Supporting Information

Analysis of Stability and (Anti)aromaticity of BN-Dibenzo[*a*,*e*]pentalenes

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ejoc201801047-sup-0001-SupMat.pdf

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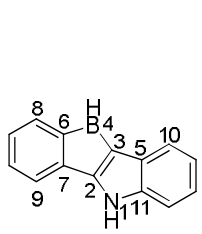
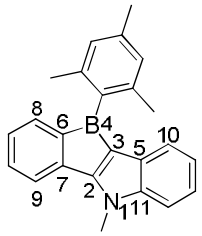
Table S1. Experimental and calculated bond lengths and bond angles for **1,4** isomer of BN-dibenzopentalene.[a]



I

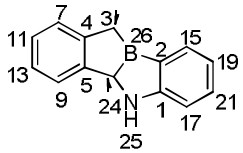


II

bond	exp/calc (Å)	angle	exp/calc (°)
N1-C2	1.359/1.357	C3B4C6	102.90/103.99
C2-C3	1.394/1.395	B4C6C7	108.45/108.17
C3-B4	1.528/1.529	C6C7C9	121.57/121.93
C3-C5	1.433/1.443	C2C7C9	131.94/131.41
B4-C6	1.613/1.594	C2C7C6	106.29/106.66
C6-C7	1.419/1.426	N1C2C3	111.76/111.14
C6-C8	1.385/1.383	N1C2C7	133.61/134.36
C7-C9	1.372/1.381	C3C2C7	114.59/114.49
C5-C10	1.402/1.402	C2C3C5	105.52/105.72
		C2C3C4	106.66/106.68
		C4C3C5	146.27/147.59
		C10C5C11	117.58/118.17

[a] Experimental data are from X-ray analysis of compound **II** (see, Supporting Information from ref. 16). Calculated data are from this work, at the B3LYP/6-311+G(d,p) level of theory.

Table S2. Spin densities in diradical state of **1,3** isomer of BN-dibenzopentalene obtained by Hirshfeld population analysis.



Atom	1	2	3	4	5	7	9	11
Spin density	0.05	0.00	-0.14	0.02	-0.03	-0.03	0.02	0.03
Atom	13	15	17	19	21	24	25	26
Spin density	-0.03	0.01	0.00	0.00	0.01	0.06	0.02	0.05

