Electronic Supplementary Material (ESI) for RSC Advances

Substituent Effects on Cyclic Electron Delocalization in Symmetric *B*- and *N*-trisubstituted Borazine Derivatives

Marija Baranac-Stojanović,[*a] Milovan Stojanović[b]

[a]Faculty of Chemistry, University of Belgrade, Studentski trg 16, P.O.Box 158, 11000 Belgrade, Serbia

[b]Center for Chemistry ICTM, University of Belgrade, P.O.Box 473, 11000 Belgrade, Serbia

Supplementary Information

Table of Contents:

Absolute energies (atomic units) and x, y, z coordinates (Å) of the optimized structures

Benzene (D_{6h})

HF/6-311+G**

E = -230.7567738 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.386233	0.000000
2	6	0	1.200513	0.693116	0.000000
3	6	0	1.200513	-0.693116	0.000000
4	6	0	0.000000	-1.386233	0.000000
5	6	0	-1.200513	-0.693116	0.000000
6	6	0	-1.200513	0.693116	0.000000
7	1	0	0.000000	2.461964	0.000000
8	1	0	2.132123	1.230982	0.000000
9	1	0	2.132123	-1.230982	0.000000
10	1	0	0.000000	-2.461964	0.000000
11	1	0	-2.132123	-1.230982	0.000000
12	1	0	-2.132123	1.230982	0.000000

B3LYP/6-311+G**

E = -232.3112416 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.394349	0.000000
2	6	0	1.207542	0.697174	0.000000
3	6	0	1.207542	-0.697174	0.000000
4	6	0	0.000000	-1.394349	0.000000
5	6	0	-1.207542	-0.697174	0.000000
6	6	0	-1.207542	0.697174	0.000000
7	1	0	0.000000	2.478493	0.000000
8	1	0	2.146438	1.239246	0.000000
9	1	0	2.146438	-1.239246	0.000000
10	1	0	0.000000	-2.478493	0.000000
11	1	0	-2.146438	-1.239246	0.000000
12	1	0	-2.146438	1.239246	0.000000

Cyclohexatriene (D_{3h})

HF/6-311+G**

E = -230.619985743 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.652196	-1.285046	0.000000
2	6	0	1.438980	0.077704	0.000000
3	6	0	0.786784	1.207341	0.000000
4	6	0	-0.786784	1.207341	0.000000
5	6	0	-1.438980	0.077704	0.000000
6	6	0	-0.652196	-1.285046	0.000000
7	1	0	1.222925	-2.196034	0.000000
8	1	0	2.513284	0.038933	0.000000
9	1	0	1.290358	2.157101	0.000000
10	1	0	-1.290358	2.157101	0.000000
11	1	0	-2.513284	0.038933	0.000000
12	1	0	-1.222925	-2.196034	0.000000

cis-Butadiene (C_{2v})

HF/6-311+G**

E = -154.9556868 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.539332	-0.497759
2	1	0	0.000000	1.169059	-1.508160
3	1	0	0.000000	2.607837	-0.377191
4	6	0	0.000000	0.740015	0.556177
5	1	0	0.000000	1.192097	1.534842
6	6	0	0.000000	-0.740015	0.556177
7	1	0	0.000000	-1.192097	1.534842
8	6	0	0.000000	-1.539332	-0.497759
9	1	0	0.000000	-1.169059	-1.508160
10	1	0	0.000000	-2.607837	-0.377191

B3LYP/6-311+G**

E = -156.0344785 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.545769	-0.502257
2	1	0	0.000000	1.171912	-1.520671
3	1	0	0.000000	2.622479	-0.382599
4	6	0	0.000000	0.735246	0.561475
5	1	0	0.000000	1.192416	1.547960
6	6	0	0.000000	-0.735246	0.561475
7	1	0	0.000000	-1.192416	1.547960
8	6	0	0.000000	-1.545769	-0.502257
9	1	0	0.000000	-1.171912	-1.520671
10	1	0	0.000000	-2.622479	-0.382599

cis-Butadiene (localized, C_{2v})

HF/6-311+G**

E = -154.928887824 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.535591	-0.505804
2	1	0	0.000000	-1.129974	-1.502395
3	1	0	0.000000	-2.608524	-0.424124
4	6	0	0.000000	-0.782524	0.569381
5	1	0	0.000000	-1.236938	1.545059
6	6	0	0.000000	0.782524	0.569381
7	1	0	0.000000	1.236938	1.545059
8	6	0	0.000000	1.535591	-0.505804
9	1	0	0.000000	1.129974	-1.502395
10	1	0	0.000000	2.608524	-0.424124

all-trans-1,3,5,7-octatetraene (C_{2h})

HF/6-311+G**

E = -308.775588 a.u.

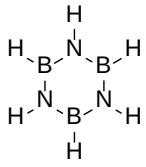
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.136047	1.835589	0.000000
2	6	0	0.392539	0.614719	0.000000
3	6	0	-0.392539	-0.614719	0.000000
4	6	0	0.136047	-1.835589	0.000000
5	6	0	-0.654755	-3.065700	0.000000
6	6	0	-0.136047	-4.284771	0.000000
7	6	0	0.654755	3.065700	0.000000
8	6	0	0.136047	4.284771	0.000000
9	1	0	-1.209073	1.950037	0.000000
10	1	0	1.465955	0.503763	0.000000
11	1	0	-1.465955	-0.503763	0.000000
12	1	0	1.209073	-1.950037	0.000000
13	1	0	-1.726910	-2.947463	0.000000
14	1	0	-0.761378	-5.159418	0.000000
15	1	0	0.928910	-4.446663	0.000000
16	1	0	1.726910	2.947463	0.000000
17	1	0	0.761378	5.159418	0.000000
18	1	0	-0.928910	4.446663	0.000000

all-trans-1,3,5,7-octatetraene (localized, C_{2h})

HF/6-311+G**

E = -308.677961440 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.136870	-1.849343	0.000000
2	6	0	-0.410012	-0.662501	0.000000
3	6	0	0.410012	0.662501	0.000000
4	6	0	-0.136870	1.849343	0.000000
5	6	0	0.682830	3.176832	0.000000
6	6	0	0.136870	4.371078	0.000000
7	6	0	-0.682830	-3.176832	0.000000
8	6	0	-0.136870	-4.371078	0.000000
9	1	0	1.208971	-1.967329	0.000000
10	1	0	-1.482085	-0.545858	0.000000
11	1	0	1.482085	0.545858	0.000000
12	1	0	-1.208971	1.967329	0.000000
13	1	0	1.753487	3.061711	0.000000
14	1	0	0.742097	5.260602	0.000000
15	1	0	-0.931766	4.510435	0.000000
16	1	0	-1.753487	-3.061711	0.000000
17	1	0	-0.742097	-5.260602	0.000000
18	1	0	0.931766	-4.510435	0.000000



(D_{3h})

HF/6-311+G**

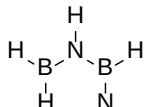
E = -241.2193277 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.250234	0.721823	0.000000
2	1	0	-2.282619	1.317871	0.000000
3	5	0	1.250234	0.721823	0.000000
4	1	0	2.282619	1.317871	0.000000
5	5	0	0.000000	-1.443646	0.000000
6	1	0	0.000000	-2.635742	0.000000
7	7	0	0.000000	1.408746	0.000000
8	1	0	0.000000	2.402926	0.000000
9	7	0	1.220010	-0.704373	0.000000
10	1	0	2.080995	-1.201463	0.000000
11	7	0	-1.220010	-0.704373	0.000000
12	1	0	-2.080995	-1.201463	0.000000

B3LYP/6-311+G**

E = -242.7485061 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.409784	0.000000
2	1	0	0.000000	2.418791	0.000000
3	7	0	1.220909	-0.704892	0.000000
4	1	0	2.094734	-1.209395	0.000000
5	7	0	-1.220909	-0.704892	0.000000
6	1	0	-2.094734	-1.209395	0.000000
7	5	0	1.256794	0.725610	0.000000
8	1	0	2.288954	1.321528	0.000000
9	5	0	0.000000	-1.451221	0.000000
10	1	0	0.000000	-2.643056	0.000000
11	5	0	-1.256794	0.725610	0.000000
12	1	0	-2.288954	1.321528	0.000000



(C_s)

HF/6-311+G**

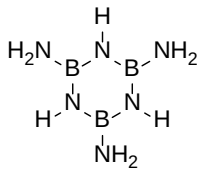
E = -161.9209493 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.693078	-1.559659	0.000000
2	1	0	0.426334	-1.972625	0.000000
3	1	0	-1.605719	-2.327533	0.000000
4	5	0	0.000000	0.923501	0.000000
5	1	0	-0.432949	2.035670	0.000000
6	7	0	-0.940602	-0.177336	0.000000
7	1	0	-1.898549	0.097138	0.000000
8	7	0	1.387667	0.745026	0.000000
9	1	0	2.011859	1.516360	0.000000
10	1	0	1.834958	-0.142052	0.000000

B3LYP/6-311+G**

E = -162.985 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.689302	-1.559325	0.000000
2	1	0	0.437879	-1.955849	0.000000
3	1	0	-1.597847	-2.332278	0.000000
4	5	0	0.000000	0.932480	0.000000
5	1	0	-0.427695	2.046543	0.000000
6	7	0	-0.943591	-0.177029	0.000000
7	1	0	-1.916339	0.100946	0.000000
8	7	0	1.385751	0.739227	0.000000
9	1	0	1.822456	-0.169933	0.000000
10	1	0	2.032938	1.509412	0.000000



(D_{3h})

HF/6-311+G**

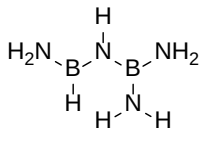
E = -406.5144865 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.415560	0.000000
2	1	0	0.000000	2.410063	0.000000
3	7	0	-1.225911	-0.707780	0.000000
4	1	0	-2.087176	-1.205031	0.000000
5	7	0	1.225911	-0.707780	0.000000
6	1	0	2.087176	-1.205031	0.000000
7	5	0	-1.261634	0.728405	0.000000
8	5	0	0.000000	-1.456810	0.000000
9	5	0	1.261634	0.728405	0.000000
10	7	0	-2.495108	1.440552	0.000000
11	1	0	-2.550576	2.431180	0.000000
12	1	0	-3.380752	0.993274	0.000000
13	7	0	2.495108	1.440552	0.000000
14	1	0	3.380752	0.993274	0.000000
15	1	0	2.550576	2.431180	0.000000
16	7	0	0.000000	-2.881103	0.000000
17	1	0	-0.830175	-3.424454	0.000000
18	1	0	0.830175	-3.424454	0.000000

B3LYP/6-311+G**

E = -409.0118103 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.419966	0.000000
2	1	0	0.000000	2.428779	0.000000
3	7	0	1.229727	-0.709983	0.000000
4	1	0	2.103384	-1.214389	0.000000
5	7	0	-1.229727	-0.709983	0.000000
6	1	0	-2.103384	-1.214389	0.000000
7	5	0	1.266800	0.731387	0.000000
8	5	0	0.000000	-1.462775	0.000000
9	5	0	-1.266800	0.731387	0.000000
10	7	0	2.504587	1.446024	0.000000
11	1	0	2.561480	2.450416	0.000000
12	1	0	3.402862	0.993098	0.000000
13	7	0	-2.504587	1.446024	0.000000
14	1	0	-3.402862	0.993098	0.000000
15	1	0	-2.561480	2.450416	0.000000
16	7	0	0.000000	-2.892048	0.000000
17	1	0	0.841383	-3.443514	0.000000
18	1	0	-0.841383	-3.443514	0.000000



