Supplementary data for the article:

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Supporting Information

Aromaticity and Stability of Azaborines

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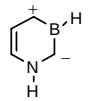
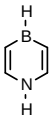
chem_201402851_sm_miscellaneous_information.pdf

Table S1. EDA and IEDA results for azaborines **2-4**.[a,b] Energies are in kcal/mol.

Molecule		ΔE ΔE_{iso}	ΔE_{prep}	ΔE_{int}	ΔE_{elstat}	ΔE_{ex}	ΔE_{rep}	ΔE_{ex+rep}	ΔE_{pol}	ΔE_{disp}	Interacting fragments
	**2**	-878.00	0.67	-878.67	-939.35	-499.10	2049.49	1550.39	-1269.83	-219.88	1 NH(t) 1 BH(t) 4 CH(q)
	**3-I**	-848.47 **29.53**	205.36 **204.69**	-1053.83 **-175.16**	-1117.62 **-178.27**	-615.89 **-116.79**	2550.56 **501.07**	1934.67 **384.28**	-1674.76 **-404.93**	-196.12 **23.76**	1 NH(t) 1 BH(t) 2 CH(q) 1 CH^+(t) 1 CH^-(t)
	**3-II**	-848.47 **29.54**	205.55 **204.89**	-1054.02 **-175.35**	-1133.64 **-194.29**	-624.71 **-125.61**	2632.43 **582.94**	2007.72 **457.33**	-1732.06 **-462.23**	-196.04 **23.84**	1 NH(t) 1 BH(t) 2 CH(q) 1 CH^+(t) 1 CH^-(t)
	**3-III**	-848.69 **29.31**	205.35 **204.68**	-1054.04 **-175.37**	-1174.53 **-235.18**	-619.24 **-120.14**	2603.80 **554.31**	1984.56 **434.17**	-1667.98 **-398.15**	-196.09 **23.79**	1 NH(t) 1 BH(t) 2 CH(q) 1 CH^+(t) 1 CH^-(t)
	**3-IV**	-848.25 **29.75**	205.57 **204.90**	-1053.82 **-175.15**	-1215.35 **-276.00**	-638.63 **-139.53**	2695.42 **645.93**	2056.79 **506.40**	-1699.16 **-429.33**	-196.09 **23.79**	1 NH(t) 1 BH(t) 2 CH(q) 1 CH^+(t) 1 CH^-(t)
	**4**	-856.11 **21.89**	0.72 **0.05**	-856.83 **21.84**	-1054.02 **-114.67**	-540.18 **-41.08**	2294.35 **244.86**	1754.17 **203.78**	-1337.62 **-67.79**	-219.37 **0.51**	1 NH(t) 1 BH(t) 4 CH(q)

[a] IEDA values are given in bold, referenced to the most stable isomer **2**. [b] ΔE = bonding energy corresponding to the formation of a given azaborine from six identical fragments: four CH groups in their electronic quartet state, one BH and one NH group in the electronic triplet state, ΔE_{prep} = preparation energy, that is the energy required to distort the six separated fragments from their equilibrium structure to the geometry and electronic state they have in the final molecule, ΔE_{int} = interaction energy, that is the energy change corresponding to the formation of molecule from the prepared fragments, which are given in the most right column in the Table, ΔE_{elstat} = electrostatic energy, ΔE_{ex} = exchange energy, ΔE_{rep} = repulsion energy, ΔE_{pol} = polarization energy, ΔE_{disp} = dispersion energy, ΔE_{iso} = energy corresponding to the isomerization of the most stable azaborine **2** into azaborines **3** and **4**.