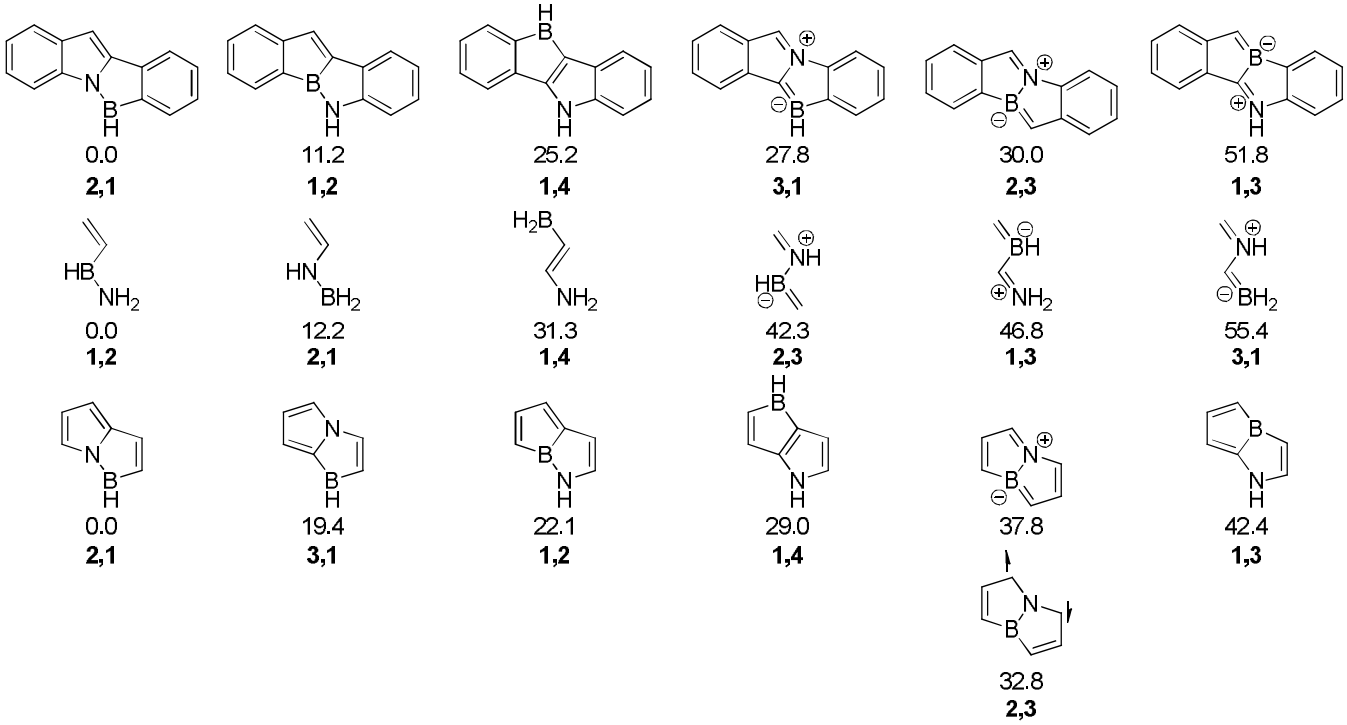


Figure S1. Relative energies (in kcal/mol) of six isomeric BN-dibenzopentalenes, BN-butadienes and BN-pentalenes, obtained at the B3LYP/6-311+G(d,p) level of theory.

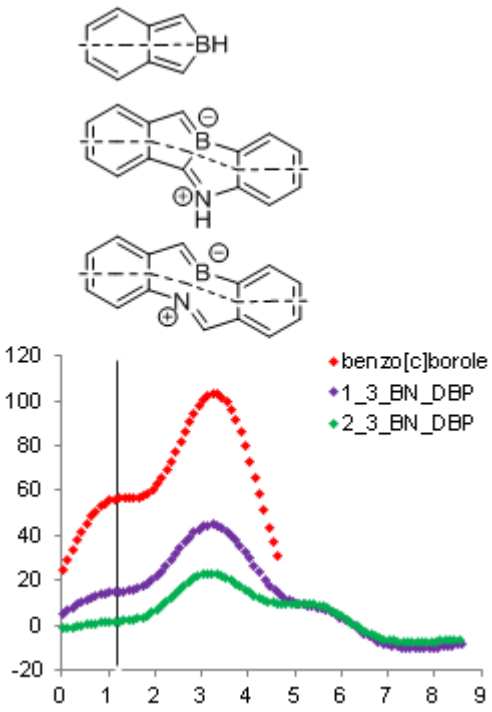


Figure S2. NICS-*XY*-scans for benzo[*c*]borole, **1,3** and **2,3** isomers of BN-dibenzopentalenes.

Section S1: Comparison of (anti)aromaticity of various isomers of BN-dibenzopentalenes

Aromaticity indices for this analysis are presented in Figure 7 in the manuscript, which is also given below.