(C_s)

HF/6-311+G**

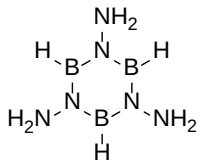
E = -272.1243532 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.542016	0.000000
2	1	0	0.481323	1.415706	0.000000
3	7	0	0.319654	-1.939107	0.000000
4	1	0	0.886580	-2.752996	0.000000
5	5	0	0.858662	-0.624457	0.000000
6	5	0	-1.420118	0.613633	0.000000
7	7	0	2.273688	-0.439436	0.000000
8	1	0	2.707391	0.452726	0.000000
9	1	0	2.919072	-1.193021	0.000000
10	7	0	-2.117943	1.840521	0.000000
11	1	0	-3.109178	1.882368	0.000000
12	1	0	-1.679772	2.732759	0.000000
13	1	0	-0.653789	-2.124857	0.000000
14	1	0	-2.072139	-0.386526	0.000000

B3LYP/6-311+G**

E = -273.8365921 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.548100	0.000000
2	1	0	0.481383	1.438983	0.000000
3	7	0	0.329855	-1.933617	0.000000
4	1	0	0.895242	-2.764791	0.000000
5	5	0	-1.423065	0.599995	0.000000
6	5	0	0.871698	-0.617136	0.000000
7	7	0	-2.147129	1.815375	0.000000
8	1	0	-1.723821	2.730644	0.000000
9	1	0	-3.152666	1.838783	0.000000
10	7	0	2.288841	-0.421638	0.000000
11	1	0	2.951198	-1.178527	0.000000
12	1	0	2.721949	0.485913	0.000000
13	1	0	-0.659691	-2.109880	0.000000
14	1	0	-2.057727	-0.412956	0.000000



(C_{3h})

HF/6-311+G**

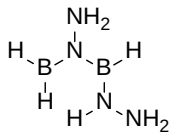
E = -406.2116237 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.411883	0.000000
2	7	0	1.222727	-0.705942	0.000000
3	7	0	-1.222727	-0.705942	0.000000
4	5	0	1.252123	0.718270	0.000000
5	5	0	-0.004022	-1.443505	0.000000
6	5	0	-1.248101	0.725235	0.000000
7	1	0	2.276706	1.317934	0.000000
8	1	0	0.003011	-2.630653	0.000000
9	1	0	-2.279717	1.312719	0.000000
10	7	0	-0.043999	2.827868	0.000000
11	1	0	0.435697	3.172527	0.806484
12	1	0	0.435697	3.172527	-0.806484
13	7	0	-2.427006	-1.452038	0.000000
14	1	0	-2.965337	-1.208939	0.806484
15	1	0	-2.965337	-1.208939	-0.806484
16	7	0	2.471005	-1.375830	0.000000
17	1	0	2.529641	-1.963588	0.806484
18	1	0	2.529641	-1.963588	-0.806484

B3LYP/6-311+G**

E = -408.7238922 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.412361	0.000000
2	7	0	1.223140	-0.706180	0.000000
3	7	0	-1.223140	-0.706180	0.000000
4	5	0	1.259173	0.722016	0.000000
5	5	0	-0.004303	-1.451484	0.000000
6	5	0	-1.254870	0.729468	0.000000
7	1	0	2.284929	1.320936	0.000000
8	1	0	0.001500	-2.639275	0.000000
9	1	0	-2.286429	1.318338	0.000000
10	7	0	-0.049082	2.854433	0.000000
11	1	0	0.459490	3.187375	0.814998
12	1	0	0.459490	3.187375	-0.814998
13	7	0	-2.447470	-1.469722	0.000000
14	1	0	-2.990093	-1.195757	0.814998
15	1	0	-2.990093	-1.195757	-0.814998
16	7	0	2.496552	-1.384710	0.000000
17	1	0	2.530602	-1.991618	0.814998
18	1	0	2.530602	-1.991618	-0.814998



(C_s)

HF/6-311+G**

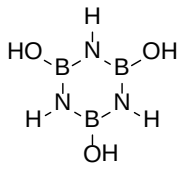
E = -271.9179978 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.923978	-0.564455	0.000000
2	7	0	-1.390315	0.400284	0.000000
3	5	0	0.574828	-1.923440	0.000000
4	5	0	0.000000	0.561924	0.000000
5	1	0	1.430554	-2.754169	0.000000
6	1	0	0.444466	1.662705	0.000000
7	7	0	2.296415	-0.183715	0.000000
8	1	0	2.742148	-0.570782	0.806631
9	1	0	2.742148	-0.570782	-0.806631
10	7	0	-2.320310	1.451643	0.000000
11	1	0	-2.194129	2.021546	0.810586
12	1	0	-2.194129	2.021546	-0.810586
13	1	0	-1.843181	-0.482313	0.000000
14	1	0	-0.570394	-2.246472	0.000000

B3LYP/6-311+G** imaginary frequency: –123.802 cm^{-1}

E = -273.6373543a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.925616	-0.568135	0.000000
2	7	0	-1.388782	0.396600	0.000000
3	5	0	0.577347	-1.926728	0.000000
4	5	0	0.000000	0.568705	0.000000
5	1	0	1.431994	-2.758992	0.000000
6	1	0	0.443298	1.670747	0.000000
7	7	0	2.323588	-0.168842	0.000000
8	1	0	2.764286	-0.586633	0.814773
9	1	0	2.764286	-0.586633	-0.814773
10	7	0	-2.353115	1.445925	0.000000
11	1	0	-2.214580	2.027588	0.820200
12	1	0	-2.214580	2.027588	-0.820200
13	1	0	-1.838024	-0.506653	0.000000
14	1	0	-0.574557	-2.235737	0.000000



(C_{3h})

HF/6-311+G**

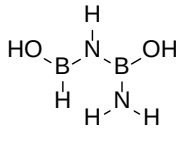
E = -466.0705299 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.413713	0.000000
2	1	0	0.034558	2.408485	0.000000
3	7	0	-1.224311	-0.706856	0.000000
4	1	0	-2.103088	-1.174314	0.000000
5	7	0	1.224311	-0.706856	0.000000
6	1	0	2.068530	-1.234170	0.000000
7	5	0	-1.252198	0.724735	0.000000
8	5	0	-0.001540	-1.446803	0.000000
9	5	0	1.253738	0.722068	0.000000
10	8	0	-2.468542	1.348387	0.000000
11	1	0	-2.442924	2.286930	0.000000
12	8	0	2.402008	1.463626	0.000000
13	1	0	3.202002	0.972169	0.000000
14	8	0	0.066533	-2.812013	0.000000
15	1	0	-0.759078	-3.259099	0.000000

B3LYP/6-311+G**

E = -468.6751267 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.417584	0.000000
2	1	0	0.036863	2.426691	0.000000
3	7	0	-1.227664	-0.708792	0.000000
4	1	0	-2.120007	-1.181421	0.000000
5	7	0	1.227664	-0.708792	0.000000
6	1	0	2.083145	-1.245270	0.000000
7	5	0	-1.257598	0.728205	0.000000
8	5	0	-0.001845	-1.453214	0.000000
9	5	0	1.259443	0.725009	0.000000
10	8	0	-2.491695	1.347764	0.000000
11	1	0	-2.458116	2.306838	0.000000
12	8	0	2.413046	1.483989	0.000000
13	1	0	3.226838	0.975372	0.000000
14	8	0	0.078649	-2.831754	0.000000
15	1	0	-0.768722	-3.282210	0.000000



(C_s)

HF/6-311+G**

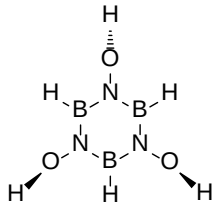
E = -311.825015 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.553650	0.000000
2	1	0	-0.447284	1.446552	0.000000
3	7	0	-0.367127	-1.924655	0.000000
4	1	0	-0.987416	-2.699603	0.000000
5	5	0	1.409978	0.620474	0.000000
6	5	0	-0.864452	-0.606283	0.000000
7	8	0	2.004305	1.845146	0.000000
8	1	0	2.942874	1.822651	0.000000
9	8	0	-2.228381	-0.462097	0.000000
10	1	0	-2.546832	0.420441	0.000000
11	1	0	2.078235	-0.368935	0.000000
12	1	0	0.595287	-2.159421	0.000000

B3LYP/6-311+G**

E = -313.6086595 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.558028	0.000000
2	1	0	-0.454228	1.464371	0.000000
3	7	0	-0.360460	-1.926189	0.000000
4	1	0	-0.979918	-2.719084	0.000000
5	5	0	-0.867417	-0.608661	0.000000
6	5	0	1.412537	0.620213	0.000000
7	8	0	-2.246240	-0.475061	0.000000
8	1	0	-2.563870	0.429733	0.000000
9	8	0	2.012448	1.856911	0.000000
10	1	0	2.971044	1.815656	0.000000
11	1	0	2.076499	-0.374162	0.000000
12	1	0	0.618432	-2.151950	0.000000



(C_s)

HF/6-311+G**

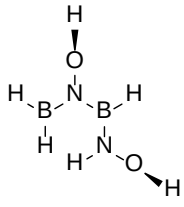
E = -465.6445867 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.084311	1.388972	0.000000
2	7	0	-0.057299	-0.694499	-1.205603
3	7	0	-0.057299	-0.694499	1.205603
4	5	0	0.030690	0.728006	-1.262493
5	5	0	-0.048578	-1.457182	0.000000
6	5	0	0.030690	0.728006	1.262493
7	1	0	0.058093	1.318318	-2.285573
8	1	0	-0.059387	-2.638469	0.000000
9	1	0	0.058093	1.318318	2.285573
10	8	0	0.045368	2.773039	0.000000
11	1	0	0.939110	3.071289	0.000000
12	8	0	0.030690	-1.388088	-2.400988
13	1	0	-0.850948	-1.519166	-2.705908
14	8	0	0.030690	-1.388088	2.400988
15	1	0	-0.850948	-1.519166	2.705908

B3LYP/6-311+G**

E = -468.2789596 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.254281	1.365985	0.000000
2	7	0	0.141044	-0.681411	1.203794
3	7	0	0.141044	-0.681411	-1.203794
4	5	0	-0.123057	0.722562	1.270202
5	5	0	0.236843	-1.448061	0.000000
6	5	0	-0.123057	0.722562	-1.270202
7	1	0	-0.225369	1.305017	2.294163
8	1	0	0.404540	-2.618312	0.000000
9	1	0	-0.225369	1.305017	-2.294163
10	8	0	-0.391740	2.783823	0.000000
11	1	0	-1.343859	2.944868	0.000000
12	8	0	0.141044	-1.401836	2.432833
13	1	0	1.059487	-1.392624	2.730473
14	8	0	0.141044	-1.401836	-2.432833
15	1	0	1.059487	-1.392624	-2.730473



(C_1)

HF/6-311+G**

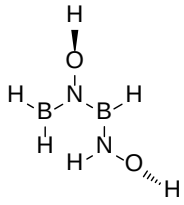
E = -311.539267 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.269548	-0.505193	-0.064829
2	1	0	0.414887	-1.678458	-0.042853
3	5	0	-1.490276	1.380115	0.032071
4	1	0	-0.652063	2.224405	0.069376
5	1	0	-2.645037	1.648203	0.049237
6	7	0	-1.075244	0.043185	-0.033525
7	7	0	1.392562	0.325346	-0.029249
8	1	0	1.407110	1.317709	-0.042102
9	8	0	-2.076573	-0.922745	-0.076046
10	1	0	-2.258407	-1.166012	0.815446
11	8	0	2.662151	-0.200072	-0.059171
12	1	0	2.931296	-0.317641	0.835841

