

Aromaticity of diazaborines and their protonated forms

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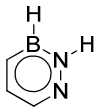
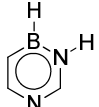
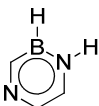
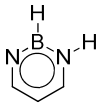
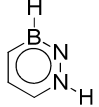
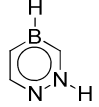
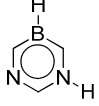
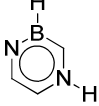
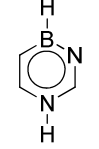
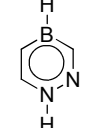
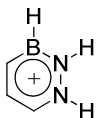
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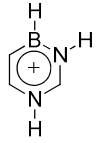
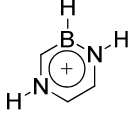
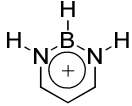
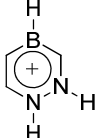
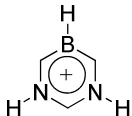
Supporting Information

Table of Contents

Table S1. Calculated bond lengths of 6-15 and 6-15-H⁺	S2
Absolute energies and x, y, z coordinates of diazaborines and their protonated forms.....	S4

Table S1. Calculated bond lengths of **6-15** and **6-15-H⁺**.

Molecule		d (Å) from boron atom in the clockwise manner					
	6	1.42472	1.34935	1.30728	1.42715	1.36783	1.51639
	7	1.44074	1.36189	1.29905	1.37285	1.37067	1.50837
	8	1.42689	1.36710	1.36650	1.36447	1.31931	1.52466
	9	1.44518	1.36068	1.36655	1.42734	1.30744	1.42586
	10	1.43169	1.31682	1.33801	1.39989	1.37996	1.51978
	11	1.51257	1.33760	1.32705	1.33962	1.39128	1.49793
	12	1.49531	1.35942	1.35347	1.31571	1.34752	1.51087
	13	1.51874	1.34535	1.35549	1.39587	1.32125	1.42804
	14	1.44920	1.28506	1.37394	1.37621	1.35902	1.52903
	15	1.53188	1.31526	1.34096	1.35789	1.36979	1.50732
	6/10-H⁺	1.42634	1.35337	1.31497	1.41671	1.36814	1.53328

	7/14-H⁺	1.46429	1.32480	1.32487	1.39416	1.35352	1.51984
	8/13-H⁺	1.42926	1.35637	1.36646	1.37145	1.32532	1.53176
	9-H⁺	1.43789	1.34383	1.38667	1.38667	1.34383	1.43789
	11/15-H⁺	1.54497	1.31657	1.34314	1.35896	1.37103	1.50746
	12-H⁺	1.50763	1.35539	1.33685	1.33685	1.35539	1.50763

Absolute energies (a.u.) and x, y, z coordinates (Å) of diazaborines and their protonated forms

6, E = -251.7653724 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.241241	0.623236	0.000000
2	6	0	0.000000	1.327565	0.000000
3	7	0	-1.194977	-0.585400	0.000000
4	1	0	2.152142	1.216219	0.000000
5	1	0	-0.016542	2.412184	0.000000
6	5	0	-0.071079	-1.461010	0.000000
7	1	0	-0.276306	-2.631856	0.000000
8	1	0	-2.146532	-0.927210	0.000000
9	6	0	1.265286	-0.744381	0.000000
10	1	0	2.224776	-1.252052	0.000000
11	7	0	-1.179495	0.763863	0.000000

7, E = -251.7938367 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.221365	-0.617654	0.000000
2	7	0	1.180555	0.636997	0.000000
3	1	0	-2.233910	-1.015084	0.000000
4	5	0	1.237419	-0.802616	0.000000
5	1	0	2.302748	-1.329935	0.000000
6	1	0	2.016729	1.206576	0.000000
7	6	0	-0.127797	-1.443998	0.000000
8	1	0	-0.299701	-2.515390	0.000000
9	1	0	0.057448	2.401829	0.000000
10	6	0	0.000000	1.316001	0.000000
11	7	0	-1.171331	0.754288	0.000000

8, E = -251.7779872 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.189113	0.658839	0.000000
2	1	0	-2.117646	1.172289	0.000000
3	5	0	1.250859	-0.766715	0.000000
4	1	0	2.309056	-1.307138	0.000000
5	1	0	2.026725	1.225420	0.000000
6	6	0	-0.126729	-1.420034	0.000000
7	1	0	-0.269933	-2.500777	0.000000
8	1	0	0.028069	2.416178	0.000000
9	6	0	0.000000	1.333354	0.000000
10	6	0	-1.175413	0.636406	0.000000
11	7	0	-1.248787	-0.726089	0.000000