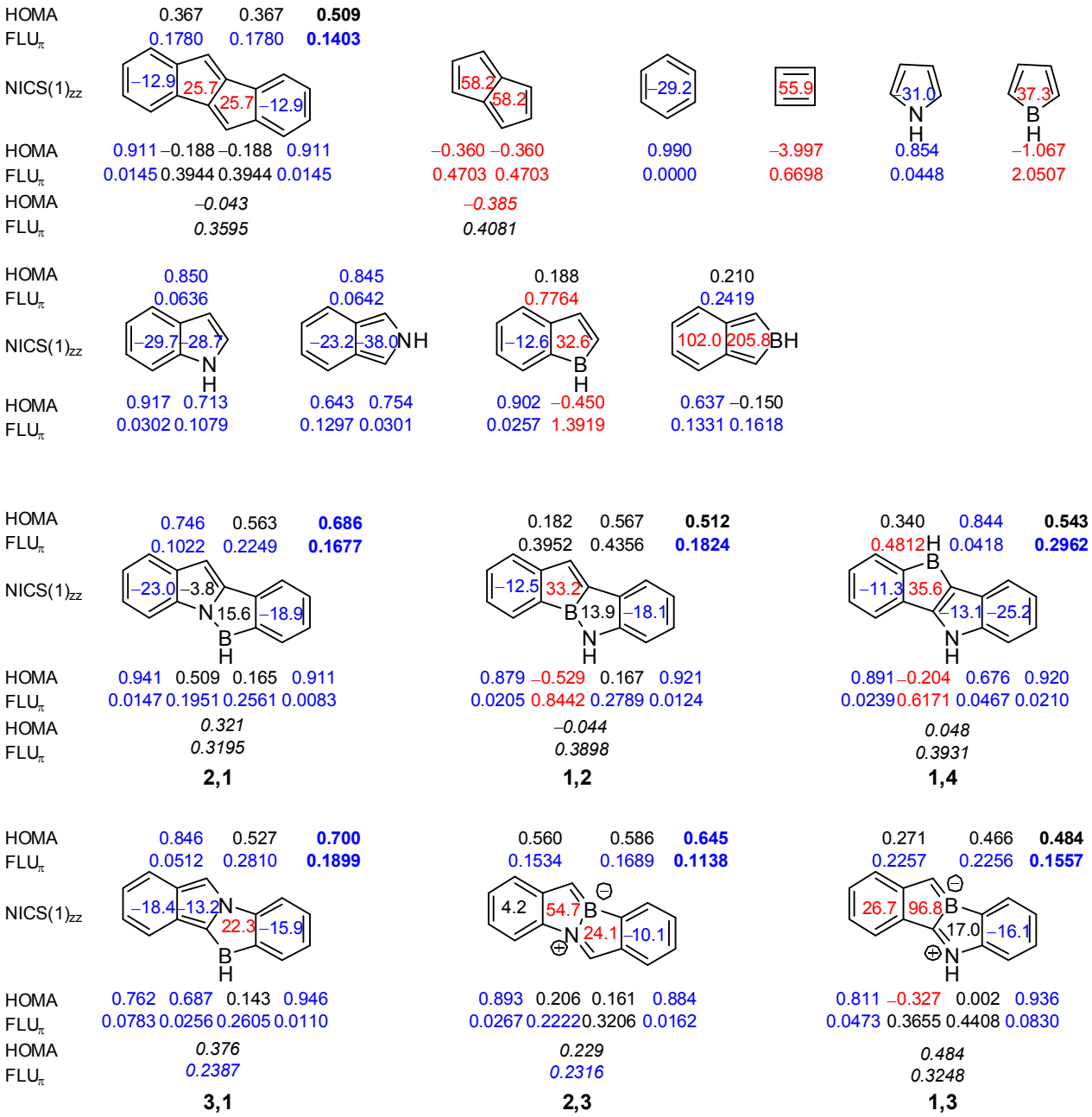


Figure 7. HOMA, FLU_{π} and $NICS(1)_{zz}$ values for dibenzopentalene and its BN-substituted analogues (benzene, cyclobutadiene, pyrrole, borole, indole, isoindole, benzo[*b*]borole and benzo[*c*]borole are also included for comparison). $NICS(1)_{zz}$ data are given inside the rings. HOMA and FLU_{π} data, which are shown below the structures, correspond to individual rings and to the central pentalene moiety (values in italic) and those which are given above the structures refer to the two benzene-fused five-membered rings and to the perimeter of a molecule (values in bold). Blue-coloured values indicate aromaticity, red-coloured ones denote antiaromaticity and those given in black describe nonaromatic system, or are at the borderline between (anti)aromaticity and nonaromaticity.

Section S1.1: Comparison of (anti)aromaticity of 2,1 and 1,4 isomers

The less stable **1,4** isomer contains one 10π-electron indole subunit and one 8π-electron benzo[*b*]borole subunit. The first one is more aromatic than the corresponding moiety in **2,1** isomer, but another benzene ring is less aromatic than that in **2,1**. Furthermore, **1,4** isomer contains an antiaromatic borole moiety, while azaborolidine moiety in **2,1** is nonaromatic. Within indole moiety, benzene in **2,1** appears to be only sligtly more aromatic, but pyrrole subunit is more aromatic in **1,4**. The perimeter of **1,4** is less delocalized than that of **2,1**. Hence, on the basis of (anti)aromaticity analysis only antiaromaticity of borole moiety, weaker aromaticity of benzene fused to it and weaker delocalization at molecular perimeter can be used to explain lower stability of **1,4** relative to **2,1**. However, this explanation does not seem to be enough to account for the large energy difference between the isomers (25.24 kcal/mol).

Section S1.2: Comparison of (anti)aromaticity of 1,2 and 1,4 isomers

The 8π-electron benzo[*b*]borole subunits in **1,2** and **1,4** isomers are both nonaromatic. As already mentioned, indole moiety in **1,4** is aromatic, but benzene-fused azaborolidine in **1,2** is nonaromatic. Aromaticities of benzene rings in the two isomers do not differ much, antiaromaticity of borole moiety in **1,2** is somewhat greater than in **1,4** and pyrrole in **1,4** is aromatic compared to azaborolidine in **1,2** which is nonaromatic. Delocalization at molecular perimeter appears to be similar (HOMA) or slightly weaker (FLU) in **1,4** isomer. Thus, (anti)aromaticity considerations do not explain lower stability of **1,4** relative to **1,2**.

Section S1.3: Comparison of (anti)aromaticity of 1,4 and 3,1 isomers

The isoindole moiety in **3,1** is similarly aromatic as indole moiety in **1,4**, while another benzene ring in **3,1** appears to be slightly more aromatic than benzene ring in **1,4**. Azaborolidine in **3,1** is nonaromatic, while **1,4** isomer contains the antiaromatic borole ring, as already discussed. The electron delocalization at molecular perimeter should stabilize **3,1** more than **1,4**. Hence, the slightly less stable **3,1** appears to be more delocalized than **1,4** isomer.