B3LYP/6-311+G** imaginary frequency: -67.768 cm^{-1}

E = -313.339597 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.268651	-0.508308	-0.066815
2	1	0	0.410121	-1.683322	-0.046798
3	5	0	-1.488268	1.394995	0.032857
4	1	0	-0.631586	2.224520	0.070307
5	1	0	-2.641267	1.673666	0.050758
6	7	0	-1.077026	0.059687	-0.034038
7	7	0	1.390924	0.322130	-0.030299
8	1	0	1.406257	1.331674	-0.041824
9	8	0	-2.110393	-0.937873	-0.079062
10	1	0	-2.283265	-1.157762	0.844598
11	8	0	2.697908	-0.206035	-0.060985
12	1	0	2.940411	-0.343676	0.863485



(C_1)

HF/6-311+G**

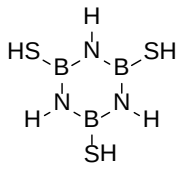
E = -311.5396443 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.270054	-0.506894	0.001883
2	1	0	0.416927	-1.678744	0.053619
3	5	0	-1.489655	1.380610	0.018323
4	1	0	-0.652325	2.225487	-0.026083
5	1	0	-2.643853	1.649890	0.049439
6	7	0	-1.074244	0.042329	0.033179
7	7	0	1.392015	0.323689	-0.051291
8	1	0	1.406013	1.315065	-0.096919
9	8	0	-2.074040	-0.924848	0.085327
10	1	0	-2.295386	-1.136462	-0.805397
11	8	0	2.661397	-0.202173	-0.080689
12	1	0	2.943372	-0.289774	0.813989

B3LYP/6-311+G**

E = -313.3399737 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.268686	-0.509209	0.001708
2	1	0	0.411142	-1.682932	0.056985
3	5	0	-1.488677	1.396016	0.019159
4	1	0	-0.633074	2.226262	-0.025652
5	1	0	-2.641360	1.674540	0.050670
6	7	0	-1.076363	0.059329	0.033444
7	7	0	1.390430	0.320608	-0.051697
8	1	0	1.404941	1.329016	-0.100794
9	8	0	-2.109297	-0.938170	0.087442
10	1	0	-2.293668	-1.155191	-0.834764
11	8	0	2.697136	-0.207270	-0.083034
12	1	0	2.950789	-0.321775	0.841725



(C_{3h})

HF/6-311+G**

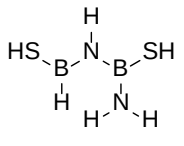
E = -1433.9416863 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.247198	0.718175	0.000000
2	5	0	-0.001641	-1.439193	0.000000
3	5	0	-1.245557	0.721017	0.000000
4	7	0	0.000000	1.412484	0.000000
5	1	0	0.006210	2.406900	0.000000
6	7	0	1.223247	-0.706242	0.000000
7	1	0	2.081332	-1.208828	0.000000
8	7	0	-1.223247	-0.706242	0.000000
9	1	0	-2.087541	-1.198072	0.000000
10	16	0	0.081370	-3.283964	0.000000
11	1	0	-1.222908	-3.546293	0.000000
12	16	0	-2.884681	1.571514	0.000000
13	1	0	-2.459726	2.832216	0.000000
14	16	0	2.803312	1.712450	0.000000
15	1	0	3.682634	0.714077	0.000000

B3LYP/6-311+G**

E = -1437.5032446 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.254149	0.722292	0.000000
2	5	0	0.001551	-1.447271	0.000000
3	5	0	1.252598	0.724979	0.000000
4	7	0	0.000000	1.416502	0.000000
5	1	0	-0.005969	2.425209	0.000000
6	7	0	-1.226726	-0.708251	0.000000
7	1	0	-2.097308	-1.217774	0.000000
8	7	0	1.226726	-0.708251	0.000000
9	1	0	2.103277	-1.207435	0.000000
10	16	0	-0.089327	-3.289331	0.000000
11	1	0	1.235447	-3.533809	0.000000
12	16	0	2.893308	1.567306	0.000000
13	1	0	2.442645	2.836833	0.000000
14	16	0	-2.803981	1.722025	0.000000
15	1	0	-3.678092	0.696977	0.000000



(C_s)

HF/6-311+G**

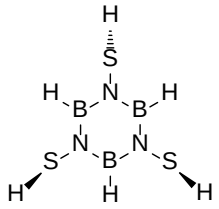
E = -957.0744674 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.347413	0.688092	0.000000
2	1	0	-2.235433	-0.097092	0.000000
3	5	0	0.513870	-1.069967	0.000000
4	7	0	0.000000	0.279213	0.000000
5	1	0	0.684125	1.004033	0.000000
6	7	0	-0.311662	-2.201296	0.000000
7	1	0	0.049043	-3.126217	0.000000
8	1	0	-1.303053	-2.152651	0.000000
9	16	0	2.344797	-1.381252	0.000000
10	1	0	2.772845	-0.121846	0.000000
11	16	0	-1.753514	2.474466	0.000000
12	1	0	-3.078708	2.366313	0.000000

B3LYP/6-311+G**

E = -959.4952595 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.362984	0.656993	0.000000
2	1	0	-2.221395	-0.164774	0.000000
3	5	0	0.554971	-1.052838	0.000000
4	7	0	0.000000	0.289096	0.000000
5	1	0	0.675447	1.042477	0.000000
6	7	0	-0.256180	-2.199755	0.000000
7	1	0	0.114220	-3.135293	0.000000
8	1	0	-1.262256	-2.155037	0.000000
9	16	0	2.387409	-1.324601	0.000000
10	1	0	2.762037	-0.030898	0.000000
11	16	0	-1.829391	2.421992	0.000000
12	1	0	-3.163031	2.239112	0.000000



(C_s)

HF/6-311+G**

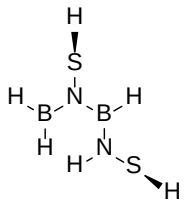
E = -1433.7323776 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000001	1.421789	0.009253
2	7	0	-1.231510	-0.711085	-0.005809
3	7	0	1.231509	-0.711086	-0.005809
4	5	0	-1.256240	0.725160	0.005144
5	5	0	-0.000001	-1.450654	-0.022851
6	5	0	1.256241	0.725159	0.005144
7	1	0	-2.279970	1.316094	0.011063
8	1	0	-0.000001	-2.632442	-0.043688
9	1	0	2.279971	1.316092	0.011063
10	16	0	0.000001	3.137484	0.080820
11	1	0	0.000001	3.399691	-1.226340
12	16	0	2.717706	-1.568402	-0.075904
13	1	0	2.941229	-1.702994	1.231543
14	16	0	-2.717707	-1.568400	-0.075904
15	1	0	-2.941230	-1.702992	1.231543

B3LYP/6-311+G** (C_1)

E = -1437.3025644 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.094635	1.414740	0.004173
2	7	0	-1.177957	-0.789631	-0.001609
3	7	0	1.272645	-0.625858	-0.001697
4	5	0	-1.309911	0.643610	0.003499
5	5	0	0.097385	-1.456676	-0.018511
6	5	0	1.212491	0.812213	0.003321
7	1	0	-2.372174	1.165305	0.008245
8	1	0	0.176182	-2.637391	-0.035611
9	1	0	2.195792	1.470782	0.007656
10	16	0	-0.211411	3.161336	0.083083
11	1	0	-0.225431	3.405786	-1.247669
12	16	0	2.844061	-1.397442	-0.078493
13	1	0	3.061974	-1.504980	1.252630
14	16	0	-2.632661	-1.763510	-0.078671
15	1	0	-2.836355	-1.896130	1.252430



(C_1)

HF/6-311+G**

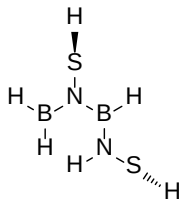
E = -956.9321737 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.352434	0.411338	0.016853
2	7	0	1.158665	0.340163	0.002800
3	5	0	-0.145362	-0.318559	-0.012994
4	5	0	1.366777	1.742741	0.011940
5	1	0	-0.193861	-1.500273	-0.041649
6	1	0	2.463905	2.192318	0.006286
7	16	0	2.543687	-0.687418	-0.078850
8	1	0	2.694706	-0.928371	1.223487
9	16	0	-2.893568	-0.290399	-0.082421
10	1	0	-3.180526	-0.376882	1.217948
11	1	0	0.425210	2.471694	0.027658
12	1	0	-1.362029	1.405172	0.014312

B3LYP/6-311+G**

E = -959.3570514 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.348550	0.407158	0.043919
2	7	0	1.155785	0.356322	0.007241
3	5	0	-0.145768	-0.324306	-0.014797
4	5	0	1.358671	1.755412	0.003253
5	1	0	-0.188175	-1.506844	-0.068047
6	1	0	2.452313	2.215922	0.001015
7	16	0	2.576362	-0.687677	-0.079508
8	1	0	2.654602	-0.991210	1.236340
9	16	0	-2.917789	-0.294717	-0.092608
10	1	0	-3.217427	-0.383771	1.226581
11	1	0	0.399086	2.466557	0.002414
12	1	0	-1.352719	1.417753	0.055142



(C_1)

HF/6-311+G**

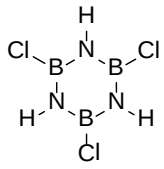
E = -956.9322831 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.352352	0.411882	0.015351
2	7	0	1.158744	0.340680	-0.005223
3	5	0	-0.145355	-0.317779	-0.019859
4	5	0	1.367123	1.743198	0.000420
5	1	0	-0.194056	-1.499227	-0.057961
6	1	0	2.464338	2.192570	-0.003527
7	16	0	-2.892847	-0.295072	0.079665
8	1	0	-3.184347	-0.309379	-1.222481
9	16	0	2.543717	-0.687485	-0.079263
10	1	0	2.683102	-0.934416	1.223207
11	1	0	0.425511	2.472223	0.009022
12	1	0	-1.362049	1.404112	0.071593

B3LYP/6-311+G**

E = -959.357133 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.348797	0.409892	-0.001252
2	7	0	-1.156091	0.356981	-0.003892
3	5	0	0.145785	-0.322851	0.023003
4	5	0	-1.359723	1.755856	-0.009637
5	1	0	0.188476	-1.506032	0.060329
6	1	0	-2.453576	2.215875	-0.013500
7	16	0	2.917484	-0.301350	-0.083545
8	1	0	3.214203	-0.298153	1.239342
9	16	0	-2.576273	-0.687531	0.082497
10	1	0	-2.641188	-1.008793	-1.229776
11	1	0	-0.400383	2.467344	-0.010119
12	1	0	1.353833	1.418726	-0.060328



(D_{3h})

HF/6-311+G**

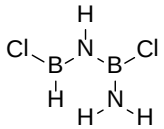
E = -1618.1691107 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.235404	0.713261	0.000000
2	5	0	-1.235404	0.713261	0.000000
3	5	0	0.000000	-1.426522	0.000000
4	7	0	0.000000	1.411381	0.000000
5	7	0	-1.222292	-0.705690	0.000000
6	7	0	1.222292	-0.705690	0.000000
7	1	0	0.000000	2.406618	0.000000
8	1	0	-2.084192	-1.203309	0.000000
9	1	0	2.084192	-1.203309	0.000000
10	17	0	0.000000	-3.211716	0.000000
11	17	0	2.781428	1.605858	0.000000
12	17	0	-2.781428	1.605858	0.000000