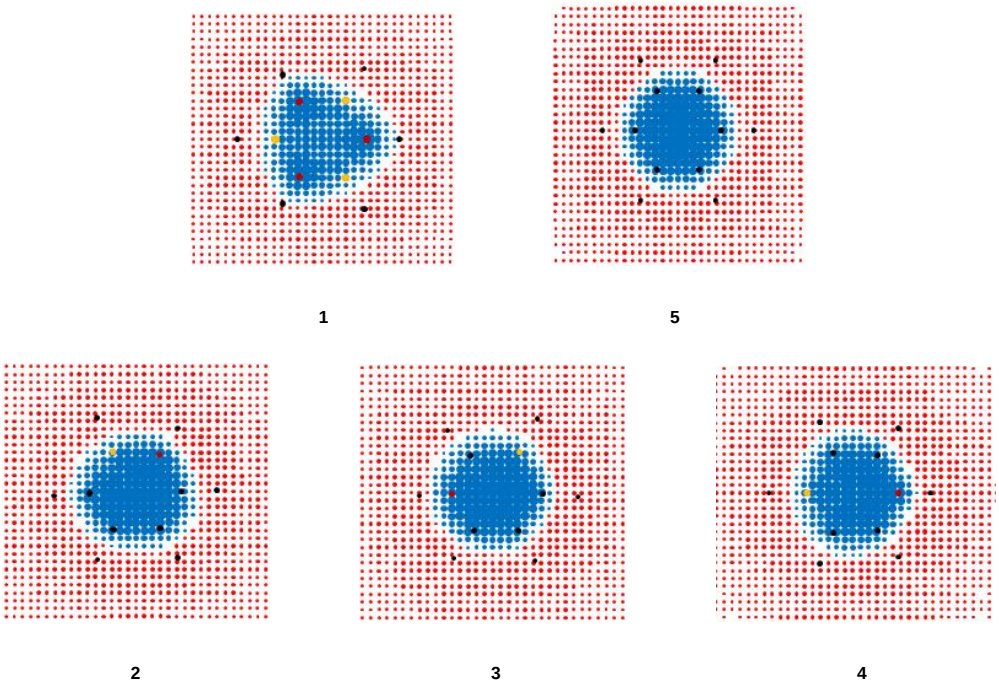


Figure 4. (De)shielding pattern arising from the π electron response to a perpendicular magnetic field, plotted in the plane of the ring. Blue and red points denote shielding and deshielding effects, respectively. The radius of points is proportional to the absolute value of the contribution (the points merge into one another inside the ring). Positions of nuclei are marked by black points (C and H), dark red points (N) and yellow points (B).

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

Borazine (**1**)

E = -242.7485014 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.256582	0.725488	0.000000
2	1	0	2.289386	1.321778	0.000000
3	5	0	-1.256582	0.725488	0.000000
4	1	0	-2.289386	1.321778	0.000000
5	5	0	0.000000	-1.450975	0.000000
6	1	0	0.000000	-2.643555	0.000000
7	7	0	0.000000	1.409279	0.000000
8	1	0	0.000000	2.418047	0.000000
9	7	0	-1.220472	-0.704640	0.000000
10	1	0	-2.094090	-1.209024	0.000000
11	7	0	1.220472	-0.704640	0.000000
12	1	0	2.094090	-1.209024	0.000000

1,2-Azaborine (**2**)

E = -235.7458969 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.190021	0.689734	0.000000
2	6	0	0.000000	1.361233	0.000000
3	6	0	-0.050299	-1.473684	0.000000
4	6	0	-1.209353	-0.733240	0.000000
5	1	0	-2.113881	1.253918	0.000000
6	1	0	0.049791	2.443903	0.000000
7	1	0	-0.134473	-2.556309	0.000000
8	1	0	-2.180872	-1.222387	0.000000
9	5	0	1.278904	-0.753082	0.000000
10	1	0	2.365429	-1.240227	0.000000
11	7	0	1.185420	0.681508	0.000000
12	1	0	2.019588	1.251703	0.000000

1,3-Azaborine (**3**)

E = -235.6987876 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.181585	-0.749093	0.000000
2	6	0	-1.176422	0.639527	0.000000
3	6	0	1.225304	0.725061	0.000000
4	6	0	0.005951	-1.479073	0.000000
5	1	0	-2.151498	-1.237906	0.000000
6	1	0	-2.072685	1.243706	0.000000
7	1	0	2.036919	1.445739	0.000000
8	1	0	-0.093075	-2.562431	0.000000
9	5	0	1.338989	-0.773348	0.000000
10	1	0	2.399622	-1.319075	0.000000
11	7	0	0.000000	1.308361	0.000000
12	1	0	-0.053716	2.319646	0.000000

1,4-Azaborine (**4**)

E = -235.7110251 a.u.

