307579
34	1	0	3.923682	5.131944	0.280252
35	1	0	2.420387	4.730592	-0.597076
36	1	0	2.415566	4.812066	1.189878
37	6	0	3.168794	-2.052751	3.074683
38	1	0	3.127248	-1.572129	4.057509

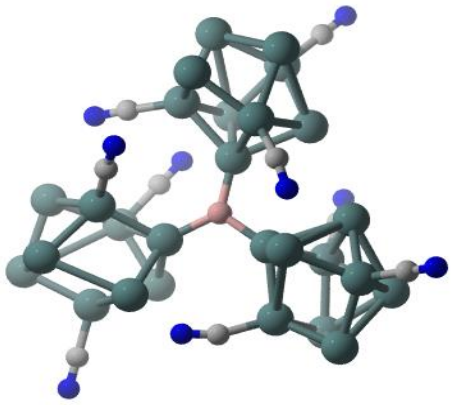
39	1	0	2.173027	-2.430145	2.820383
40	1	0	3.885633	-2.879561	3.099458
41	6	0	2.413604	-4.854636	0.392748
42	1	0	3.068931	-4.658324	-0.461319
43	1	0	2.771857	-4.302912	1.265506
44	1	0	2.408708	-5.927028	0.615379
45	6	0	0.417006	4.300043	-2.667189
46	1	0	1.248547	3.617383	-2.466081
47	1	0	0.124281	4.205604	-3.718033
48	1	0	0.721881	5.330863	-2.461294
49	6	0	-3.335691	5.577072	3.576829
50	1	0	-2.656327	5.220461	4.357833
51	1	0	-3.151100	6.639135	3.388111
52	1	0	-4.371856	5.434806	3.899062
53	6	0	-5.339350	0.322194	-1.043792
54	1	0	-5.002496	-0.429979	-1.761945
55	1	0	-5.581380	-0.154917	-0.090792
56	1	0	-6.229774	0.827268	-1.436257
57	6	0	-2.843436	-1.721338	-3.320930
58	1	0	-3.854776	-2.020275	-3.615122
59	1	0	-2.846248	-0.678193	-2.989130
60	1	0	-2.166071	-1.826395	-4.174355
61	6	0	-4.387710	-5.438157	2.887063
62	1	0	-5.386454	-5.500335	2.444045
63	1	0	-4.060602	-6.434936	3.199291
64	1	0	-4.412128	-4.772576	3.756049



$B[Ge_9(BO)_3]_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.022082	-0.009436	-0.106183
2	32	0	0.276989	2.042860	-0.308249
3	32	0	1.639374	3.124431	1.654100
4	32	0	-1.378909	4.012436	0.173231
5	32	0	-0.218454	4.871558	2.453331
6	32	0	2.804502	3.133222	-0.806682
7	32	0	2.335393	5.688984	1.305268
8	32	0	-0.289537	6.458208	0.069478
9	32	0	-0.167263	3.948003	-2.283911