Section S1.4: Comparison of (anti)aromaticity of 3,1 and 2,3 isomers

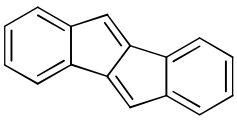
There is an aromatic substructure in the more stable **3,1** (isoindole) and one very weakly aromatic benzene-fused azaborolidine, while **2,3** consists of two weakly aromatic benzene-fused azaborolidine moieties. Benzene fused to azaborolidine in **3,1** is more aromatic than the corresponding ring in **2,3** and the other benzene is slightly less aromatic according to HOMA and FLU_{π}, or slightly more aromatic according to $NICS(1)_{zz}$. The more stable isomer contains one aromatic pyrrole moiety and one nonaromatic azaborolidine, while the less stable isomer has two nonaromatic azaborolidine moieties. The perimeter of **2,3**, however, appears to be

somewhat more delocalized than that of **3,1**. Thus, aromaticity content is slightly higher in the more stable **3,1** isomer. However, there is one thing which should be kept in mind: the less stable isomer should, in fact, significantly gain from aromatic stabilization so as to compensate its charge separation instability and form the structure which is by only 2.16 kcal/mol higher in energy.

Section S1.5: Comparison of (anti)aromaticity of 2,3 and 1,3 isomers

The energy difference between the two charge-separated **2,3** and **1,3** is large (21.86 kcal/mol) so that the more stable **2,3** should be significantly more delocalized than **1,3** isomer. First, its perimeter is, indeed, slightly more delocalized. Next, it consists of two weakly aromatic benzene-fused azaborolidines, as mentioned above, while the less stable **1,3** consists of nonaromatic benzo[*c*]borole moiety and nonaromatic benzene-fused azaborolidine. Benzene fused to azaborolidine is slightly less aromatic in **2,3** and another benzene is aromatic in **2,3**, but slightly paratropic in **1,3**. The two azaborolidine moieties in **2,3** are nonaromatic. In **1,3**, azaborolidine is nonaromatic, as well, and borole is antiaromatic. All in all, although the more stable **2,3** isomer seems to be somewhat more delocalized this can not explain the large energy difference between the isomers.

Absolute energies and X, Y, Z coordinates of optimized structures



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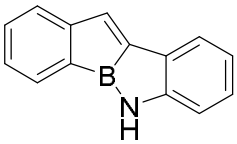

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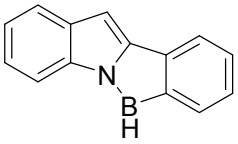

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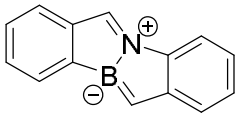

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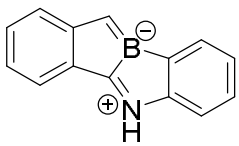

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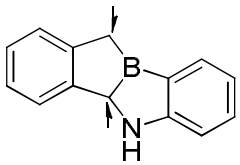

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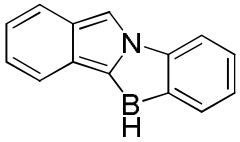

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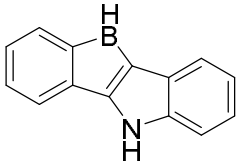
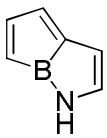
5	6	0	1.175150	-1.392187	0.000000
6	1	0	1.579899	1.937332	0.000000
7	6	0	3.478845	-0.465240	0.000000
8	1	0	4.157897	0.380447	0.000000
9	6	0	1.702035	-2.701038	0.000000
10	1	0	1.039338	-3.558714	0.000000
11	6	0	3.958083	-1.755929	0.000000
12	1	0	5.026949	-1.935777	0.000000
13	6	0	3.070964	-2.865748	0.000000
14	1	0	3.488047	-3.866845	0.000000
15	6	0	-1.468835	2.553109	0.000000
16	1	0	-0.652347	3.265943	0.000000
17	6	0	-3.601697	0.704106	0.000000
18	1	0	-4.430911	0.004502	0.000000
19	6	0	-2.802251	2.993797	0.000000
20	1	0	-3.007983	4.058137	0.000000
21	6	0	-3.855127	2.084166	0.000000
22	1	0	-4.876680	2.446952	0.000000
23	5	0	-1.629460	-1.196384	0.000000
24	1	0	-2.172526	-2.251355	0.000000
25	6	0	-0.147248	-0.885329	0.000000
26	7	0	0.000000	0.508533	0.000000



E = -619.2758111 a.u.

