Supplementary material for the article:

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Aromaticity of diazaborines and their protonated forms

Milovan Stojanović,[†] and Marija Baranac-Stojanović,[*‡]

[†]*Center for Chemistry ICTM, University of Belgrade, Njegoševa 12, P.O.Box 473, 11000 Belgrade, Serbia*

[‡]*Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, P.O.Box 158, 11000 Belgrade, Serbia*

Supporting Information

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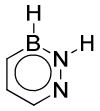
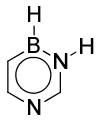
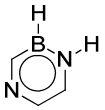
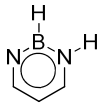
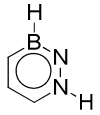
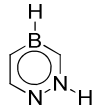
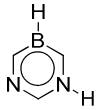
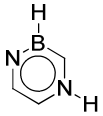
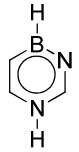
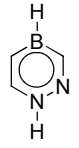
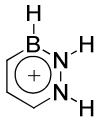
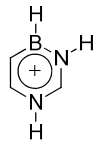
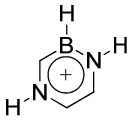
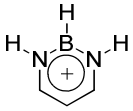
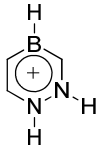
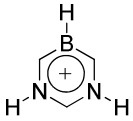
Table S1. Calculated bond lengths of **6-15** and **6-15**-H^+.

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