B3LYP/6-311+G**

E = -1621.7782558 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.415349	0.000000
2	1	0	0.000000	2.425075	0.000000
3	7	0	1.225728	-0.707674	0.000000
4	1	0	2.100176	-1.212537	0.000000
5	7	0	-1.225728	-0.707674	0.000000
6	1	0	-2.100176	-1.212537	0.000000
7	5	0	1.243178	0.717749	0.000000
8	5	0	0.000000	-1.435499	0.000000
9	5	0	-1.243178	0.717749	0.000000
10	17	0	-2.789062	1.610266	0.000000
11	17	0	2.789062	1.610266	0.000000
12	17	0	0.000000	-3.220531	0.000000



(C_s)

HF/6-311+G**

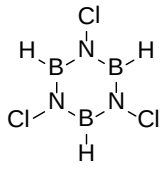
E = -1079.8898596 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.324555	0.730681	0.000000
2	1	0	-2.248953	-0.005221	0.000000
3	5	0	0.464448	-1.078851	0.000000
4	7	0	-0.358762	-2.200059	0.000000
5	1	0	-1.350607	-2.151610	0.000000
6	1	0	0.012144	-3.121027	0.000000
7	7	0	0.000000	0.282452	0.000000
8	1	0	0.713519	0.980117	0.000000
9	17	0	2.245681	-1.333037	0.000000
10	17	0	-1.675930	2.477851	0.000000

B3LYP/6-311+G**

E = -1082.3418264 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.287507	0.000000
2	1	0	0.717977	1.002378	0.000000
3	7	0	-0.338969	-2.202088	0.000000
4	1	0	0.034534	-3.136752	0.000000
5	5	0	-1.332791	0.722642	0.000000
6	5	0	0.484320	-1.075968	0.000000
7	17	0	2.266383	-1.314692	0.000000
8	17	0	-1.710275	2.461025	0.000000
9	1	0	-2.245894	-0.033793	0.000000
10	1	0	-1.345303	-2.150809	0.000000



(D_{3h})

HF/6-311+G**

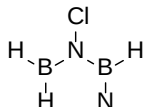
E = -1617.8258525 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.397280	0.000000
2	7	0	1.210080	-0.698640	0.000000
3	7	0	-1.210080	-0.698640	0.000000
4	5	0	0.000000	-1.463477	0.000000
5	1	0	0.000000	-2.641379	0.000000
6	5	0	-1.267408	0.731739	0.000000
7	1	0	-2.287501	1.320690	0.000000
8	5	0	1.267408	0.731739	0.000000
9	1	0	2.287501	1.320690	0.000000
10	17	0	0.000000	3.104101	0.000000
11	17	0	2.688230	-1.552051	0.000000
12	17	0	-2.688230	-1.552051	0.000000

B3LYP/6-311+G**

E = -1621.461356 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.392414	0.000000
2	7	0	-1.205866	-0.696207	0.000000
3	7	0	1.205866	-0.696207	0.000000
4	5	0	0.000000	-1.472076	0.000000
5	1	0	0.000000	-2.651556	0.000000
6	5	0	1.274855	0.736038	0.000000
7	1	0	2.296315	1.325778	0.000000
8	5	0	-1.274855	0.736038	0.000000
9	1	0	-2.296315	1.325778	0.000000
10	17	0	0.000000	3.137967	0.000000
11	17	0	-2.717559	-1.568983	0.000000
12	17	0	2.717559	-1.568983	0.000000



(C_s)

HF/6-311+G**

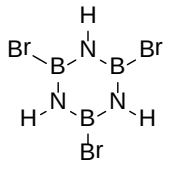
E = -1079.6595181 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.884699	-0.802409	0.000000
2	7	0	-1.392543	0.178604	0.000000
3	5	0	0.000000	0.354669	0.000000
4	1	0	0.450823	1.443981	0.000000
5	5	0	0.538303	-2.170479	0.000000
6	1	0	1.370606	-3.010984	0.000000
7	17	0	2.559776	-0.418420	0.000000
8	17	0	-2.469314	1.485763	0.000000
9	1	0	-1.877200	-0.687417	0.000000
10	1	0	-0.618704	-2.444738	0.000000

B3LYP/6-311+G**

E = -1082.1277512 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.878033	-0.817448	0.000000
2	7	0	-1.388484	0.170922	0.000000
3	5	0	0.538301	-2.179603	0.000000
4	1	0	1.362363	-3.029821	0.000000
5	5	0	0.000000	0.355331	0.000000
6	1	0	0.452384	1.445760	0.000000
7	17	0	2.594971	-0.409936	0.000000
8	17	0	-2.502370	1.490680	0.000000
9	1	0	-1.879294	-0.710341	0.000000
10	1	0	-0.628011	-2.431211	0.000000



(D_{3h})

HF/6-311+G**

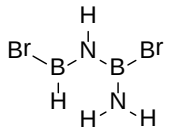
E = -7956.7333491 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.412686	0.000000
2	1	0	0.000000	2.407493	0.000000
3	7	0	1.223422	-0.706343	0.000000
4	1	0	2.084950	-1.203747	0.000000
5	7	0	-1.223422	-0.706343	0.000000
6	1	0	-2.084950	-1.203747	0.000000
7	5	0	1.232820	0.711769	0.000000
8	5	0	0.000000	-1.423538	0.000000
9	5	0	-1.232820	0.711769	0.000000
10	35	0	0.000000	-3.375577	0.000000
11	35	0	2.923335	1.687788	0.000000
12	35	0	-2.923335	1.687788	0.000000

B3LYP/6-311+G**

E = -7963.5207673 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.416024	0.000000
2	1	0	0.000000	2.425392	0.000000
3	7	0	1.226313	-0.708012	0.000000
4	1	0	2.100451	-1.212696	0.000000
5	7	0	-1.226313	-0.708012	0.000000
6	1	0	-2.100451	-1.212696	0.000000
7	5	0	1.241318	0.716675	0.000000
8	5	0	0.000000	-1.433351	0.000000
9	5	0	-1.241318	0.716675	0.000000
10	35	0	0.000000	-3.384406	0.000000
11	35	0	2.930981	1.692203	0.000000
12	35	0	-2.930981	1.692203	0.000000



(C_s)

HF/6-311+G**

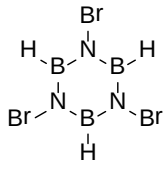
E = -5305.6004925 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.149780	0.000000
2	1	0	0.816938	-0.422646	0.000000
3	7	0	-2.507393	0.045747	0.000000
4	1	0	-3.345530	-0.486307	0.000000
5	5	0	0.191606	1.533842	0.000000
6	5	0	-1.254682	-0.553426	0.000000
7	35	0	1.994477	2.271244	0.000000
8	35	0	-1.173413	-2.519816	0.000000
9	1	0	-2.641730	1.030270	0.000000
10	1	0	-0.699806	2.307943	0.000000

B3LYP/6-311+G**

E = -5310.1709541 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.147332	0.000000
2	1	0	0.854096	-0.397118	0.000000
3	7	0	-2.505212	-0.065467	0.000000
4	1	0	-3.336430	-0.633031	0.000000
5	5	0	0.128242	1.542566	0.000000
6	5	0	-1.226937	-0.619711	0.000000
7	35	0	1.887527	2.367473	0.000000
8	35	0	-1.059170	-2.577651	0.000000
9	1	0	-2.673422	0.928766	0.000000
10	1	0	-0.806798	2.270299	0.000000



(D_{3h})

HF/6-311+G**

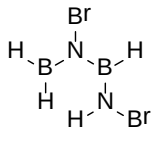
E = -7956.4299676 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.402388	0.000000
2	7	0	1.214503	-0.701194	0.000000
3	7	0	-1.214503	-0.701194	0.000000
4	5	0	0.000000	-1.461304	0.000000
5	1	0	0.000000	-2.640482	0.000000
6	5	0	-1.265526	0.730652	0.000000
7	1	0	-2.286725	1.320241	0.000000
8	5	0	1.265526	0.730652	0.000000
9	1	0	2.286725	1.320241	0.000000
10	35	0	0.000000	3.255372	0.000000
11	35	0	2.819235	-1.627686	0.000000
12	35	0	-2.819235	-1.627686	0.000000

B3LYP/6-311+G**

E = -7963.2456699 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.394739	0.000000
2	7	0	1.207879	-0.697369	0.000000
3	7	0	-1.207879	-0.697369	0.000000
4	5	0	0.000000	-1.471385	0.000000
5	1	0	0.000000	-2.651922	0.000000
6	5	0	-1.274257	0.735692	0.000000
7	1	0	-2.296632	1.325961	0.000000
8	5	0	1.274257	0.735692	0.000000
9	1	0	2.296632	1.325961	0.000000
10	35	0	0.000000	3.292964	0.000000
11	35	0	2.851790	-1.646482	0.000000
12	35	0	-2.851790	-1.646482	0.000000



(C_s)

HF/6-311+G**

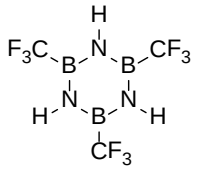
E = -5305.3959943 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.537425	-1.239419	0.000000
2	7	0	-1.388010	0.333039	0.000000
3	5	0	0.000000	0.115911	0.000000
4	1	0	0.732356	1.041421	0.000000
5	5	0	-0.179228	-2.455959	0.000000
6	1	0	0.378587	-3.499965	0.000000
7	35	0	2.400367	-1.344379	0.000000
8	35	0	-2.137756	2.009481	0.000000
9	1	0	-2.083899	-0.374962	0.000000
10	1	0	-1.368193	-2.400162	0.000000

B3LYP/6-311+G**

E = -5309.9843964 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.512290	-1.260181	0.000000
2	7	0	-1.384541	0.330324	0.000000
3	5	0	0.000000	0.113898	0.000000
4	1	0	0.742381	1.033016	0.000000
5	5	0	-0.200576	-2.469173	0.000000
6	1	0	0.339076	-3.523834	0.000000
7	35	0	2.428834	-1.365748	0.000000
8	35	0	-2.156939	2.038371	0.000000
9	1	0	-2.096980	-0.383851	0.000000
10	1	0	-1.392171	-2.381754	0.000000



(C_{3v})

HF/6-311+G**

E = -1248.3842993 a.u.