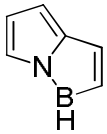
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.948255	-0.797855	0.000000
2	6	0	-1.757921	0.613998	0.000000
3	6	0	2.124325	0.969520	0.000000
4	6	0	1.729453	-0.400375	0.000000
5	6	0	3.475282	1.266819	0.000000
6	1	0	3.809264	2.299589	0.000000
7	6	0	2.653301	-1.426801	0.000000
8	1	0	2.349973	-2.468994	0.000000
9	6	0	4.430453	0.227616	0.000000
10	1	0	5.488130	0.466389	0.000000
11	6	0	4.024216	-1.097099	0.000000
12	1	0	4.763771	-1.889972	0.000000
13	6	0	-2.894121	1.434907	0.000000
14	1	0	-2.787163	2.513606	0.000000
15	6	0	-3.206491	-1.392007	0.000000
16	1	0	-3.326322	-2.469955	0.000000
17	6	0	-4.154803	0.849551	0.000000
18	1	0	-5.036787	1.480109	0.000000
19	6	0	-4.312391	-0.546879	0.000000
20	1	0	-5.308883	-0.972873	0.000000
21	1	0	-0.510953	-2.388595	0.000000
22	6	0	0.257763	-0.415363	0.000000
23	7	0	-0.681147	-1.395122	0.000000
24	6	0	-0.333655	0.848610	0.000000
25	5	0	0.806594	1.866664	0.000000
26	1	0	0.771081	3.055394	0.000000



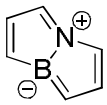
E = -311.8934866 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.131868	-0.028471	0.000000
2	6	0	1.403874	-1.170990	0.000000
3	6	0	0.000000	-0.785924	0.000000
4	6	0	-1.276651	-1.204316	0.000000
5	6	0	-2.200770	0.011112	0.000000
6	6	0	-1.553567	1.195854	0.000000
7	1	0	1.778338	2.069258	0.000000
8	1	0	-1.667143	-2.217951	0.000000
9	1	0	3.210071	0.065920	0.000000
10	1	0	1.835352	-2.162457	0.000000
11	1	0	-2.068396	2.147527	0.000000
12	1	0	-3.281192	-0.107662	0.000000
13	5	0	-0.028593	0.785801	0.000000
14	7	0	1.329631	1.167539	0.000000



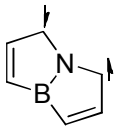
E = -311.9287431 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.236719	0.073735	0.000000
2	6	0	-1.389267	1.136747	0.000000
3	6	0	0.000000	0.682882	0.000000
4	6	0	1.295064	1.131822	0.000000
5	6	0	2.144967	-0.037536	0.000000
6	6	0	1.330888	-1.137386	0.000000
7	1	0	-1.623227	-2.367639	0.000000
8	1	0	1.623585	2.160347	0.000000
9	1	0	-3.313856	0.173824	0.000000
10	1	0	-1.661495	2.185728	0.000000
11	1	0	1.576484	-2.187665	0.000000
12	1	0	3.223781	-0.044040	0.000000
13	7	0	0.009609	-0.707608	0.000000
14	5	0	-1.352425	-1.213776	0.000000



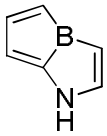
E = -311.8684848 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.424074	1.211635	0.000000
2	6	0	-2.174890	-0.079848	0.000000
3	6	0	-1.342825	-1.138869	0.000000
4	6	0	1.225980	-1.096617	0.000000
5	6	0	2.188637	-0.023569	0.000000
6	6	0	1.525732	1.189516	0.000000
7	1	0	-1.961594	2.151071	0.000000
8	1	0	1.444433	-2.160103	0.000000
9	1	0	-3.253670	-0.165797	0.000000
10	1	0	-1.541955	-2.199221	0.000000
11	1	0	2.060135	2.131769	0.000000
12	1	0	3.256612	-0.193860	0.000000
13	5	0	0.000936	0.875063	0.000000
14	7	0	0.000000	-0.616095	0.000000



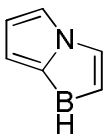
E = -311.8764822 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.493101	-1.195787	0.000000
2	6	0	-2.184196	0.032515	0.000000
3	6	0	-1.287078	1.116768	0.000000
4	6	0	1.287434	1.116660	0.000000
5	6	0	2.184042	0.032763	0.000000
6	6	0	1.493027	-1.195856	0.000000
7	1	0	-2.012739	-2.145120	0.000000
8	1	0	1.513940	2.174334	0.000000
9	1	0	-3.258675	0.161699	0.000000
10	1	0	-1.514018	2.174334	0.000000
11	1	0	2.013055	-2.144975	0.000000
12	1	0	3.258573	0.161534	0.000000
13	5	0	-0.000180	-0.847326	0.000000
14	7	0	0.000000	0.630349	0.000000



E = -311.8611637 a.u.