10	32	0	1.785222	5.496699	-1.316071
11	32	0	1.637173	-1.265612	-0.201831
12	32	0	1.939315	-3.172501	1.559265
13	32	0	4.142148	-0.799498	0.397404
14	32	0	4.338712	-2.451733	2.492064
15	32	0	1.398687	-3.960025	-0.992513
16	32	0	3.869447	-4.965533	1.042168
17	32	0	5.778631	-2.899071	0.008951
18	32	0	3.552223	-1.627028	-2.165492
19	32	0	3.966928	-4.148848	-1.507454
20	32	0	-1.941438	-0.776079	0.158588
21	32	0	-2.843895	-3.188687	-0.347033
22	32	0	-3.680756	-0.106817	-1.695491
23	32	0	-4.293714	-2.560949	-2.537018
24	32	0	-3.246126	-2.202373	2.167341
25	32	0	-5.495491	-3.491422	-0.107588
26	32	0	-6.222127	-0.788622	-1.214136
27	32	0	-4.131048	0.829617	0.820385
28	32	0	-5.621931	-1.264862	1.360825
29	5	0	2.839710	6.760829	-2.486389
30	5	0	-3.378654	3.970272	-0.135610
31	5	0	-3.094944	1.469357	-2.818921
32	5	0	-7.177861	-1.036785	2.628584
33	5	0	-1.740739	-4.876797	-0.189976
34	5	0	0.266385	-3.563800	2.624809
35	5	0	4.613292	-5.462362	-2.896945
36	8	0	5.011802	-6.259255	-3.750953
37	8	0	-0.993238	-5.863310	-0.141405
38	8	0	-0.818995	-3.697664	3.207149
39	8	0	-8.123927	-0.907252	3.410835
40	8	0	-2.614735	2.428622	-3.438283
41	8	0	-4.605288	3.881200	-0.277182
42	8	0	3.471482	7.535894	-3.210141
43	5	0	5.131161	0.955251	0.173319
44	8	0	5.702108	2.047452	0.055465
45	5	0	2.625954	1.855624	2.885373
46	8	0	3.195671	1.050039	3.630001



$B[Ge_9(CN)_3]_3$

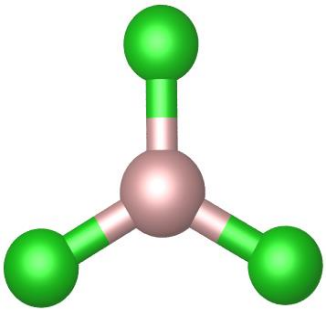
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.092868	0.124827	0.038727
2	32	0	0.717686	-1.760379	0.339757
3	32	0	-0.461001	-4.104012	-0.035498
4	32	0	2.185540	-2.691647	-1.702304
5	32	0	0.653857	-4.708382	-2.448601
6	32	0	1.119886	-6.274528	-0.021932
7	32	0	0.541774	-3.563979	2.398920
8	6	0	-2.380968	-4.273364	0.123411
9	32	0	3.413237	-2.315756	0.728447
10	32	0	3.477957	-5.005959	-1.328559
11	6	0	2.747490	-1.064962	-2.644589
12	32	0	2.872295	-4.807956	1.320231
13	7	0	-3.561583	-4.335710	0.230143
14	7	0	2.895405	0.083909	-2.911349
15	6	0	4.256141	-5.735881	2.305374
16	7	0	5.086200	-6.311871	2.928919
17	32	0	-2.101105	0.667126	-0.075547
18	32	0	-3.809248	-0.955007	-1.146244
19	32	0	-4.012617	-0.428505	2.041986
20	32	0	-5.815770	-1.709550	0.370604
21	32	0	-5.869047	0.503569	-1.845599
22	32	0	-3.257911	2.479342	-1.731001
23	6	0	-2.877489	-2.017829	-2.504847
24	32	0	-3.212665	2.047124	1.961830
25	32	0	-7.219157	0.664417	0.357104
26	6	0	-2.497458	-1.647445	2.594791
27	32	0	-5.133334	2.413263	0.198758
28	7	0	-2.242328	-2.659989	-3.275202
29	7	0	-1.616723	-2.362818	2.945123
30	6	0	-6.008340	4.160718	0.143161
31	7	0	-6.535428	5.224694	0.116791
32	32	0	1.280561	1.691490	-0.113847
33	32	0	0.934870	4.273447	-0.072115
34	32	0	2.648235	2.417842	2.030941
35	32	0	1.974227	4.979874	2.236094
36	32	0	2.947183	5.762598	-0.759215
37	32	0	2.288014	2.136666	-2.587274

38	6	0	-0.930833	4.437391	-0.661170
39	32	0	4.164923	1.353315	0.005864
40	32	0	4.685395	4.085232	1.227413
41	6	0	3.104251	1.046221	3.341792
42	32	0	4.243745	3.567127	-1.461935
43	7	0	-2.035124	4.169789	-1.011211
44	7	0	3.320485	0.186040	4.132161
45	6	0	5.950758	3.717458	-2.371411
46	7	0	6.980821	3.821001	-2.952172

Table S1. Comparison of Ionization potential and electronegativity of Boron, Ligands and charge on the Boron in complexes.

