

Supplementary data for article:

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Does Aromaticity Account for an Enhanced Thermodynamic Stability?

The Case of Monosubstituted Azaborines and the Stereoelectronic Chameleonism of NH₂ group

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Supplementary Information

Table of Contents

Table S1	S2
Table S2	S4
Table S3	S5
Table S4	S10
Absolute energies and x, y, z coordinates of the optimized structures.....	S11

Table S1. Contribution of various energy components to the total binding interactions between two radical fragments, the ring and the substituent, and energy changes (values in bold) upon constitutional isomerization.^a Values are in kcal/mol, calculated at the UB3LYP/6-311+G(d,p) level.

Entry	Compound	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}
		ΔE_{iso}	$\Delta \Delta E_{\text{def}}$	$\Delta \Delta E_{\text{int}}$	$\Delta \Delta E_{\text{elstat}}$	$\Delta \Delta E_{\text{Pauli}}$	$\Delta \Delta E_{\text{oi}}$	$\Delta \Delta E_{\text{disp}}$
1	2-nitro-1,2-azaborine	-86.67	6.29	-92.96	-174.07	327.59	-223.63	-22.85
2	3-nitro-1,2-azaborine	-67.15	9.34	-76.49	-163.57	349.59	-239.70	-22.81
3	2-nitro → 3-nitro	19.52	3.05	16.47	10.50	22.00	-16.07	0.04
4	5-nitro-1,2-azaborine	-65.29	13.29	-78.58	-163.81	350.13	-241.48	-23.42
5	2-nitro → 5-nitro	21.38	7.00	14.38	10.26	22.54	-17.85	-0.57
6	4-nitro-1,2-azaborine	-64.77	5.72	-70.49	-154.31	327.49	-221.68	-21.99
7	2-nitro → 4-nitro	21.90	-0.57	22.47	19.76	-0.10	1.95	0.86
8	6-nitro-1,2-azaborine	-64.71	10.06	-74.77	-162.83	348.78	-237.67	-23.05
9	2-nitro → 6-nitro	21.96	3.77	18.19	11.24	21.19	-14.04	-0.20
10	1-nitro-1,2-azaborine	-41.56	10.29	-51.85	-139.20	330.71	-222.09	-21.27
11	2-nitro → 1-nitro	45.11	4.00	41.11	34.87	3.12	1.54	1.58
12	2-amino-1,2-azaborine	-124.95	2.51	-127.46	-260.75	554.17	-395.16	-25.72
13	4-amino-1,2-azaborine	-102.03	6.07	-108.10	-244.42	533.42	-372.44	-24.66
14	2-amino → 4-amino	22.92	3.56	19.36	16.33	-20.75	22.72	1.06
15	6-amino-1,2-azaborine	-99.68	8.59	-108.27	-227.57	481.17	-336.99	-24.88
16	2-amino → 6-amino	25.26	6.07	19.19	33.18	-73.00	58.17	0.84
17	3-amino-1,2-azaborine	-98.46	7.69	-106.15	-232.62	507.33	-356.05	-24.81
18	2-amino → 3-amino	26.49	5.18	21.31	28.13	-46.84	39.11	0.91
19	5-amino-1,2-azaborine	-93.73	10.49	-104.22	-206.89	433.88	-306.42	-24.79
20	2-amino → 5-amino	31.22	7.98	23.24	53.86	-120.29	88.74	0.93
21	1-amino-1,2-azaborine	-71.34	8.59	-79.93	-170.25	370.54	-257.86	-22.36
22	2-amino → 1-amino	53.62	6.08	47.53	90.50	-183.63	137.30	3.36
23	3-nitro-1,3-azaborine	-87.32	6.56	-93.88	-171.35	322.26	-222.17	-22.62
24	2-nitro-1,3-azaborine	-68.41	10.63	-79.04	-175.40	376.04	-256.20	-23.48
25	3-nitro → 2-nitro	18.91	4.07	14.84	-4.05	53.78	-34.03	-0.86
26	4-nitro-1,3-azaborine	-65.97	7.97	-73.94	-161.42	345.30	-235.34	-22.48
27	3-nitro → 4-nitro	21.34	1.40	19.94	9.93	23.04	-13.17	0.14
28	6-nitro-1,3-azaborine	-65.54	15.97	-81.51	-173.11	372.69	-256.90	-24.19
29	3-nitro → 6-nitro	21.78	9.41	12.37	-1.76	50.43	-34.73	-1.57
30	5-nitro-1,3-azaborine	-63.11	8.64	-71.75	-157.35	334.70	-226.90	-22.20
31	3-nitro → 5-nitro	24.21	2.08	22.13	14.00	12.44	-4.73	0.42
32	1-nitro-1,3-azaborine	-37.93	2.32	-40.25	-121.29	287.26	-186.95	-19.27
33	3-nitro → 1-nitro	49.38	-4.25	53.63	50.06	-35.00	35.22	3.35
34	3-amino-1,3-azaborine	-121.13	2.71	-123.84	-251.75	529.20	-375.84	-25.45
35	4-amino-1,3-azaborine	-102.66	8.24	-110.90	-266.70	606.23	-425.39	-25.04
36	3-amino → 4-amino	18.46	5.52	12.94	-14.95	77.03	-49.55	0.41
37	2-amino-1,3-azaborine	-99.78	7.47	-107.25	-241.38	522.87	-363.93	-24.81
38	3-amino → 2-amino	21.34	4.75	16.59	10.37	-6.33	11.91	0.64