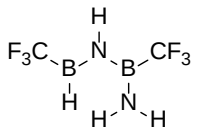
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.423299	-0.042679
2	5	0	-1.232613	-0.711650	-0.042679
3	5	0	1.232613	-0.711650	-0.042679
4	7	0	0.000000	-1.412313	-0.048133
5	1	0	0.000000	-2.409014	-0.077222
6	7	0	-1.223099	0.706156	-0.048133
7	1	0	-2.086267	1.204507	-0.077222
8	7	0	1.223099	0.706156	-0.048133
9	1	0	2.086267	1.204507	-0.077222
10	6	0	0.000000	3.037384	-0.000627
11	6	0	-2.630451	-1.518692	-0.000627
12	6	0	2.630451	-1.518692	-0.000627
13	9	0	0.000000	3.478472	1.251783
14	9	0	1.066203	3.560622	-0.590818
15	9	0	-1.066203	3.560622	-0.590818
16	9	0	3.012445	-1.739236	1.251783
17	9	0	3.616691	-0.856952	-0.590818
18	9	0	2.550488	-2.703670	-0.590818
19	9	0	-3.012445	-1.739236	1.251783
20	9	0	-3.616691	-0.856952	-0.590818
21	9	0	-2.550488	-2.703670	-0.590818

B3LYP/6-311+G**

E = -1254.2188791 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.431384	-0.037311
2	5	0	-1.239615	-0.715692	-0.037311
3	5	0	1.239615	-0.715692	-0.037311
4	7	0	0.000000	-1.413929	-0.041563
5	1	0	0.000000	-2.425658	-0.072346
6	7	0	-1.224499	0.706965	-0.041563
7	1	0	-2.100682	1.212829	-0.072346
8	7	0	1.224499	0.706965	-0.041563
9	1	0	2.100682	1.212829	-0.072346
10	6	0	0.000000	3.039974	-0.002003
11	6	0	-2.632695	-1.519987	-0.002003
12	6	0	2.632695	-1.519987	-0.002003
13	9	0	0.000000	3.502431	1.278205
14	9	0	1.091663	3.576403	-0.607888
15	9	0	-1.091663	3.576403	-0.607888
16	9	0	3.033194	-1.751215	1.278205
17	9	0	3.643088	-0.842794	-0.607888

18	9	0	2.551425	-2.733610	-0.607888
19	9	0	-3.033194	-1.751215	1.278205
20	9	0	-3.643088	-0.842794	-0.607888
21	9	0	-2.551425	-2.733610	-0.607888



(C_s)

HF/6-311+G** imaginary frequences: –51.297, –27.088 cm^{-1}

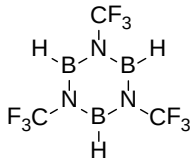
E = -833.3645315 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.951871	1.259023	0.000000
2	5	0	-0.556484	-1.255206	0.000000
3	7	0	-0.139744	0.123788	0.000000
4	1	0	0.849364	0.267556	0.000000
5	7	0	-1.871947	-1.695280	0.000000
6	1	0	-2.108851	-2.660773	0.000000
7	6	0	-0.248290	2.715698	0.000000
8	6	0	0.607110	-2.387069	0.000000
9	9	0	0.529699	-3.177209	1.064343
10	9	0	1.830907	-1.869247	0.000000
11	9	0	0.529699	-3.177209	-1.064343
12	9	0	0.529699	2.881121	1.066059
13	9	0	0.529699	2.881121	-1.066059
14	9	0	-1.113772	3.715960	0.000000
15	1	0	-2.658531	-1.088305	0.000000
16	1	0	-2.134657	1.200283	0.000000

B3LYP/6-311+G** imaginary frequences: –49.717, –27.079 cm^{-1}

E = -837.2991095a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.954045	1.259820	0.000000
2	5	0	-0.554633	-1.263835	0.000000
3	7	0	-0.139403	0.124638	0.000000
4	1	0	0.865799	0.267666	0.000000
5	7	0	-1.874538	-1.696041	0.000000
6	1	0	-2.124009	-2.672763	0.000000
7	6	0	-0.263280	2.715218	0.000000
8	6	0	0.607328	-2.390159	0.000000
9	9	0	0.535235	-3.202299	1.089277
10	9	0	1.859668	-1.855052	0.000000
11	9	0	0.535235	-3.202299	-1.089277
12	9	0	0.535235	2.892535	1.091908
13	9	0	0.535235	2.892535	-1.091908
14	9	0	-1.151767	3.736608	0.000000
15	1	0	-2.665976	-1.071153	0.000000
16	1	0	-2.138716	1.187529	0.000000



(C_{3h})

HF/6-311+G**

E = -1248.3452299 a.u.

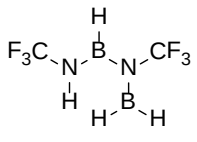
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.974606	1.079721	0.000000
2	1	0	1.778598	1.933886	0.000000
3	5	0	0.447763	-1.383894	0.000000
4	1	0	0.785495	-2.507254	0.000000
5	5	0	-1.422369	0.304173	0.000000
6	1	0	-2.564094	0.573368	0.000000
7	7	0	-0.431989	1.354583	0.000000
8	7	0	1.389097	-0.303178	0.000000
9	7	0	-0.957108	-1.051405	0.000000
10	6	0	-0.928582	2.679663	0.000000
11	6	0	2.784948	-0.535656	0.000000
12	6	0	-1.856365	-2.144007	0.000000
13	9	0	3.358426	0.000000	1.057916
14	9	0	3.358426	0.000000	-1.057916
15	9	0	3.075531	-1.811612	0.000000
16	9	0	-1.679213	-2.908482	1.057916
17	9	0	-1.679213	-2.908482	-1.057916
18	9	0	-3.106668	-1.757682	0.000000
19	9	0	-1.679213	2.908482	1.057916
20	9	0	0.031137	3.569294	0.000000
21	9	0	-1.679213	2.908482	-1.057916

B3LYP/6-311+G**

E = -1254.1610161 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.980405	1.082667	0.000000
2	1	0	1.784998	1.939920	0.000000
3	5	0	0.447415	-1.390390	0.000000
4	1	0	0.787522	-2.515814	0.000000
5	5	0	-1.427820	0.307722	0.000000
6	1	0	-2.572519	0.575893	0.000000
7	7	0	-0.429685	1.355448	0.000000
8	7	0	1.388695	-0.305606	0.000000
9	7	0	-0.959010	-1.049842	0.000000
10	6	0	-0.925077	2.697042	0.000000
11	6	0	2.798245	-0.547381	0.000000
12	6	0	-1.873168	-2.149661	0.000000
13	9	0	3.386075	0.000000	1.083816
14	9	0	3.386075	0.000000	-1.083816
15	9	0	3.092295	-1.852938	0.000000
16	9	0	-1.693037	-2.932427	1.083816
17	9	0	-1.693037	-2.932427	-1.083816

18	9	0	-3.150839	-1.751537	0.000000
19	9	0	-1.693037	2.932427	1.083816
20	9	0	0.058544	3.604475	0.000000
21	9	0	-1.693037	2.932427	-1.083816



(C_1)

HF/6-311+G**

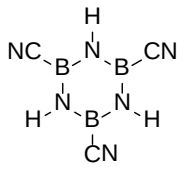
E = -833.3429929 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.345198	2.028898	0.003714
2	1	0	-2.399448	2.555387	0.010745
3	5	0	0.058974	-0.100832	-0.012608
4	1	0	0.064756	-1.278915	-0.015151
5	7	0	1.292579	0.584332	-0.022163
6	7	0	-1.218575	0.608221	-0.001836
7	6	0	2.535008	-0.058129	-0.001370
8	6	0	-2.358142	-0.235505	0.001031
9	9	0	3.492064	0.833429	-0.147816
10	9	0	2.656959	-0.946467	-0.963512
11	9	0	2.762335	-0.698286	1.129097
12	9	0	-2.378242	-1.016515	-1.060847
13	9	0	-3.480883	0.435900	0.010495
14	9	0	-2.365983	-1.025723	1.056277
15	1	0	1.365336	1.575345	0.004310
16	1	0	-0.354999	2.680734	0.001342

B3LYP/6-311+G**

E = -837.2650935 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.319386	2.024621	0.013202
2	1	0	-2.367861	2.566789	0.028861
3	5	0	0.051101	-0.138883	-0.021726
4	1	0	0.036050	-1.317283	-0.017465
5	7	0	1.285326	0.542907	-0.050774
6	7	0	-1.217479	0.604443	-0.002062
7	6	0	2.555595	-0.061803	-0.005317
8	6	0	-2.387091	-0.224335	0.001699
9	9	0	3.461245	0.720398	-0.632609
10	9	0	2.562148	-1.268045	-0.588384
11	9	0	3.011793	-0.233326	1.260653
12	9	0	-2.423215	-1.019882	-1.089119
13	9	0	-3.522206	0.482478	0.017175
14	9	0	-2.404711	-1.037370	1.079966
15	1	0	1.334067	1.553092	-0.016677
16	1	0	-0.312279	2.655806	0.010335



(D_{3h})

HF/6-311+G**

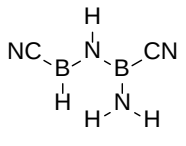
E = -516.5435175 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.235147	0.713112	0.000000
2	5	0	-1.235147	0.713112	0.000000
3	5	0	0.000000	-1.426225	0.000000
4	7	0	0.000000	1.411463	0.000000
5	1	0	0.000000	2.407662	0.000000
6	7	0	-1.222363	-0.705732	0.000000
7	1	0	-2.085097	-1.203831	0.000000
8	7	0	1.222363	-0.705732	0.000000
9	1	0	2.085097	-1.203831	0.000000
10	6	0	-2.590319	1.495521	0.000000
11	6	0	0.000000	-2.991043	0.000000
12	6	0	2.590319	1.495521	0.000000
13	7	0	-3.570183	2.061246	0.000000
14	7	0	0.000000	-4.122492	0.000000
15	7	0	3.570183	2.061246	0.000000

B3LYP/6-311+G**

E = -519.6020044 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.246252	0.719524	0.000000
2	5	0	0.000000	-1.439047	0.000000
3	5	0	-1.246252	0.719524	0.000000
4	7	0	0.000000	1.413970	0.000000
5	1	0	0.000000	2.424644	0.000000
6	7	0	1.224534	-0.706985	0.000000
7	1	0	2.099803	-1.212322	0.000000
8	7	0	-1.224534	-0.706985	0.000000
9	1	0	-2.099803	-1.212322	0.000000
10	6	0	-2.585472	1.492723	0.000000
11	6	0	0.000000	-2.985446	0.000000
12	6	0	2.585472	1.492723	0.000000
13	7	0	-3.585433	2.070051	0.000000
14	7	0	0.000000	-4.140101	0.000000
15	7	0	3.585433	2.070051	0.000000



(C_s)

HF/6-311+G**

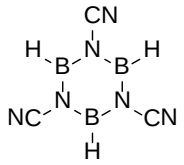
E = -345.4739209 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.257185	0.901570	0.000000
2	1	0	-2.262689	0.279136	0.000000
3	5	0	0.292054	-1.120947	0.000000
4	7	0	0.000000	0.292058	0.000000
5	1	0	0.795597	0.895108	0.000000
6	7	0	-0.657244	-2.131933	0.000000
7	1	0	-0.401549	-3.092154	0.000000
8	1	0	-1.637631	-1.970685	0.000000
9	6	0	-1.357731	2.461889	0.000000
10	6	0	1.810032	-1.537061	0.000000
11	7	0	-1.442939	3.591041	0.000000
12	7	0	2.902773	-1.831665	0.000000

B3LYP/6-311+G**

E = -347.5578826 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.281748	0.867792	0.000000
2	1	0	-2.257057	0.190698	0.000000
3	5	0	0.347433	-1.112173	0.000000
4	7	0	0.000000	0.299696	0.000000
5	1	0	0.786579	0.938559	0.000000
6	7	0	-0.587862	-2.143233	0.000000
7	1	0	-1.584667	-1.991073	0.000000
8	1	0	-0.316773	-3.113520	0.000000
9	6	0	1.857166	-1.482551	0.000000
10	6	0	-1.448524	2.401244	0.000000
11	7	0	2.980604	-1.749337	0.000000
12	7	0	-1.593936	3.547886	0.000000