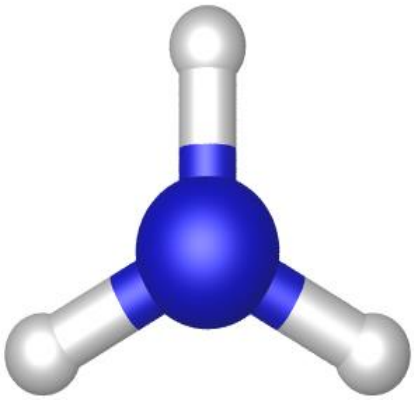
	Electron affinity	Ionization energy	Electro-negativity	
Boron	0.280	8.302	4.31	
Ligands	Electron affinity	Ionization energy	Electro-negativity	Charge on Boron
C_6F_5	4.42	9.09	6.75	0.884
$C_6(BO)_5$	3.85	10.60	7.22	0.970
$C_6(CN)_5$	4.25	11.31	7.78	1.030
$Ge_9(CH_3)_3$	2.67	5.74	4.21	-0.721
Ge_9H_3	2.87	6.58	4.72	-0.696
$Ge_9(BO)_3$	4.22	7.00	5.60	-0.690
$Ge_9(CN)_3$	4.14	7.14	5.64	-0.680

S7. Optimized geometries and Cartesian coordinates of BF_3, NH_3 and BF_3-NH_3 molecules.



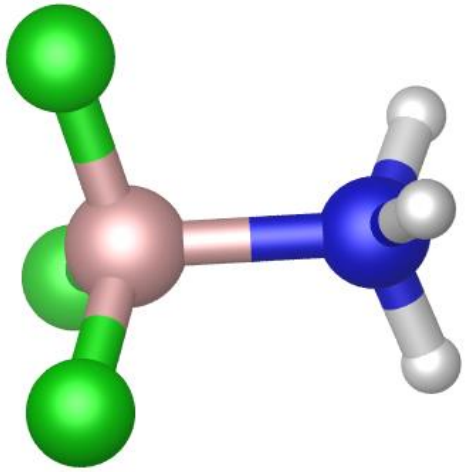
BF_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.000000
2	9	0	0.000000	1.351688	0.000000
3	9	0	1.170596	-0.675844	0.000000
4	9	0	-1.170596	-0.675844	0.000000



NH_3

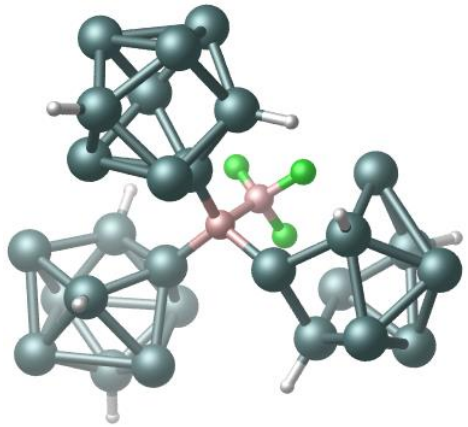
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.053023
2	1	0	0.000000	0.993460	-0.123721
3	1	0	-0.860362	-0.496730	-0.123721
4	1	0	0.860362	-0.496730	-0.123721



BF_3-NH_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000000	0.000000	-0.186035
2	9	0	0.000000	1.368069	-0.545215
3	9	0	1.184783	-0.684035	-0.545215
4	9	0	-1.184783	-0.684035	-0.545215
5	7	0	0.000000	-0.000000	1.465526
6	1	0	-0.000000	-0.969215	1.797430
7	1	0	-0.839365	0.484607	1.797430
8	1	0	0.839365	0.484607	1.797430