39	5-amino-1,3-azaborine	-96.34	7.74	-104.08	-223.01	475.72	-332.43	-24.36
40	3-amino → 5-amino	24.78	5.02	19.76	28.74	-53.48	43.41	1.09
41	6-amino-1,3-azaborine	-95.59	12.20	-107.79	-207.16	414.54	-290.35	-24.82
42	3-amino → 6-amino	25.53	9.48	16.05	44.59	-114.66	85.49	0.63
43	1-amino-1,3-azaborine	-71.95	3.47	-75.42	-179.26	395.97	-270.31	-21.82
44	3-amino → 1-amino	49.17	0.75	48.42	72.49	-133.23	105.53	3.63
45	4-nitro-1,4-azaborine	-86.39	5.50	-91.89	-176.84	335.03	-228.18	-21.90
46	3-nitro-1,4-azaborine	-64.74	10.99	-75.73	-162.89	347.97	-238.17	-22.64
47	4-nitro → 3-nitro	21.64	5.48	16.16	13.95	12.94	-9.99	-0.74
48	2-nitro-1,4-azaborine	-62.65	9.10	-71.75	-162.68	346.18	-232.89	-22.36
49	4-nitro → 2-nitro	23.74	3.60	20.14	14.16	11.15	-4.71	-0.46
50	1-nitro-1,4-azaborine	-39.70	18.16	-57.86	-144.22	342.63	-234.28	-21.99
51	4-nitro → 1-nitro	46.69	12.66	34.03	32.62	7.60	-6.10	-0.09
52	4-amino-1,4-azaborine	-127.11	2.72	-129.83	-261.96	553.99	-396.32	-25.54
53	2-amino-1,4-azaborine	-98.11	8.01	-106.12	-226.19	474.70	-330.26	-24.37
54	4-amino → 2-amino	29.00	5.29	23.71	35.77	-79.29	66.06	1.17
55	3-amino-1,4-azaborine	-94.86	9.02	-103.88	-224.99	486.46	-340.83	-24.52
56	4-amino → 3-amino	32.25	6.30	25.95	36.98	-67.53	55.49	1.02
57	1-amino-1,4-azaborine	-70.00	16.50	-86.50	-181.58	396.49	-278.60	-22.81
58	4-amino → 1-amino	57.10	13.77	43.33	80.38	-157.50	117.72	2.73