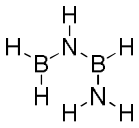
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.281854	-0.727168
2	6	0	0.000000	1.205460	0.635086
3	6	0	0.000000	-1.205460	0.635086
4	6	0	0.000000	-1.281854	-0.727168
5	1	0	0.000000	2.282079	-1.149721
6	1	0	0.000000	2.066403	1.296178
7	1	0	0.000000	-2.066403	1.296178
8	1	0	0.000000	-2.282079	-1.149721
9	5	0	0.000000	0.000000	-1.548895
10	1	0	0.000000	0.000000	-2.743214
11	7	0	0.000000	0.000000	1.286466
12	1	0	0.000000	0.000000	2.294496

Benzene (**5**)

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

Reference structures used for calculations of ECREs

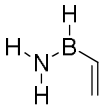


E = -162.985 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.689291	-1.559315	0.000000
2	1	0	0.437893	-1.955829	0.000000
3	1	0	-1.597821	-2.332285	0.000000
4	5	0	0.000000	0.932480	0.000000
5	1	0	-0.427696	2.046542	0.000000
6	7	0	-0.943599	-0.177023	0.000000
7	1	0	-1.916346	0.100949	0.000000
8	7	0	1.385749	0.739216	0.000000
9	1	0	2.032938	1.509399	0.000000
10	1	0	1.822435	-0.169953	0.000000

E = -156.0344785 a.u.

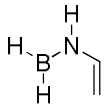
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.545768	-0.502283
2	1	0	0.000000	1.171952	-1.520698
3	1	0	0.000000	2.622457	-0.382453
4	6	0	0.000000	0.735245	0.561487
5	1	0	0.000000	1.192506	1.547927
6	6	0	0.000000	-0.735245	0.561487
7	1	0	0.000000	-1.192506	1.547927
8	6	0	0.000000	-1.545768	-0.502283
9	1	0	0.000000	-1.171952	-1.520698
10	1	0	0.000000	-2.622457	-0.382453



E = -159.5025744 a.u.

imaginary frequency: -111.4 cm^{-1}

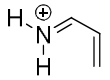
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.001411	-0.208985	0.000000
2	1	0	-2.065809	0.024307	0.000000
3	6	0	-0.675124	-1.507380	0.000000
4	1	0	0.358173	-1.848582	0.000000
5	1	0	-1.420728	-2.297529	0.000000
6	7	0	1.388397	0.827084	0.000000
7	1	0	1.849318	-0.070625	0.000000
8	1	0	2.028663	1.604857	0.000000
9	5	0	0.000000	0.995505	0.000000
10	1	0	-0.409181	2.118653	0.000000



E = -159.481795 a.u.

imaginary frequency: -45.87 cm^{-1}

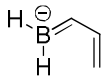
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.879259	0.000000
2	1	0	-0.540984	1.820537	0.000000
3	6	0	1.332573	0.884498	0.000000
4	1	0	1.921999	-0.023051	0.000000
5	1	0	1.860774	1.828350	0.000000
6	7	0	-0.847503	-0.250855	0.000000
7	1	0	-1.826623	-0.002004	0.000000
8	5	0	-0.529951	-1.616796	0.000000
9	1	0	0.604277	-1.972822	0.000000
10	1	0	-1.432604	-2.393587	0.000000



E = -172.4490176 a.u.

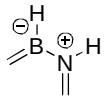
imaginary frequency: -58.47 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.883634	0.000000
2	1	0	-0.396940	1.895566	0.000000
3	6	0	-0.941773	-0.203743	0.000000
4	1	0	-1.982509	0.097392	0.000000
5	6	0	-0.619103	-1.509858	0.000000
6	1	0	0.400802	-1.882580	0.000000
7	1	0	-1.395229	-2.266441	0.000000
8	7	0	1.296441	0.798603	0.000000
9	1	0	1.790953	-0.087782	0.000000
10	1	0	1.873097	1.633422	0.000000



E = -142.811853 a.u.