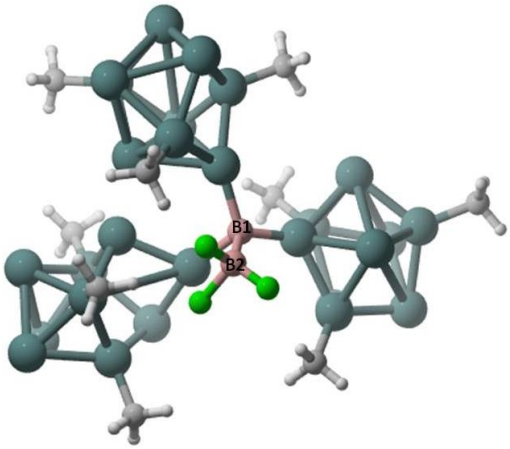
S8. Optimized geometry and Cartesian coordinates of $BF_3[B(Ge_9H_3)_3]$, $BF_3[B(Ge_9(CH_3)_3)_3]$ and $BF_3[B(Ge_9(CN)_3)_3]$ molecules.



$BF_3[B(Ge_9H_3)_3]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.208375	-0.006756	-0.317159
2	32	0	1.968153	-0.079577	0.880244
3	32	0	3.576300	-2.038474	0.816955
4	32	0	3.670903	1.803620	0.942120
5	32	0	4.855208	-0.194444	2.540161
6	32	0	3.849917	-2.199543	-1.797788
7	32	0	6.217772	-1.576593	0.536641
8	1	0	3.167000	-3.291525	1.629866
9	32	0	6.290516	1.236924	0.623240
10	32	0	3.941507	2.112906	-1.660103
11	1	0	3.322037	3.021820	1.832252
12	32	0	5.423220	-0.077951	-1.666019
13	1	0	6.572319	-0.073218	-2.718714
14	32	0	-0.962825	-1.751933	-0.089858
15	32	0	-2.681763	-2.509030	-1.842264
16	32	0	-2.794582	-2.158120	1.647921
17	32	0	-4.762554	-2.561119	-0.138334
18	32	0	-0.456963	-4.105812	-1.455031
19	32	0	-3.700354	-4.927556	-1.393568
20	1	0	-2.630427	-1.975577	-3.297635
21	32	0	-3.807871	-4.624335	1.625827
22	32	0	-0.553934	-3.800648	1.718493
23	1	0	-2.825020	-1.387251	2.997940
24	32	0	-1.740728	-5.618252	0.263198
25	1	0	-1.399654	-7.119320	0.421013
26	32	0	-0.929145	1.745823	-0.020466
27	32	0	-2.604731	2.608427	-1.768852
28	32	0	-0.087102	4.174309	0.094167
29	32	0	-1.516355	5.042534	-2.010265
30	32	0	-3.602318	1.704255	0.670812
31	32	0	-4.158919	4.566843	-0.863471
32	1	0	-3.165465	1.660272	-2.862327
33	32	0	-1.950740	5.995272	0.643026

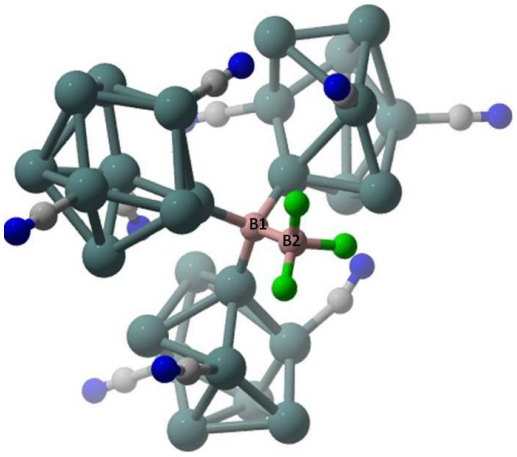
34	32	0	-1.267343	3.075090	2.352398
35	1	0	1.399081	4.508133	0.418299
36	32	0	-3.556330	4.138102	1.689572
37	1	0	-4.607486	4.551562	2.747175
38	5	0	1.014684	0.024276	-1.894984
39	9	0	0.144242	0.058601	-2.988399
40	9	0	1.958815	-1.170730	-2.147217
41	9	0	2.004310	1.182638	-2.080749