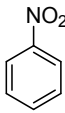
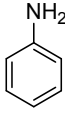
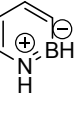
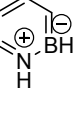
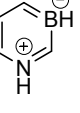
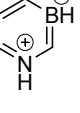
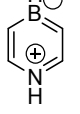
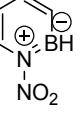
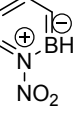
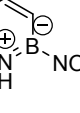
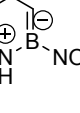

^a ΔE_{tot} = total binding energy between two fragments, ΔE_{def} = deformation energy, ΔE_{int} = interaction energy, ΔE_{elstat} = electrostatic energy, ΔE_{Pauli} = Pauli repulsion, ΔE_{oi} = orbital interaction energy, ΔE_{disp} = dispersion energy, ΔE_{iso} = isomerization energy.^b

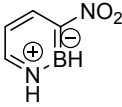
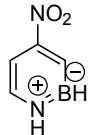
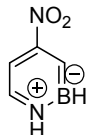
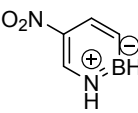
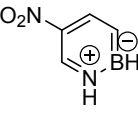
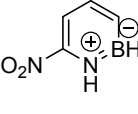
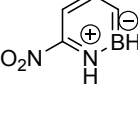
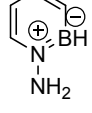
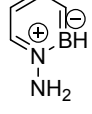
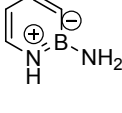
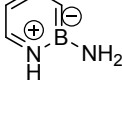
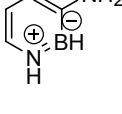
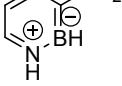
Table S2. Contribution of various energy components to the total binding interactions between six radical fragments and energy changes (values in bold) upon constitutional isomerization.^a Values are in kcal/mol, calculated at the UB3LYP/6-311+G(d,p) level.