(D_{3h})

HF/6-311+G**

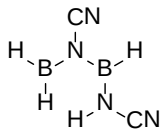
E = -516.4101955 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.270771	0.733680	0.000000
2	1	0	2.288583	1.321315	0.000000
3	5	0	0.000000	-1.467360	0.000000
4	1	0	0.000000	-2.642628	0.000000
5	5	0	-1.270771	0.733680	0.000000
6	1	0	-2.288584	1.321314	0.000000
7	7	0	1.227712	-0.708819	0.000000
8	7	0	-1.227711	-0.708820	0.000000
9	7	0	0.000000	1.417639	0.000000
10	6	0	2.397660	-1.384290	0.000000
11	6	0	-2.397660	-1.384290	0.000000
12	6	0	0.000000	2.768580	0.000000
13	7	0	-3.375615	-1.948912	0.000000
14	7	0	3.375615	-1.948912	0.000000
15	7	0	0.000000	3.897824	0.000000

B3LYP/6-311+G**

E = -519.4683504 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.274422	0.735788	0.000000
2	1	0	2.294562	1.324766	0.000000
3	5	0	-1.274422	0.735788	0.000000
4	1	0	-2.294562	1.324766	0.000000
5	5	0	0.000000	-1.471576	0.000000
6	1	0	0.000000	-2.649532	0.000000
7	7	0	0.000000	1.421956	0.000000
8	7	0	-1.231450	-0.710978	0.000000
9	7	0	1.231450	-0.710978	0.000000
10	6	0	0.000000	2.779293	0.000000
11	6	0	-2.406938	-1.389646	0.000000
12	6	0	2.406938	-1.389646	0.000000
13	7	0	-3.406292	-1.966624	0.000000
14	7	0	0.000000	3.933248	0.000000
15	7	0	3.406292	-1.966624	0.000000



(C_s)

HF/6-311+G**

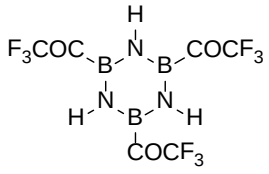
E = -345.3868317 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.492839	-2.156499	0.000000
2	1	0	-0.662190	-2.419741	0.000000
3	1	0	1.324559	-2.994151	0.000000
4	5	0	0.000000	0.386746	0.000000
5	1	0	0.457270	1.471645	0.000000
6	7	0	0.885963	-0.773502	0.000000
7	7	0	-1.409491	0.218574	0.000000
8	1	0	-1.846990	-0.676992	0.000000
9	6	0	2.212100	-0.502689	0.000000
10	6	0	-2.267333	1.249816	0.000000
11	7	0	3.318921	-0.275655	0.000000
12	7	0	-2.996171	2.114189	0.000000

B3LYP/6-311+G**

E = -347.4703736 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.520141	-2.137518	0.000000
2	1	0	-0.639096	-2.396906	0.000000
3	1	0	1.354289	-2.975310	0.000000
4	5	0	0.000000	0.400469	0.000000
5	1	0	0.439051	1.495124	0.000000
6	7	0	0.908468	-0.754728	0.000000
7	7	0	-1.404210	0.197051	0.000000
8	1	0	-1.803147	-0.735437	0.000000
9	6	0	2.237120	-0.464816	0.000000
10	6	0	-2.307031	1.195391	0.000000
11	7	0	3.364512	-0.216121	0.000000
12	7	0	-3.087675	2.047273	0.000000



(C_{3h})

HF/6-311+G**

E = -1586.6285138 a.u.

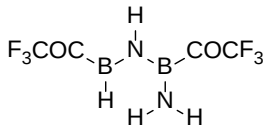
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.068863	1.423204	0.000000
2	7	0	-1.253000	0.648267	0.000000
3	5	0	-1.198099	-0.771239	0.000000
4	7	0	0.065084	-1.409263	0.000000
5	5	0	1.266962	-0.651964	0.000000
6	7	0	1.187916	0.760996	0.000000
7	6	0	-0.026160	3.049388	0.000000
8	1	0	-2.155355	1.073760	0.000000
9	1	0	0.147774	-2.403472	0.000000
10	1	0	2.007581	1.329712	0.000000
11	8	0	1.004309	3.631013	0.000000
12	6	0	2.653927	-1.502039	0.000000
13	8	0	2.642394	-2.685264	0.000000
14	6	0	-2.627767	-1.547349	0.000000
15	8	0	-3.646704	-0.945749	0.000000
16	6	0	-1.332350	3.863237	0.000000
17	6	0	-2.679487	-3.085468	0.000000
18	6	0	4.011837	-0.777769	0.000000
19	9	0	-1.133865	5.147179	0.000000
20	9	0	-2.047284	3.546001	1.064909
21	9	0	-2.047284	3.546001	-1.064909
22	9	0	4.094569	0.000000	1.064909
23	9	0	4.094569	0.000000	-1.064909
24	9	0	5.024520	-1.591633	0.000000
25	9	0	-2.047284	-3.546001	1.064909
26	9	0	-3.890655	-3.555545	0.000000
27	9	0	-2.047284	-3.546001	-1.064909

B3LYP/6-311+G**

E = -1594.2517056 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.056173	1.433790	0.000000
2	7	0	-1.248162	0.660693	0.000000
3	5	0	-1.213612	-0.765542	0.000000
4	7	0	0.051904	-1.411287	0.000000
5	5	0	1.269785	-0.668248	0.000000
6	7	0	1.196258	0.750594	0.000000
7	6	0	0.005594	3.046549	0.000000
8	1	0	-2.161726	1.099755	0.000000
9	1	0	0.128447	-2.421987	0.000000
10	1	0	2.033278	1.322232	0.000000
11	8	0	1.059058	3.637627	0.000000

12	6	0	2.635592	-1.528119	0.000000
13	8	0	2.620749	-2.735984	0.000000
14	6	0	-2.641185	-1.518430	0.000000
15	8	0	-3.679806	-0.901643	0.000000
16	6	0	-1.313575	3.873698	0.000000
17	6	0	-2.697934	-3.074438	0.000000
18	6	0	4.011508	-0.799260	0.000000
19	9	0	-1.112642	5.185866	0.000000
20	9	0	-2.048889	3.548780	1.090498
21	9	0	-2.048889	3.548780	-1.090498
22	9	0	4.097778	0.000000	1.090498
23	9	0	4.097778	0.000000	-1.090498
24	9	0	5.047413	-1.629357	0.000000
25	9	0	-2.048889	-3.548780	1.090498
26	9	0	-3.934771	-3.556509	0.000000
27	9	0	-2.048889	-3.548780	-1.090498



HF/6-311+G** (C_s)

E = -1058.8622148 a.u.

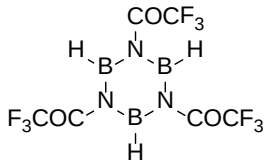
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.931368	-0.455267	0.000000
2	5	0	-1.622185	-0.905641	0.000000
3	7	0	-0.457148	-0.052949	0.000000
4	5	0	-0.421556	1.339610	0.000000
5	1	0	-3.687116	-1.102489	0.000000
6	1	0	0.441356	-0.492277	0.000000
7	6	0	1.062749	2.011338	0.000000
8	8	0	2.050212	1.358500	0.000000
9	6	0	-1.487025	-2.537338	0.000000
10	8	0	-2.445385	-3.231899	0.000000
11	6	0	-0.104147	-3.216156	0.000000
12	6	0	1.184653	3.544013	0.000000
13	9	0	0.577328	4.031625	1.066212
14	9	0	0.577328	4.031625	-1.066212
15	9	0	2.418068	3.960532	0.000000
16	9	0	0.577328	-2.829971	1.064870
17	9	0	-0.171263	-4.514347	0.000000
18	9	0	0.577328	-2.829971	-1.064870
19	1	0	-3.200885	0.500576	0.000000
20	1	0	-1.396089	2.012489	0.000000

B3LYP/6-311+G** (C_1)

E = -1063.9889954 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.345985	1.291703	-0.030676
2	7	0	-0.179517	0.427189	-0.064245
3	5	0	1.165399	0.792270	0.016703
4	7	0	-1.289302	2.676998	0.032772
5	6	0	-2.860401	0.702982	-0.066759
6	1	0	-0.338744	-0.572324	-0.167245
7	1	0	-2.141312	3.219375	0.042642
8	8	0	-3.822645	1.428275	-0.153154
9	6	0	2.221312	-0.430350	-0.067235
10	8	0	1.874842	-1.581543	-0.195492
11	6	0	-3.110998	-0.831291	0.039843
12	6	0	3.739291	-0.109279	0.020079
13	9	0	-4.390984	-1.166618	-0.068963
14	9	0	-2.648114	-1.278035	1.230890
15	9	0	-2.415213	-1.477894	-0.929738
16	9	0	4.000669	0.503894	1.197538
17	9	0	4.515840	-1.185852	-0.075293
18	9	0	4.074762	0.749103	-0.970830
19	1	0	-0.438688	3.217157	0.058263

20	1	0	1.517966	1.919001	0.137694



(C_3)

HF/6-311+G**

E = -1586.5897268 a.u.

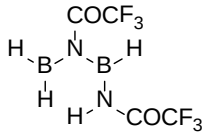
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.398154	1.374247	-0.349197
2	7	0	-1.389210	-0.342312	-0.349197
3	7	0	0.991055	-1.031935	-0.349197
4	5	0	-1.007003	1.053000	-0.359420
5	1	0	-1.827584	1.886145	-0.372673
6	5	0	-0.408423	-1.398590	-0.359420
7	1	0	-0.719658	-2.525807	-0.372673
8	5	0	1.415426	0.345590	-0.359420
9	1	0	2.547242	0.639661	-0.372673
10	6	0	0.857777	2.698824	-0.410316
11	8	0	1.862534	3.023969	-0.920098
12	6	0	0.000000	3.793750	0.272968
13	9	0	-0.562401	3.348689	1.375917
14	9	0	-0.945969	4.211813	-0.536918
15	9	0	0.752353	4.809064	0.583115
16	6	0	1.908362	-2.092269	-0.410316
17	8	0	1.687567	-3.124986	-0.920098
18	6	0	-2.766139	-0.606555	-0.410316
19	8	0	-3.550101	0.101018	-0.920098
20	6	0	3.285484	-1.896875	0.272968
21	6	0	-3.285484	-1.896875	0.272968
22	9	0	-3.174552	-2.925139	-0.536918
23	9	0	-2.618849	-2.161398	1.375917
24	9	0	-4.540948	-1.752975	0.583115
25	9	0	4.120521	-1.286674	-0.536918
26	9	0	3.788595	-3.056089	0.583115
27	9	0	3.181250	-1.187291	1.375917

B3LYP/6-311+G**

E = -1594.2066389 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.407157	1.373515	-0.342694
2	7	0	-1.393077	-0.334149	-0.342694
3	7	0	0.985920	-1.039366	-0.342694
4	5	0	-1.003613	1.064020	-0.346881
5	1	0	-1.824015	1.901999	-0.353765
6	5	0	-0.419662	-1.401164	-0.346881
7	1	0	-0.735172	-2.530643	-0.353765

8	5	0	1.423275	0.337144	-0.346881
9	1	0	2.559187	0.628643	-0.353765
10	6	0	0.882542	2.710932	-0.403168
11	8	0	1.922001	3.029223	-0.899858
12	6	0	0.000000	3.817752	0.263867
13	9	0	-0.567541	3.381431	1.406338
14	9	0	-0.978392	4.216974	-0.570012
15	9	0	0.754619	4.873986	0.554973
16	6	0	1.906465	-2.119770	-0.403168
17	8	0	1.662384	-3.179113	-0.899858
18	6	0	-2.789007	-0.591162	-0.403168
19	8	0	-3.584385	0.149890	-0.899858
20	6	0	3.306270	-1.908876	0.263867
21	6	0	-3.306270	-1.908876	0.263867
22	9	0	-3.162811	-2.955799	-0.570012
23	9	0	-2.644634	-2.182220	1.406338
24	9	0	-4.598305	-1.783474	0.554973
25	9	0	4.141203	-1.261175	-0.570012
26	9	0	3.843686	-3.090512	0.554973
27	9	0	3.212175	-1.199211	1.406338



(C_1)

HF/6-311+G**

E = -1058.8466269 a.u.