$BF_3[B(Ge_9(CH_3)_3)_3]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.855638	-0.037388	0.998624
2	32	0	-0.420990	-1.459838	0.045702
3	32	0	-3.909523	-2.172768	1.646518
4	32	0	-2.831778	-4.330923	0.672961
5	32	0	-5.606622	-4.158140	1.085619
6	32	0	-2.856966	-0.623861	-0.191749
7	32	0	-5.718928	-1.863451	-0.479235
8	32	0	-4.871877	-4.402610	-1.464987
9	32	0	-1.302354	-3.674898	-1.389753
10	32	0	-3.377707	-2.209146	-2.151206
11	32	0	0.095957	1.969801	0.813178
12	32	0	0.353154	4.185726	-0.498497
13	32	0	-1.714249	3.018793	2.280220
14	32	0	-0.970228	5.482889	1.641262
15	32	0	-0.856193	2.533612	-2.181720
16	32	0	-1.779983	5.982414	-0.884599
17	32	0	-3.625270	4.451965	0.890187
18	32	0	-2.620838	1.916329	-0.093096
19	32	0	-3.074964	3.911407	-1.826854
20	32	0	2.865736	-0.262676	0.447469
21	32	0	3.790857	-0.443995	-1.945901
22	32	0	4.111388	-2.436777	1.070547
23	32	0	4.696459	-2.959061	-1.527721
24	32	0	4.684350	1.637532	-0.375958
25	32	0	6.419740	-0.762787	-2.066098
26	32	0	6.683789	-2.395521	0.432594

27	32	0	4.946638	-0.098335	2.250071
28	32	0	6.782281	0.272845	0.392038
29	6	0	8.518569	1.199727	0.792205
30	1	0	8.895409	1.683414	-0.114563
31	1	0	8.354778	1.954023	1.569269
32	1	0	9.248802	0.465252	1.147258
33	6	0	2.757659	0.159737	-3.570952
34	1	0	2.556227	-0.714421	-4.199552
35	1	0	1.807016	0.606154	-3.257178
36	1	0	3.337874	0.894126	-4.137607
37	6	0	2.191778	4.909197	-0.848462
38	1	0	2.609285	5.330022	0.071414
39	1	0	2.840731	4.101429	-1.201600
40	1	0	2.124138	5.689977	-1.614291
41	6	0	-2.195972	-5.803962	1.880629
42	1	0	-1.245017	-5.489723	2.326263
43	1	0	-2.922936	-6.007333	2.672498
44	1	0	-2.036675	-6.713387	1.289331
45	6	0	-3.745390	-1.438499	-3.968051
46	1	0	-2.852765	-0.918133	-4.331715
47	1	0	-3.998202	-2.251400	-4.657807
48	1	0	-4.584103	-0.736155	-3.915414
49	6	0	-3.907700	-1.466039	3.514375
50	1	0	-2.878719	-1.183704	3.760049
51	1	0	-4.561952	-0.589978	3.582929
52	1	0	-4.260522	-2.242374	4.200421
53	6	0	-2.720680	2.277283	3.851717
54	1	0	-3.756180	2.043189	3.589715
55	1	0	-2.190766	1.377679	4.172554
56	1	0	-2.702986	3.032209	4.645553
57	6	0	-4.862811	3.727154	-2.737787
58	1	0	-5.681049	3.827976	-2.019679
59	1	0	-4.937923	4.513509	-3.497044
60	1	0	-4.915618	2.747331	-3.223631
61	5	0	0.413958	-0.692195	2.560994
62	9	0	-0.423497	-2.093469	2.032316
63	9	0	1.392199	-1.220052	3.423574
64	9	0	-0.623393	-0.043647	3.307360
65	6	0	3.330201	-3.747973	2.376527
66	1	0	2.703942	-3.192586	3.080594
67	1	0	2.720789	-4.476405	1.831873
68	1	0	4.136601	-4.260929	2.910033