9, E = -251.8041313 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.107181	-1.370417	0.000000
2	6	0	1.157873	-0.709397	0.000000
3	6	0	1.174399	0.657056	0.000000
4	7	0	-1.265882	-0.764773	0.000000
5	1	0	2.094465	1.230767	0.000000
6	1	0	-0.098927	-2.464640	0.000000
7	1	0	2.082702	-1.271269	0.000000
8	1	0	0.060809	2.353390	0.000000
9	1	0	-2.260902	1.326609	0.000000
10	5	0	-1.273504	0.661071	0.000000
11	7	0	0.000000	1.344249	0.000000

10, E = -251.7348337 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.150038	-0.789086	0.000000
2	6	0	-1.160802	0.610766	0.000000
3	7	0	1.222828	0.787632	0.000000
4	1	0	-2.107026	-1.301788	0.000000
5	1	0	-2.059735	1.212845	0.000000
6	5	0	1.339615	-0.639289	0.000000
7	1	0	2.436876	-1.104198	0.000000
8	6	0	0.057998	-1.456113	0.000000
9	1	0	0.034929	-2.542785	0.000000
10	7	0	0.000000	1.276202	0.000000
11	1	0	-0.045868	2.292135	0.000000

11, E = -251.7255578 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	1.310104	-0.812390	0.000000
2	1	0	2.358532	-1.375764	0.000000
3	1	0	-0.220870	-2.525069	0.000000
4	6	0	1.207430	0.696691	0.000000
5	1	0	2.017393	1.420782	0.000000
6	1	0	-2.181338	-1.067485	0.000000
7	6	0	-0.044095	-1.452645	0.000000
8	6	0	-1.178944	-0.647802	0.000000
9	7	0	-1.193332	0.691736	0.000000
10	7	0	0.000000	1.272267	0.000000
11	1	0	-0.077256	2.283999	0.000000

12, E = -251.7385302 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.161326	0.585326	0.000000
2	6	0	1.228640	0.698668	0.000000
3	6	0	-0.066331	-1.428071	0.000000
4	7	0	-1.218417	-0.729145	0.000000
5	1	0	2.044446	1.414312	0.000000
6	1	0	-2.072546	1.172132	0.000000
7	1	0	-0.074568	2.291774	0.000000
8	1	0	2.333433	-1.394335	0.000000
9	1	0	-0.234572	-2.505230	0.000000
10	7	0	0.000000	1.280458	0.000000
11	5	0	1.305365	-0.794677	0.000000

13, E = -251.7496744 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.003153	-1.489712	0.000000
2	1	0	-0.059434	2.307366	0.000000
3	1	0	-2.083140	1.186842	0.000000
4	5	0	1.257922	-0.807904	0.000000
5	1	0	2.296477	-1.396383	0.000000
6	6	0	1.211652	0.710128	0.000000
7	1	0	2.040229	1.410708	0.000000
8	1	0	-2.070934	-1.313189	0.000000
9	6	0	-1.114531	-0.785088	0.000000
10	6	0	-1.169601	0.609695	0.000000
11	7	0	0.000000	1.294822	0.000000

14, E = -251.7728654 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.207861	0.605935	0.000000
2	7	0	-1.303702	-0.696398	0.000000
3	1	0	2.078066	1.254349	0.000000
4	1	0	-0.015954	2.275193	0.000000
5	5	0	-0.093621	-1.493826	0.000000
6	1	0	-0.175385	-2.684586	0.000000
7	6	0	1.243743	-0.752615	0.000000
8	1	0	2.221042	-1.223928	0.000000
9	1	0	-2.065786	1.241154	0.000000
10	6	0	-1.192931	0.583874	0.000000
11	7	0	0.000000	1.265510	0.000000

15, E = -251.7292137 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.017770	2.263079	0.000000
2	5	0	-0.050335	-1.527033	0.000000
3	1	0	-0.145750	-2.714382	0.000000
4	1	0	2.244366	-1.212604	0.000000
5	6	0	-1.277729	-0.610425	0.000000
6	1	0	-2.307589	-0.963318	0.000000
7	1	0	2.051563	1.257716	0.000000
8	6	0	1.253364	-0.770469	0.000000
9	6	0	1.188863	0.597800	0.000000
10	7	0	0.000000	1.253911	0.000000
11	7	0	-1.222876	0.703695	0.000000