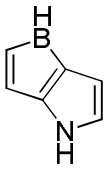
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.113595	0.050031	0.000000
2	6	0	0.000000	-0.704716	0.000000
3	6	0	1.242628	-1.198470	0.000000
4	6	0	2.207115	-0.008288	0.000000
5	6	0	1.596103	1.193036	0.000000
6	1	0	1.583533	-2.228636	0.000000
7	1	0	-3.191708	-0.080135	0.000000
8	1	0	-1.715335	-2.028694	0.000000
9	1	0	2.146290	2.125240	0.000000
10	1	0	3.281896	-0.168842	0.000000
11	6	0	-1.426462	1.250956	0.000000
12	1	0	-1.968140	2.186947	0.000000
13	5	0	0.040456	0.872708	0.000000
14	7	0	-1.339078	-1.094959	0.000000



E = -311.8977572 a.u.

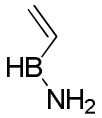
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.236039	-0.101573	0.000000
2	6	0	-0.022117	0.809299	0.000000
3	6	0	-1.365472	1.165262	0.000000
4	6	0	-2.147836	-0.026994	0.000000
5	6	0	-1.266535	-1.094184	0.000000
6	1	0	-1.749709	2.174681	0.000000
7	1	0	3.297372	-0.308444	0.000000
8	1	0	1.889155	2.363193	0.000000
9	1	0	-1.453622	-2.157052	0.000000
10	1	0	-3.224036	-0.099021	0.000000
11	7	0	0.000000	-0.579424	0.000000
12	6	0	1.318291	-1.093047	0.000000
13	1	0	1.451756	-2.167880	0.000000
14	5	0	1.454972	1.259583	0.000000



E = -311.8824521 a.u.

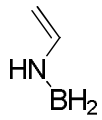
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.279799	0.214054	0.000000
2	6	0	-1.346875	1.188905	0.000000
3	6	0	2.131189	-0.101533	0.000000
4	6	0	1.347059	-1.237687	0.000000
5	1	0	-2.030526	-2.275332	0.000000
6	1	0	1.589213	1.963357	0.000000
7	1	0	-3.342622	0.423739	0.000000
8	1	0	-1.521996	2.259991	0.000000
9	1	0	1.729386	-2.247626	0.000000
10	1	0	3.201257	0.026556	0.000000
11	6	0	-0.019167	-0.823510	0.000000
12	6	0	0.000000	0.566180	0.000000
13	7	0	1.281504	1.003223	0.000000
14	5	0	-1.517936	-1.202340	0.000000



E = -159.5065865 a.u.

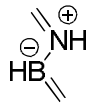
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.287801	-1.439924	0.000000
2	1	0	2.226602	-0.892555	0.000000
3	1	0	1.365708	-2.523750	0.000000

4	6	0	0.112146	-0.797239	0.000000
5	1	0	-0.791406	-1.411118	0.000000
6	1	0	0.982638	1.434000	0.000000
7	1	0	-2.124365	0.899159	0.000000
8	1	0	-1.347552	2.396301	0.000000
9	7	0	-1.244473	1.393859	0.000000
10	5	0	0.000000	0.752785	0.000000



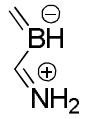
E = -159.4871499 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.116342	1.421130	0.000000
2	1	0	-2.102620	0.968827	0.000000
3	1	0	-1.063691	2.501049	0.000000
4	6	0	0.000000	0.690828	0.000000
5	1	0	0.979637	1.156259	0.000000
6	1	0	-0.857444	-1.156031	0.000000
7	1	0	2.269884	-0.968738	0.000000
8	1	0	1.081623	-2.687334	0.000000
9	5	0	1.205714	-1.503704	0.000000
10	7	0	0.051727	-0.709609	0.000000



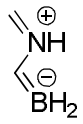
E = -159.4391643 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.007336	-1.630101	0.000000
2	1	0	-2.007713	-1.196059	0.000000
3	1	0	-1.013953	-2.715770	0.000000
4	1	0	1.346433	-1.184597	0.000000
5	1	0	-0.976191	0.933673	0.000000
6	1	0	1.921120	1.356053	0.000000
7	1	0	0.550689	2.641137	0.000000
8	7	0	0.000000	0.644279	0.000000
9	6	0	0.868026	1.606029	0.000000
10	5	0	0.203096	-0.839992	0.000000



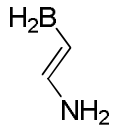
E = -159.4320663 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.975416	1.097772	0.000000
2	1	0	0.937782	2.474220	0.000000
3	1	0	-0.962998	1.146208	0.000000
4	1	0	1.161661	-1.409446	0.000000
5	1	0	-2.154123	-1.011523	0.000000
6	1	0	-1.347347	-2.637637	0.000000
7	6	0	-1.211228	-1.558172	0.000000
8	6	0	0.000000	0.635747	0.000000
9	5	0	0.081345	-0.883099	0.000000
10	7	0	1.035750	1.470065	0.000000