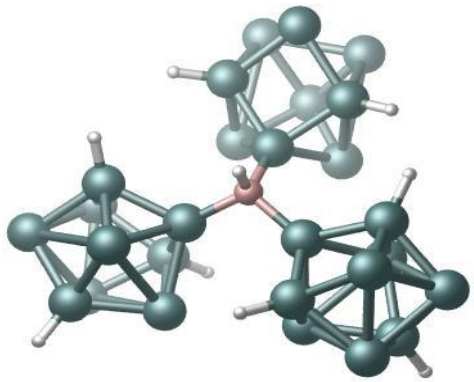


$BF_3[B(Ge_9(CN)_3)_3]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.018949	-0.292303	0.906733
2	32	0	-0.255188	1.807976	0.621629
3	32	0	1.766655	4.382800	1.240861
4	32	0	-0.624167	2.868992	-1.682221
5	32	0	1.343900	4.505117	-2.105390
6	32	0	0.767020	6.402728	-0.387388
7	32	0	-0.561458	3.448098	2.550407
8	6	0	2.925068	2.950234	0.287060
9	32	0	-2.745068	3.237648	0.092761
10	32	0	-1.688020	5.307874	-1.835748
11	6	0	-1.288885	1.364394	-2.789382
12	32	0	-1.359449	5.397261	0.879105
13	7	0	3.735128	2.161050	-0.083752
14	7	0	-1.728783	0.297378	-3.058343
15	6	0	-2.499099	6.772837	1.641861
16	7	0	-3.175248	7.626852	2.112769
17	32	0	1.763643	-1.161338	0.032844
18	32	0	3.333490	-0.944835	-1.959196
19	32	0	4.411391	-0.780325	1.631301
20	32	0	4.934149	0.848225	-1.092928
21	32	0	5.661318	-2.401961	-2.031807
22	32	0	2.154858	-3.811986	-0.515796
23	6	0	2.257306	-0.491489	-3.527455
24	32	0	2.666306	-2.649186	2.211054
25	32	0	6.557328	-0.893681	0.215563
26	6	0	4.433351	0.725696	2.878845
27	32	0	4.723845	-3.672526	-0.038522
28	7	0	1.597179	-0.219609	-4.476391
29	7	0	4.484535	1.670809	3.595406
30	6	0	5.730829	-5.184378	0.662035
31	7	0	6.345736	-6.100159	1.103172
32	32	0	-1.734481	-1.294685	0.208443
33	32	0	-2.391590	-3.808982	0.584686
34	32	0	-3.810514	-1.158913	1.805180
35	32	0	-4.284434	-3.714255	2.390097
36	32	0	-4.459724	-4.736325	-0.708198
37	32	0	-2.033558	-1.796668	-2.411220

38	6	0	-0.604799	-4.634634	0.624343
39	32	0	-4.208601	-0.146555	-0.760017
40	32	0	-5.967338	-2.208403	0.400519
41	6	0	-4.314233	0.572290	2.574823
42	32	0	-4.582910	-2.470715	-2.016069
43	7	0	0.571724	-4.812687	0.510347
44	7	0	-4.524522	1.656650	3.012538
45	6	0	-5.869743	-2.251720	-3.452302
46	7	0	-6.641506	-2.136783	-4.346954
47	5	0	0.213298	-0.402385	2.640280
48	9	0	0.847291	-1.795857	3.019541
49	9	0	-0.983290	-0.331169	3.404224
50	9	0	1.190817	0.544512	3.136902

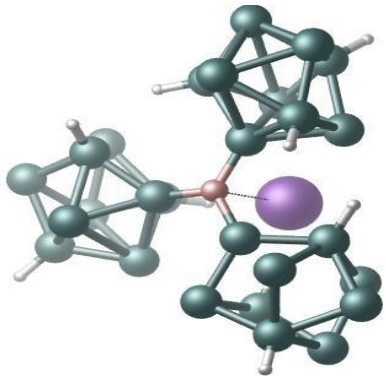
S9. Optimized geometries and Cartesian coordinates of $H[B(Ge_9H_3)_3]$ and $K[B(Ge_9H_3)_3]$ molecules.