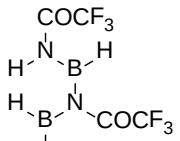
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.394865	1.085138	-0.169945
2	7	0	1.072708	0.640113	-0.221651
3	5	0	-0.311885	0.160743	-0.153870
4	1	0	-0.506578	-0.989316	-0.055337
5	5	0	1.455558	2.020340	-0.142057
6	1	0	2.584244	2.339712	-0.249601
7	6	0	-2.749784	0.885021	-0.063785
8	8	0	-3.533384	1.764419	-0.109258
9	6	0	-3.253234	-0.562694	0.126174
10	9	0	-2.744498	-1.092873	1.218552
11	9	0	-2.911119	-1.313842	-0.897388
12	9	0	-4.548576	-0.578904	0.230654
13	6	0	2.024596	-0.366951	-0.444101
14	8	0	1.818236	-1.341930	-1.063616
15	6	0	3.427087	-0.200861	0.195419
16	9	0	4.224384	0.472263	-0.603576
17	9	0	3.368593	0.427286	1.349524
18	9	0	3.953469	-1.374403	0.402105
19	1	0	0.619588	2.844556	0.006285
20	1	0	-1.211604	2.060120	-0.278627

B3LYP/6-311+G**

E = -1063.9698734 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.395553	1.087480	-0.175750
2	7	0	1.069669	0.628614	-0.221126
3	5	0	-0.323318	0.151253	-0.158562
4	1	0	-0.527499	-1.000500	-0.062758
5	5	0	1.450481	2.009760	-0.148504
6	1	0	2.581581	2.332022	-0.236096
7	6	0	-2.764947	0.901253	-0.067696
8	8	0	-3.555228	1.806594	-0.113367
9	6	0	-3.275831	-0.559595	0.125507
10	9	0	-2.757084	-1.108116	1.244081
11	9	0	-2.933054	-1.336365	-0.921133
12	9	0	-4.600129	-0.570217	0.234914
13	6	0	2.031073	-0.396723	-0.426278
14	8	0	1.805769	-1.415728	-1.010772
15	6	0	3.456300	-0.188372	0.186960
16	9	0	4.239537	0.521971	-0.647191
17	9	0	3.408009	0.452316	1.371650
18	9	0	4.031532	-1.373278	0.384843
19	1	0	0.600993	2.830322	-0.030874

20	1	0	-1.192887	2.077323	-0.279140



(C_1)

HF/6-311+G**

E = -1058.8479135 a.u.

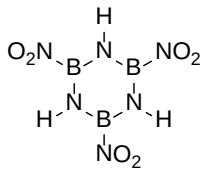
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.256573	1.070502	-0.050325
2	7	0	1.138132	0.320030	0.003361
3	5	0	-0.240603	0.046123	-0.250970
4	1	0	-0.538786	-1.012754	-0.656419
5	5	0	-0.971538	2.441407	0.286506
6	1	0	-1.854309	3.205668	0.445999
7	6	0	-2.606801	0.758343	-0.286585
8	8	0	-3.382352	1.493254	-0.769499
9	6	0	-3.115634	-0.636276	0.160845
10	9	0	-2.433458	-1.101757	1.185119
11	9	0	-3.022684	-1.498802	-0.824690
12	9	0	-4.367068	-0.551470	0.515418
13	6	0	2.143962	-0.593803	-0.188156
14	8	0	2.021782	-1.709366	-0.539320
15	6	0	3.553499	-0.017717	0.065128
16	9	0	3.906917	0.741190	-0.951625
17	9	0	3.565203	0.739797	1.147166
18	9	0	4.432997	-0.960295	0.210873
19	1	0	1.424401	1.207079	0.351990
20	1	0	0.155736	2.776280	0.432300

B3LYP/6-311+G**

E = -1063.9704158 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.257358	1.078785	-0.048257
2	7	0	1.129689	0.308584	0.014834
3	5	0	-0.250057	0.031605	-0.227579
4	1	0	-0.553808	-1.037085	-0.610365
5	5	0	-0.949319	2.445914	0.282206
6	1	0	-1.823251	3.225221	0.432827
7	6	0	-2.631214	0.781397	-0.274695
8	8	0	-3.420630	1.554998	-0.728800
9	6	0	-3.137555	-0.638068	0.148033
10	9	0	-2.461943	-1.120101	1.210822
11	9	0	-3.006745	-1.511059	-0.867245
12	9	0	-4.427076	-0.572123	0.476891

13	6	0	2.150466	-0.612328	-0.161397
14	8	0	2.032066	-1.760762	-0.486026
15	6	0	3.573172	-0.011197	0.057158
16	9	0	4.017839	0.528490	-1.095017
17	9	0	3.559131	0.978378	0.985389
18	9	0	4.434161	-0.941048	0.452427
19	1	0	1.421335	1.221202	0.342441
20	1	0	0.187270	2.755951	0.430520



(D_{3h})

HF/6-311+G**

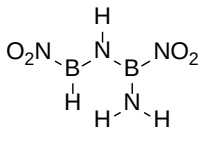
E = -851.8875584 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.394703	0.000000
2	7	0	1.226455	0.708094	0.000000
3	5	0	1.207848	-0.697351	0.000000
4	7	0	0.000000	-1.416188	0.000000
5	5	0	-1.207848	-0.697351	0.000000
6	7	0	-1.226455	0.708094	0.000000
7	1	0	2.092250	1.207961	0.000000
8	1	0	0.000000	-2.415922	0.000000
9	1	0	-2.092250	1.207961	0.000000
10	7	0	2.556032	-1.475726	0.000000
11	8	0	3.557819	-0.833316	0.000000
12	8	0	2.500583	-2.664504	0.000000
13	7	0	0.000000	2.951451	0.000000
14	8	0	1.057237	3.497820	0.000000
15	8	0	-1.057237	3.497820	0.000000
16	7	0	-2.556032	-1.475726	0.000000
17	8	0	-2.500583	-2.664504	0.000000
18	8	0	-3.557819	-0.833316	0.000000

B3LYP/6-311+G**

E = -856.5211549 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.407383	0.000000
2	7	0	1.228015	0.708995	0.000000
3	5	0	1.218830	-0.703692	0.000000
4	7	0	0.000000	-1.417990	0.000000
5	5	0	-1.218830	-0.703692	0.000000
6	7	0	-1.228015	0.708995	0.000000
7	1	0	2.107052	1.216507	0.000000
8	1	0	0.000000	-2.433014	0.000000
9	1	0	-2.107052	1.216507	0.000000
10	7	0	2.562440	-1.479426	0.000000
11	8	0	3.599644	-0.820038	0.000000
12	8	0	2.509995	-2.707364	0.000000
13	7	0	0.000000	2.958851	0.000000
14	8	0	1.089648	3.527402	0.000000
15	8	0	-1.089648	3.527402	0.000000
16	7	0	-2.562440	-1.479426	0.000000
17	8	0	-2.509995	-2.707364	0.000000
18	8	0	-3.599644	-0.820038	0.000000



(C_s)

HF/6-311+G** imaginary frequency: –17.681 cm^{-1}

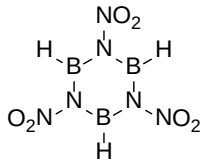
E = -569.0378169 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.561467	1.446516	0.000000
2	7	0	0.000000	0.186173	0.000000
3	5	0	0.689805	-1.063934	0.000000
4	7	0	2.037221	-1.319784	0.000000
5	1	0	-1.002718	0.134966	0.000000
6	1	0	2.372291	-2.257638	0.000000
7	7	0	-0.434367	2.654075	0.000000
8	8	0	0.039616	3.744644	0.000000
9	8	0	-1.604058	2.417608	0.000000
10	7	0	-0.240810	-2.335086	0.000000
11	8	0	-1.418152	-2.156129	0.000000
12	8	0	0.282017	-3.404859	0.000000
13	1	0	1.704589	1.719207	0.000000
14	1	0	2.739783	-0.617190	0.000000

B3LYP/6-311+G** imaginary frequency: –16.478 cm^{-1}

E = -572.1711302 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.792432	-1.002726	0.000000
2	7	0	2.162703	-1.139675	0.000000
3	5	0	0.437271	1.508281	0.000000
4	7	0	0.000000	0.194854	0.000000
5	1	0	2.574408	-2.062669	0.000000
6	1	0	-1.011303	0.052270	0.000000
7	7	0	-0.021477	-2.345745	0.000000
8	8	0	0.606678	-3.401982	0.000000
9	8	0	-1.248483	-2.269252	0.000000
10	7	0	-0.671355	2.604215	0.000000
11	8	0	-0.305547	3.776909	0.000000
12	8	0	-1.849249	2.241777	0.000000
13	1	0	1.556821	1.879032	0.000000
14	1	0	2.815279	-0.371568	0.000000



(D_3)

HF/6-311+G**

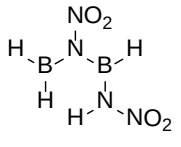
E = -851.6743145 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.283143	0.740823	0.000000
2	1	0	-2.291707	1.323118	0.000000
3	5	0	0.000000	-1.481646	0.000000
4	1	0	0.000000	-2.646236	0.000000
5	5	0	1.283143	0.740823	0.000000
6	1	0	2.291707	1.323118	0.000000
7	7	0	0.000000	1.402596	0.000000
8	7	0	-1.214684	-0.701298	0.000000
9	7	0	1.214684	-0.701298	0.000000
10	7	0	-2.428308	-1.401984	0.000000
11	8	0	-3.338444	-0.882093	0.538454
12	8	0	-2.433137	-2.450131	-0.538454
13	7	0	2.428308	-1.401984	0.000000
14	8	0	3.338444	-0.882093	-0.538454
15	8	0	2.433137	-2.450131	0.538454
16	7	0	0.000000	2.803968	0.000000
17	8	0	-0.905307	3.332224	-0.538454
18	8	0	0.905307	3.332224	0.538454

B3LYP/6-311+G**

E = -856.3149005 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.281578	0.739920	0.000000
2	1	0	-2.295855	1.325513	0.000000
3	5	0	0.000000	-1.479839	0.000000
4	1	0	0.000000	-2.651025	0.000000
5	5	0	1.281578	0.739920	0.000000
6	1	0	2.295855	1.325513	0.000000
7	7	0	0.000000	1.398855	0.000000
8	7	0	-1.211444	-0.699427	0.000000
9	7	0	1.211444	-0.699427	0.000000
10	7	0	-2.482667	-1.433369	0.000000
11	8	0	-3.419517	-0.871087	0.514793
12	8	0	-2.464142	-2.525845	-0.514793
13	7	0	2.482667	-1.433369	0.000000
14	8	0	3.419517	-0.871087	-0.514793
15	8	0	2.464142	-2.525845	0.514793
16	7	0	0.000000	2.866737	0.000000
17	8	0	-0.955375	3.396932	-0.514793
18	8	0	0.955375	3.396932	0.514793