6/10-H⁺, E = -252.1111958 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.223466	-0.751263	0.000000
2	6	0	-1.155373	0.663813	0.000000
3	7	0	1.187102	0.641789	0.000000
4	1	0	-2.211432	-1.197150	0.000000
5	1	0	-2.032653	1.298738	0.000000
6	5	0	1.284779	-0.781199	0.000000
7	1	0	2.364289	-1.252631	0.000000
8	1	0	1.983831	1.268811	0.000000
9	6	0	-0.073525	-1.492512	0.000000
10	1	0	-0.158817	-2.574135	0.000000
11	7	0	0.000000	1.291705	0.000000
12	1	0	0.035356	2.307680	0.000000

7/14-H⁺, E = -252.1589068 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.235165	0.639020	0.000000
2	7	0	-1.191976	-0.678598	0.000000
3	1	0	2.084707	1.310841	0.000000
4	1	0	-0.018828	2.299721	0.000000
5	5	0	0.010297	-1.514465	0.000000
6	1	0	-0.127250	-2.684170	0.000000
7	1	0	-2.117303	-1.096990	0.000000
8	6	0	1.301558	-0.712873	0.000000
9	1	0	2.285165	-1.166366	0.000000
10	1	0	-2.073533	1.228567	0.000000
11	6	0	-1.160159	0.645817	0.000000
12	7	0	0.000000	1.285589	0.000000

8/13-H⁺, E = -252.1489026 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.028993	-1.387521	0.000000
2	1	0	-0.070678	2.349704	0.000000
3	1	0	-2.097896	1.215559	0.000000
4	5	0	1.308330	-0.750279	0.000000
5	1	0	2.306670	-1.372977	0.000000
6	1	0	-0.033481	-2.401529	0.000000
7	6	0	1.203569	0.777899	0.000000
8	1	0	2.034720	1.473382	0.000000
9	1	0	-2.072343	-1.297779	0.000000
10	6	0	-1.154370	-0.724662	0.000000
11	6	0	-1.184465	0.641468	0.000000
12	7	0	0.000000	1.332778	0.000000

9-H⁺, E = -252.1964365 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.194622	0.682741
2	6	0	0.000000	0.000000	1.386815
3	6	0	0.000000	-1.194622	0.682741
4	7	0	0.000000	-1.201732	-0.661069
5	1	0	0.000000	2.151706	1.192330
6	1	0	0.000000	0.000000	2.466967
7	1	0	0.000000	-2.151706	1.192330
8	5	0	0.000000	0.000000	-1.450609
9	1	0	0.000000	0.000000	-2.625488
10	7	0	0.000000	1.201732	-0.661069
11	1	0	0.000000	2.108974	-1.115954
12	1	0	0.000000	-2.108974	-1.115954

11/15-H⁺, E = -252.0702445 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.989906	1.174040	0.000000
2	1	0	-0.079821	2.277990	0.000000
3	5	0	0.064134	-1.575350	0.000000
4	1	0	0.013586	-2.753484	0.000000
5	1	0	2.318952	-1.127716	0.000000
6	6	0	-1.227806	-0.728106	0.000000
7	1	0	-2.248806	-1.096774	0.000000
8	1	0	2.041141	1.328306	0.000000
9	6	0	1.311161	-0.728387	0.000000
10	6	0	1.204322	0.638473	0.000000
11	7	0	0.000000	1.268061	0.000000
12	7	0	-1.157411	0.586582	0.000000

12-H⁺, E = -252.1023553 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.000000	1.999894	1.187702
2	1	0	0.000000	0.000000	2.389571
3	5	0	0.000000	0.000000	-1.567433
4	1	0	0.000000	0.000000	-2.746012
5	1	0	0.000000	-2.274192	-1.077481
6	6	0	0.000000	1.249388	-0.723644
7	1	0	0.000000	2.274192	-1.077481
8	1	0	0.000000	-1.999894	1.187702
9	6	0	0.000000	-1.249388	-0.723644
10	6	0	0.000000	0.000000	1.310682
11	7	0	0.000000	-1.149427	0.628058
12	7	0	0.000000	1.149427	0.628058