$H[B(Ge_9H_3)_3]$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.176539	-0.156375	1.303044
2	32	0	-1.365460	-1.468807	0.651143
3	32	0	-3.003151	-2.757264	2.125012
4	32	0	-1.535978	-3.203591	-1.202612
5	32	0	-2.593985	-4.940330	0.587117
6	32	0	-4.064041	-0.456736	1.077729
7	32	0	-5.189741	-3.657149	0.940119
8	1	0	-2.885571	-2.703357	3.670545
9	32	0	-3.977336	-4.039190	-1.805044
10	32	0	-2.788729	-0.842319	-1.808796
11	1	0	-0.325211	-3.490897	-2.125063
12	32	0	-5.092339	-1.756095	-0.952233
13	1	0	-6.419639	-1.284599	-1.595962
14	32	0	-0.378870	1.773683	0.576977
15	32	0	0.635159	3.049192	-1.457499
16	32	0	-1.092002	3.648401	2.254395
17	32	0	1.143774	4.424399	0.867608
18	32	0	-1.835893	2.224431	-1.879378
19	32	0	-0.189052	5.524997	-1.532136

20	1	0	1.922661	2.315761	-1.912705
21	32	0	-1.392447	5.950608	1.069485
22	32	0	-3.128112	2.674085	0.904843
23	1	0	-0.688418	3.226518	3.691846
24	32	0	-2.649822	4.564088	-0.903683
25	1	0	-3.892170	5.198890	-1.589241
26	32	0	2.099852	-0.727868	0.664617
27	32	0	4.202336	0.699482	1.080371
28	32	0	2.982644	-1.021901	-1.720449
29	32	0	4.959170	0.790345	-1.499683
30	32	0	3.970515	-1.696115	2.450822
31	32	0	6.507120	-0.510171	0.547222
32	1	0	4.200844	1.854510	2.122403
33	32	0	5.444996	-2.018688	-1.878350
34	32	0	2.894031	-3.265376	-0.074509
35	1	0	2.034593	-1.296874	-2.924564
36	32	0	5.398794	-2.924085	0.625075
37	1	0	6.281547	-4.142666	0.986057
38	1	0	0.122859	-0.112203	2.500282