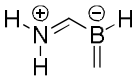
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.360922	0.922471	0.000000
2	1	0	1.966563	0.021528	0.000000
3	1	0	1.885437	1.873835	0.000000
4	6	0	0.000000	0.874101	0.000000
5	1	0	-0.483531	1.859153	0.000000
6	6	0	-0.912118	-0.248900	0.000000
7	1	0	-1.960743	0.065090	0.000000
8	5	0	-0.618197	-1.690723	0.000000
9	1	0	0.507661	-2.143265	0.000000
10	1	0	-1.517224	-2.508763	0.000000



E = -159.4301881 a.u.

imaginary frequency: -137.34 cm^{-1}

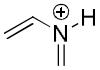
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.293388	0.942568	0.000000
2	1	0	1.864953	0.023853	0.000000
3	1	0	1.801781	1.898413	0.000000
4	6	0	-0.534319	-1.644370	0.000000
5	1	0	0.503175	-1.975095	0.000000
6	1	0	-1.239015	-2.470715	0.000000
7	5	0	-0.984581	-0.273997	0.000000
8	1	0	-2.110700	0.123191	0.000000
9	7	0	0.000000	0.883732	0.000000
10	1	0	-0.451704	1.795023	0.000000



E = -159.4238269 a.u.

imaginary frequency: -107.75 cm^{-1}

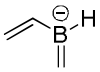
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.930914	0.000000
2	1	0	-0.285097	1.984300	0.000000
3	6	0	-0.672597	-1.574146	0.000000
4	1	0	0.357550	-1.937462	0.000000
5	1	0	-1.386013	-2.395096	0.000000
6	7	0	1.318989	0.779317	0.000000
7	1	0	1.721850	-0.147591	0.000000
8	1	0	1.959135	1.558542	0.000000
9	5	0	-1.071340	-0.172217	0.000000
10	1	0	-2.208063	0.202568	0.000000



E = -172.4256625 a.u.

imaginary frequency: -142.89 cm^{-1}

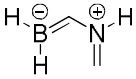
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.283559	0.901591	0.000000
2	1	0	1.864942	-0.012553	0.000000
3	1	0	1.778901	1.865277	0.000000
4	6	0	-0.883623	-0.271565	0.000000
5	1	0	-1.922144	0.028498	0.000000
6	6	0	-0.489722	-1.540645	0.000000
7	1	0	0.544094	-1.865251	0.000000
8	1	0	-1.242448	-2.318780	0.000000
9	7	0	0.000000	0.858588	0.000000
10	1	0	-0.484630	1.756406	0.000000



E = -142.8095564 a.u.

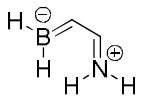
imaginary frequency: -136.73 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.347783	1.007923	0.000000
2	1	0	1.936948	0.092300	0.000000
3	1	0	1.916843	1.938453	0.000000
4	6	0	0.000000	0.975646	0.000000
5	1	0	-0.468919	1.969165	0.000000
6	6	0	-0.585045	-1.673940	0.000000
7	1	0	0.452890	-2.020753	0.000000
8	1	0	-1.302229	-2.497855	0.000000
9	5	0	-0.987751	-0.272817	0.000000
10	1	0	-2.173206	0.025000	0.000000



E = -159.409765 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.311015	0.847942	0.000000
2	1	0	1.870250	-0.074194	0.000000
3	1	0	1.796929	1.810698	0.000000
4	6	0	-0.907923	-0.234871	0.000000
5	1	0	-1.924201	0.142266	0.000000
6	5	0	-0.567951	-1.678769	0.000000
7	1	0	0.564253	-2.068887	0.000000
8	1	0	-1.452003	-2.480427	0.000000
9	7	0	0.000000	0.808362	0.000000
10	1	0	-0.434023	1.727435	0.000000



E = -159.453561 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.980300	-0.108160	0.000000
2	1	0	-1.991207	0.289746	0.000000
3	6	0	0.000000	0.853930	0.000000
4	1	0	-0.267693	1.909150	0.000000
5	7	0	1.336205	0.651959	0.000000
6	1	0	1.981645	1.421118	0.000000
7	1	0	1.706733	-0.285654	0.000000
8	5	0	-0.731286	-1.591929	0.000000
9	1	0	0.386040	-2.036340	0.000000
10	1	0	-1.630718	-2.376712	0.000000