(C_1)

HF/6-311+G**

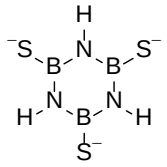
E = -568.9040309 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.095293	-0.296804	-0.078492
2	1	0	-0.104524	-1.438543	-0.316832
3	5	0	1.338827	1.867657	0.081927
4	1	0	0.360048	2.531968	0.066078
5	1	0	2.412223	2.334588	0.181980
6	7	0	1.157686	0.446436	0.016875
7	7	0	-1.309855	0.429588	0.083502
8	1	0	-1.395571	1.391790	0.322082
9	7	0	2.314375	-0.350450	0.022743
10	8	0	3.257288	0.071400	-0.544777
11	8	0	2.242903	-1.376591	0.601740
12	7	0	-2.555865	-0.120065	-0.038151
13	8	0	-3.454864	0.623292	0.174119
14	8	0	-2.637106	-1.257181	-0.339241

B3LYP/6-311+G**

E = -572.039589 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.099877	-0.269522	0.051531
2	1	0	0.110621	-1.425468	0.246085
3	5	0	-1.342037	1.883586	-0.130153
4	1	0	-0.361953	2.553113	-0.168503
5	1	0	-2.424529	2.345715	-0.196621
6	7	0	-1.151581	0.477393	-0.031107
7	7	0	1.316033	0.450324	-0.070309
8	1	0	1.417287	1.440122	-0.253944
9	7	0	-2.367684	-0.364511	-0.008933
10	8	0	-3.334813	0.107836	0.537789
11	8	0	-2.272204	-1.442514	-0.548301
12	7	0	2.600275	-0.130887	0.042940
13	8	0	3.523669	0.648960	-0.114974
14	8	0	2.669607	-1.315535	0.280230



(D_{3h})

HF/6-311+G**

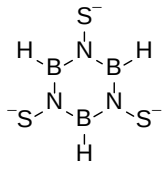
E = -1431.9819317 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.283633	0.741106	0.000000
2	5	0	-1.283633	0.741106	0.000000
3	5	0	0.000000	-1.482212	0.000000
4	7	0	0.000000	1.405310	0.000000
5	1	0	0.000000	2.397693	0.000000
6	7	0	-1.217034	-0.702655	0.000000
7	1	0	-2.076463	-1.198846	0.000000
8	7	0	1.217034	-0.702655	0.000000
9	1	0	2.076463	-1.198846	0.000000
10	16	0	-2.893310	1.670453	0.000000
11	16	0	0.000000	-3.340907	0.000000
12	16	0	2.893310	1.670453	0.000000

B3LYP/6-311+G**

E = -1435.5558622 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.292824	0.746412	0.000000
2	5	0	-1.292824	0.746412	0.000000
3	5	0	0.000000	-1.492824	0.000000
4	7	0	0.000000	1.408912	0.000000
5	1	0	0.000000	2.416817	0.000000
6	7	0	-1.220153	-0.704456	0.000000
7	1	0	-2.093025	-1.208408	0.000000
8	7	0	1.220153	-0.704456	0.000000
9	1	0	2.093025	-1.208408	0.000000
10	16	0	-2.899957	1.674291	0.000000
11	16	0	0.000000	-3.348582	0.000000
12	16	0	2.899957	1.674291	0.000000



(D_{3h})

HF/6-311+G**

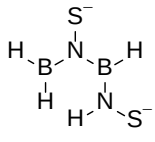
E = -1431.743253 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.431633	0.000000
2	1	0	0.000000	2.628705	0.000000
3	5	0	1.239831	-0.715817	0.000000
4	1	0	2.276525	-1.314353	0.000000
5	5	0	-1.239831	-0.715817	0.000000
6	1	0	-2.276525	-1.314353	0.000000
7	7	0	-1.245760	0.719240	0.000000
8	7	0	1.245760	0.719240	0.000000
9	7	0	0.000000	-1.438480	0.000000
10	16	0	-2.791590	1.611725	0.000000
11	16	0	2.791590	1.611725	0.000000
12	16	0	0.000000	-3.223450	0.000000

B3LYP/6-311+G**

E = -1435.3396517 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.436954	0.000000
2	7	0	-1.244531	-0.718829	0.000000
3	7	0	1.244531	-0.718829	0.000000
4	5	0	0.000000	-1.444588	0.000000
5	1	0	0.000000	-2.641431	0.000000
6	5	0	1.250648	0.721858	0.000000
7	1	0	2.287329	1.320014	0.000000
8	5	0	-1.250648	0.721858	0.000000
9	1	0	-2.287329	1.320014	0.000000
10	16	0	0.000000	3.258376	0.000000
11	16	0	-2.822287	-1.628854	0.000000
12	16	0	2.822287	-1.628854	0.000000



(C_s)

HF/6-311+G** imaginary frequency: –61.584 cm^{-1}

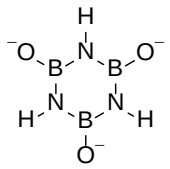
E = -955.6985147 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.577221	-2.088182	0.000000
2	1	0	0.590893	-2.407180	0.000000
3	1	0	-1.373918	-2.991445	0.000000
4	5	0	0.000000	0.375852	0.000000
5	1	0	-0.449384	1.479876	0.000000
6	7	0	-0.959179	-0.759460	0.000000
7	7	0	1.387534	0.209839	0.000000
8	1	0	1.757872	-0.710495	0.000000
9	16	0	-2.709405	-0.361816	0.000000
10	16	0	2.669540	1.426706	0.000000

B3LYP/6-311+G** imaginary frequency: –82.765 cm^{-1}

E = -958.1426809 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.988091	-0.737846	0.000000
2	7	0	1.380598	0.172466	0.000000
3	5	0	-0.639854	-2.083224	0.000000
4	1	0	-1.461110	-2.963429	0.000000
5	5	0	0.000000	0.389330	0.000000
6	1	0	-0.418717	1.505821	0.000000
7	16	0	-2.744356	-0.260902	0.000000
8	16	0	2.750009	1.328117	0.000000
9	1	0	1.713126	-0.780465	0.000000
10	1	0	0.527992	-2.410241	0.000000



(D_{3h})

HF/6-311+G**

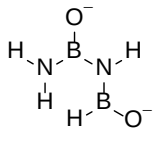
E = -463.8746512 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.336296	0.771511	0.000000
2	5	0	0.000000	-1.543022	0.000000
3	5	0	-1.336296	0.771511	0.000000
4	7	0	0.000000	1.414497	0.000000
5	1	0	0.000000	2.411413	0.000000
6	7	0	1.224990	-0.707249	0.000000
7	1	0	2.088345	-1.205707	0.000000
8	7	0	-1.224990	-0.707249	0.000000
9	1	0	-2.088345	-1.205707	0.000000
10	8	0	0.000000	-2.873590	0.000000
11	8	0	-2.488602	1.436795	0.000000
12	8	0	2.488602	1.436795	0.000000

B3LYP/6-311+G**

E = -466.5343174 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.340382	0.773870	0.000000
2	5	0	0.000000	-1.547740	0.000000
3	5	0	-1.340382	0.773870	0.000000
4	7	0	0.000000	1.417664	0.000000
5	1	0	0.000000	2.429606	0.000000
6	7	0	1.227733	-0.708832	0.000000
7	1	0	2.104101	-1.214803	0.000000
8	7	0	-1.227733	-0.708832	0.000000
9	1	0	-2.104101	-1.214803	0.000000
10	8	0	0.000000	-2.897250	0.000000
11	8	0	-2.509092	1.448625	0.000000
12	8	0	2.509092	1.448625	0.000000

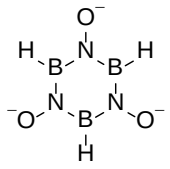


(C_s)

HF/6-311+G** imaginary frequency: -419.777 cm^{-1}

E = -310.4816853 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.458744	0.737870	0.000000
2	1	0	2.062112	-0.382456	0.000000
3	5	0	-0.981593	-0.525923	0.000000
4	7	0	0.000000	0.587227	0.000000
5	1	0	-0.466536	1.471476	0.000000
6	7	0	-0.359312	-1.886750	0.000000
7	1	0	-0.938021	-2.693373	0.000000
8	1	0	0.620129	-2.045896	0.000000
9	8	0	-2.279563	-0.384173	0.000000
10	8	0	2.136031	1.845070	0.000000



(D_{3h})

HF/6-311+G**

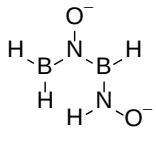
E = -463.4529932 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.422951	0.000000
2	1	0	0.000000	2.639198	0.000000
3	5	0	1.232312	-0.711475	0.000000
4	1	0	2.285613	-1.319599	0.000000
5	5	0	-1.232312	-0.711475	0.000000
6	1	0	-2.285613	-1.319599	0.000000
7	7	0	1.241897	0.717010	0.000000
8	7	0	0.000000	-1.434020	0.000000
9	7	0	-1.241897	0.717010	0.000000
10	8	0	0.000000	-2.839942	0.000000
11	8	0	2.459462	1.419971	0.000000
12	8	0	-2.459462	1.419971	0.000000

B3LYP/6-311+G**

E = -466.1539202 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.440397	0.000000
2	7	0	1.247421	-0.720199	0.000000
3	7	0	-1.247421	-0.720199	0.000000
4	5	0	0.000000	-1.440987	0.000000
5	1	0	0.000000	-2.651768	0.000000
6	5	0	-1.247932	0.720494	0.000000
7	1	0	-2.296499	1.325884	0.000000
8	5	0	1.247932	0.720494	0.000000
9	1	0	2.296499	1.325884	0.000000
10	8	0	0.000000	2.864889	0.000000
11	8	0	-2.481067	-1.432444	0.000000
12	8	0	2.481067	-1.432444	0.000000



(C_s)

HF/6-311+G** imaginary frequency: -109.256 cm^{-1}

E = -310.192787 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.666086	-1.859098	0.000000
2	1	0	0.491053	-2.233781	0.000000
3	1	0	-1.521316	-2.722500	0.000000
4	5	0	0.000000	0.605135	0.000000
5	1	0	-0.465681	1.711275	0.000000
6	7	0	-0.983187	-0.526601	0.000000
7	7	0	1.375295	0.455737	0.000000
8	1	0	1.771366	-0.458449	0.000000
9	8	0	-2.310103	-0.134015	0.000000
10	8	0	2.348885	1.442679	0.000000

B3LYP/6-311+G** imaginary frequency: -127.568 cm^{-1}

E = -312.0412406 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.011681	-0.497708	0.000000
2	7	0	1.376815	0.427748	0.000000
3	5	0	0.000000	0.629291	0.000000
4	1	0	-0.434325	1.747072	0.000000
5	5	0	-0.709815	-1.862012	0.000000
6	1	0	-1.584434	-2.700801	0.000000
7	8	0	-2.318263	-0.049630	0.000000
8	8	0	2.424036	1.345022	0.000000
9	1	0	1.716853	-0.530471	0.000000
10	1	0	0.448857	-2.225606	0.000000