E = -159.4182372 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.173907	-1.068929	0.000000
2	1	0	-1.060392	-2.815174	0.000000
3	1	0	1.147190	-1.136944	0.000000
4	1	0	-0.973082	0.875723	0.000000
5	1	0	1.944738	1.271300	0.000000
6	1	0	0.567301	2.557231	0.000000
7	7	0	0.000000	0.574029	0.000000
8	6	0	0.896235	1.530152	0.000000
9	6	0	0.117244	-0.793231	0.000000
10	5	0	-1.106544	-1.624586	0.000000



E = -159.4567771 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.026915	0.944105	0.000000
2	1	0	-1.040734	2.354749	0.000000
3	1	0	0.933074	1.127586	0.000000
4	1	0	-0.918891	-1.320528	0.000000
5	1	0	2.375029	-0.890974	0.000000
6	1	0	1.419811	-2.715002	0.000000
7	6	0	0.000000	0.570096	0.000000
8	7	0	-1.106013	1.352033	0.000000
9	6	0	0.037533	-0.796165	0.000000

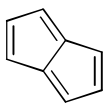
10	5	0	1.355104	-1.521551	0.000000

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

E = -154.7211606 a.u.

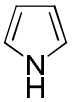
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.666663	0.788598
2	6	0	0.000000	0.666663	-0.788598
3	6	0	0.000000	-0.666663	-0.788598
4	6	0	0.000000	-0.666663	0.788598
5	1	0	0.000000	1.433070	1.551212
6	1	0	0.000000	1.433070	-1.551212
7	1	0	0.000000	-1.433070	-1.551212
8	1	0	0.000000	-1.433070	1.551212



E = -308.4476026 a.u.

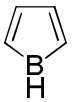
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.161909	1.278414	0.000000
2	6	0	0.039457	2.170561	0.000000
3	6	0	1.161909	1.413435	0.000000
4	6	0	0.728939	0.004299	0.000000

5	6	0	-0.728939	-0.004299	0.000000
6	6	0	1.161909	-1.278414	0.000000
7	6	0	-0.039457	-2.170561	0.000000
8	6	0	-1.161909	-1.413435	0.000000
9	1	0	-2.184118	1.635809	0.000000
10	1	0	2.184118	-1.635809	0.000000
11	1	0	-0.007794	3.250790	0.000000
12	1	0	2.181459	1.771258	0.000000
13	1	0	-2.181459	-1.771258	0.000000
14	1	0	0.007794	-3.250790	0.000000



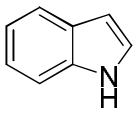
E = -210.2305244 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.125066	0.331227
2	6	0	0.000000	0.712442	-0.982383
3	6	0	0.000000	-0.712442	-0.982383
4	6	0	0.000000	-1.125066	0.331227
5	7	0	0.000000	0.000000	1.121620
6	1	0	0.000000	0.000000	2.127701
7	1	0	0.000000	2.112538	0.763194
8	1	0	0.000000	1.359292	-1.845779
9	1	0	0.000000	-1.359292	-1.845779
10	1	0	0.000000	-2.112538	0.763194



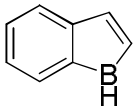
E = -180.266767 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.252594	0.349642
2	6	0	0.000000	-0.759099	-0.899378
3	6	0	0.000000	0.759099	-0.899378
4	6	0	0.000000	1.252594	0.349642
5	1	0	0.000000	0.000000	2.506389
6	1	0	0.000000	-2.311376	0.575203
7	1	0	0.000000	-1.331622	-1.822428
8	1	0	0.000000	1.331622	-1.822428
9	1	0	0.000000	2.311376	0.575203
10	5	0	0.000000	0.000000	1.316978



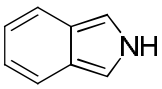
E = -363.9139334 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.492494	-0.617847	0.000000
2	6	0	0.000000	0.715798	0.000000
3	6	0	-1.366463	1.007033	0.000000
4	6	0	-2.250326	-0.063337	0.000000
5	6	0	-1.785636	-1.393382	0.000000
6	6	0	-0.428556	-1.678581	0.000000
7	6	0	1.926949	-0.533055	0.000000
8	6	0	2.252493	0.795733	0.000000
9	1	0	-1.727510	2.029826	0.000000
10	1	0	-3.317396	0.127970	0.000000
11	1	0	-2.504586	-2.204819	0.000000
12	1	0	-0.081903	-2.706274	0.000000
13	1	0	2.626640	-1.354130	0.000000
14	1	0	3.220182	1.272284	0.000000
15	1	0	1.062564	2.559758	0.000000
16	7	0	1.096611	1.554458	0.000000