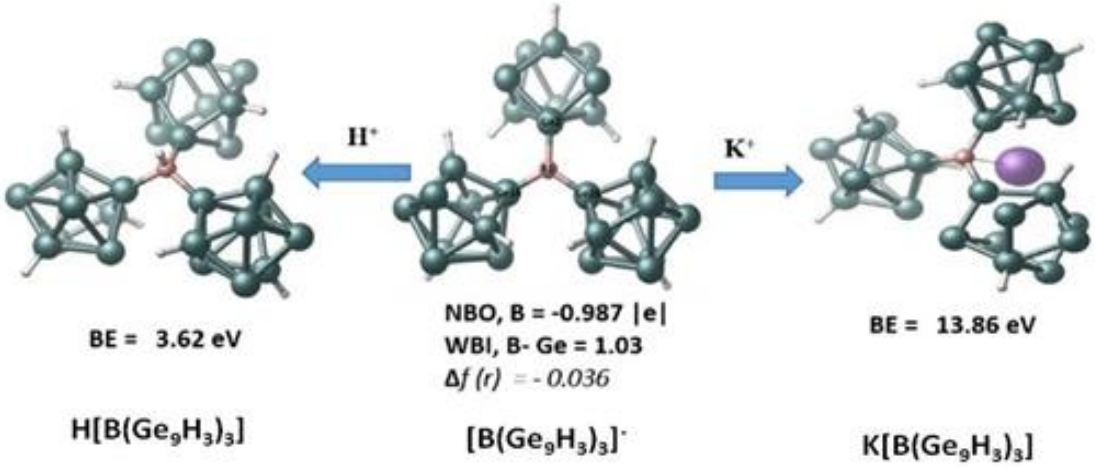


$K[B(Ge_9H_3)_3]$

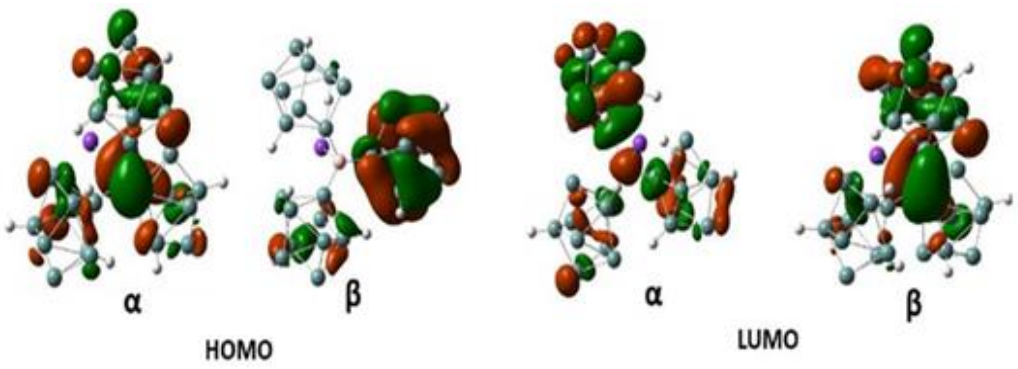
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.012881	0.108591	-0.566684
2	32	0	1.245648	-1.559043	-0.508039
3	32	0	2.092286	-2.468501	1.789475
4	32	0	3.688502	-1.835628	-1.248329
5	32	0	4.710433	-2.330362	1.187115
6	32	0	0.269570	-3.985006	0.400643
7	32	0	3.387965	-4.801501	1.761250
8	1	0	1.410192	-1.952806	3.113175
9	32	0	4.639367	-4.304655	-0.942528
10	32	0	1.776624	-3.535911	-2.367492
11	1	0	4.290823	-1.041299	-2.442801
12	32	0	2.236544	-5.403899	-0.568012
13	1	0	2.066662	-6.886354	-0.977530
14	32	0	-1.976249	-0.287341	-0.816126
15	32	0	-3.652459	1.429092	0.134059
16	32	0	-3.488908	-2.463875	1.295650
17	32	0	-4.686464	0.332767	2.246942
18	32	0	-4.217753	0.508142	-2.406737
19	32	0	-6.219332	0.896932	-0.331873

20	1	0	-3.271256	2.935960	0.050477
21	32	0	-6.068780	-1.692970	1.338865
22	32	0	-3.033032	-2.538574	-1.383792
23	1	0	-2.425554	-1.634394	2.237949
24	32	0	-5.489101	-1.540585	-1.281401
25	1	0	-6.564353	-2.149017	-2.234086
26	32	0	0.818011	1.989715	-0.225415
27	32	0	-0.216020	4.181911	-1.211101
28	32	0	3.392897	2.445040	-0.060977
29	32	0	2.285211	3.667775	-2.276782
30	32	0	-0.472384	3.967587	1.406929
31	32	0	1.457803	6.173348	-1.009840
32	1	0	-1.241569	3.732166	-2.289126
33	32	0	3.908173	4.997153	-0.244475
34	32	0	2.140044	2.729755	2.228338
35	1	0	4.104728	1.160508	-0.561920
36	32	0	1.838550	5.247991	1.522800
37	1	0	1.987382	6.300833	2.656037
38	19	0	-0.640532	0.251163	2.818346

S10. Optimized geometries of $[B(Ge_9H_3)_3]^-$ and its complex with H and K along with binding energies.



S11. Frontier molecular orbitals of $K[B(Ge_9H_3)_3]$.



Frontier MO's of $K[B(Ge_9H_3)_3]$