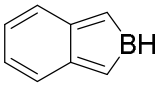
E = -333.9741906 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.696905	0.000000
2	6	0	0.528467	-0.621102	0.000000
3	6	0	-0.341233	-1.697059	0.000000
4	6	0	-1.735676	-1.474333	0.000000
5	6	0	-2.233624	-0.181793	0.000000
6	6	0	-1.360238	0.928052	0.000000
7	6	0	1.121168	1.677877	0.000000
8	6	0	2.333005	1.075302	0.000000
9	1	0	0.038083	-2.714251	0.000000
10	1	0	-2.418511	-2.316515	0.000000
11	1	0	-3.305571	-0.017069	0.000000
12	1	0	-1.762279	1.936069	0.000000
13	1	0	0.942603	2.750081	0.000000
14	1	0	3.261229	1.633926	0.000000
15	5	0	2.093801	-0.470785	0.000000
16	1	0	2.904229	-1.341410	0.000000



E = -363.8993747 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.724993	0.250562
2	6	0	0.000000	-0.724993	0.250562
3	6	0	0.000000	-1.429764	-0.983569
4	6	0	0.000000	-0.714590	-2.153361
5	6	0	0.000000	0.714590	-2.153361
6	6	0	0.000000	1.429764	-0.983569
7	6	0	0.000000	1.134368	1.582091
8	1	0	0.000000	-2.514413	-0.996396
9	1	0	0.000000	-1.237129	-3.103541
10	1	0	0.000000	1.237129	-3.103541
11	1	0	0.000000	2.514413	-0.996396
12	1	0	0.000000	2.114907	2.028263
13	1	0	0.000000	0.000000	3.356011
14	1	0	0.000000	-2.114907	2.028263
15	6	0	0.000000	-1.134368	1.582091
16	7	0	0.000000	0.000000	2.348380



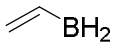
E = -333.9148163 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.713893	0.281479
2	6	0	0.000000	-0.713893	0.281479
3	6	0	0.000000	-1.408705	-0.895460
4	6	0	0.000000	-0.682931	-2.139602
5	6	0	0.000000	0.682931	-2.139602
6	6	0	0.000000	1.408705	-0.895460
7	6	0	0.000000	1.173943	1.686831
8	6	0	0.000000	-1.173943	1.686831
9	1	0	0.000000	-2.493603	-0.907536
10	1	0	0.000000	-1.231632	-3.074096
11	1	0	0.000000	1.231632	-3.074096
12	1	0	0.000000	2.493603	-0.907536
13	1	0	0.000000	2.242036	1.894380
14	1	0	0.000000	-2.242036	1.894380
15	5	0	0.000000	0.000000	2.631207
16	1	0	0.000000	0.000000	3.819491

$H_2B{=}NH_2$

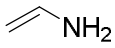
E = -82.0741592 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	-0.779548
2	1	0	0.000000	1.042920	-1.357574
3	1	0	0.000000	-1.042920	-1.357574
4	7	0	0.000000	0.000000	0.611871
5	1	0	0.000000	0.843612	1.164894
6	1	0	0.000000	-0.843612	1.164894



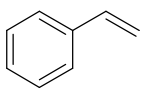
E = -104.0604251 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.174136	-0.173059	0.000000
2	1	0	-1.205294	-1.259267	0.000000
3	1	0	-2.135431	0.335077	0.000000
4	6	0	0.000000	0.484132	0.000000
5	1	0	-0.033758	1.572991	0.000000
6	5	0	1.340393	-0.271128	0.000000
7	1	0	2.384151	0.305733	0.000000
8	1	0	1.333183	-1.465334	0.000000



E = -133.9951231 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.252323	-0.196546	0.014605
2	1	0	1.333880	-1.278465	0.019053
3	1	0	2.170480	0.373812	0.004085
4	6	0	0.069444	0.428238	-0.000603
5	1	0	0.029333	1.513774	-0.010783
6	7	0	-1.184732	-0.169493	-0.079542
7	1	0	-1.221609	-1.157099	0.129853
8	1	0	-1.949565	0.344272	0.330576



E = -309.7307788 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.778877	-1.044542	0.000002
2	6	0	-0.406058	-1.279710	-0.000006

3	6	0	0.514224	-0.220293	-0.000004
4	6	0	0.008774	1.090567	-0.000005
5	6	0	-1.360375	1.327526	-0.000005
6	6	0	-2.262479	0.261398	0.000007
7	1	0	-2.468949	-1.880956	0.000011
8	1	0	-0.036113	-2.300088	-0.000005
9	1	0	0.690681	1.932898	-0.000007
10	1	0	-1.728255	2.347693	0.000003
11	1	0	-3.330079	0.449776	0.000009
12	6	0	1.953593	-0.528632	-0.000001
13	1	0	2.186106	-1.591483	-0.000006
14	6	0	2.973649	0.335153	0.000006
15	1	0	2.833848	1.410395	0.000010
16	1	0	3.998052	-0.017035	0.000008