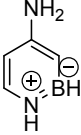
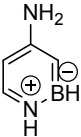
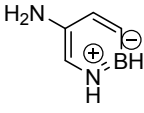
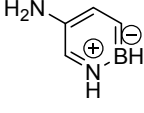
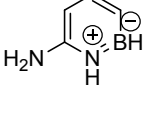
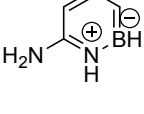
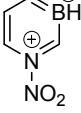
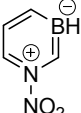
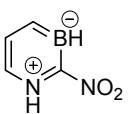
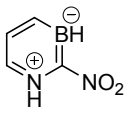
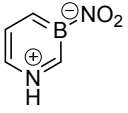
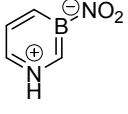
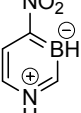
Entry	Compound	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}	Interacting fragments
		ΔE_{iso}	$\Delta \Delta E_{\text{def}}$	$\Delta \Delta E_{\text{int}}$	$\Delta \Delta E_{\text{elstat}}$	$\Delta \Delta E_{\text{Pauli}}$	$\Delta \Delta E_{\text{oi}}$	$\Delta \Delta E_{\text{disp}}$	
1	1,4-azaborine ^b	-856.11	0.72	-856.83	-1054.02	1754.17	-1337.62	-219.37	4×CH(q), NH(t), BH(t)
2	1,3-azaborine ^b	-848.25	205.57	-1053.82	-1215.35	2056.79	-1699.16	-196.09	2×CH(q), C(6)H ⁺ (t), NH(t), BH(t), C(2) ⁻ (t)
3	1,4 → 1,3^b	7.88	204.85	-196.97	-161.33	302.62	-361.54	23.28	
4	2-nitro-1,4-azaborine	-855.64	1.30	-856.94	-1063.78	1858.51	-1441.05	-210.62	3×CH(q), NH(t), BH(t), CNO ₂ (q)
5	2-nitro-1,3-azaborine	-853.20	154.03	-1007.23	-1210.85	2118.30	-1722.26	-192.42	2×CH(q), C(6)H ⁺ (t), NH(t), BH(t), CNO ₂ ⁻ (t)
6	2-NO₂-1,4 → 2-NO₂-1,3	2.44	152.73	-150.29	-147.07	259.79	-281.21	18.20	
7	1,4-azaborine ^b	-856.11	0.72	-856.83	-1054.02	1754.17	-1337.62	-219.37	4×CH(q), NH(t), BH(t)
8	1,3-azaborine ^b	-848.69	205.35	-1054.04	-1174.53	1984.56	-1667.98	-196.09	2×CH(q), C(4)H ⁺ (t), NH(t), BH(t), C(2) ⁻ (t)
9	1,4 → 1,3^b	7.43	204.63	-197.20	-120.51	230.39	-330.36	23.28	
10	3-amino-1,4-azaborine	-860.78	1.75	-862.53	-1089.14	1766.59	-1321.67	-218.31	3×CH(q), NH(t), BH(t), CNH ₂ (q)
11	4-amino-1,3-azaborine	-860.35	126.37	-986.72	-1150.73	1945.43	-1582.22	-199.20	2×CH(q), C(2)H ⁻ (t), NH(t), BH(t), CNH ₂ ⁺ (t)
12	3-NH₂-1,4 → 4-NH₂-1,3	0.43	124.62	-124.19	-61.59	178.84	-260.55	19.11	
13	1,2-azaborine ^b	-878.00	0.67	-878.67	-939.35	1550.39	-1269.83	-219.88	4×CH(q), NH(t), BH(t)
14	1,4-azaborine ^b	-856.11	0.72	-856.83	-1054.02	1754.17	-1337.62	-219.37	4×CH(q), NH(t), BH(t)
15	1,2 → 1,4^b	21.89	0.05	21.84	-114.67	203.78	-67.79	0.51	
16	2-nitro-1,2-azaborine	-2972.28	-2091.84	-880.94	-942.60	1585.67	-1307.32	-216.69	4×CH(q), NH(t), BNO ₂ (t)
17	4-nitro-1,4-azaborine	-2952.22	-2092.15	-860.07	-1025.71	1748.48	-1367.44	-215.40	4×CH(q), NH(t), BNO ₂ (t)
18	2-NO₂-1,2 → 4-NO₂-1,4	20.56	-0.31	20.87	-83.11	162.81	-60.12	1.29	
19	2-amino-1,2-azaborine	-864.02	2.06	-866.08	-1077.81	1747.22	-1313.82	-221.67	4×CH(q), NH(t), BNH ₂ (t)
20	4-amino-1,4-azaborine	-845.90	1.97	-847.87	-1074.23	1755.45	-1307.93	-221.16	4×CH(q), NH(t), BNH ₂ (t)
21	2-NH₂-1,2 → 4-NH₂-1,4	18.12	-0.09	18.21	3.58	8.23	5.89	0.51	

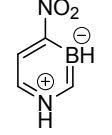
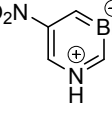
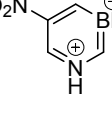
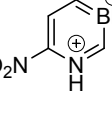
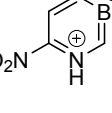
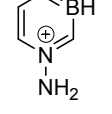
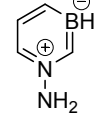
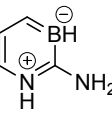
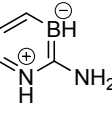
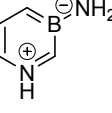
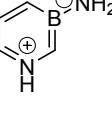
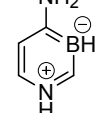
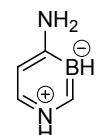
^a Labeling of various energy terms is the same as in Table S1. ^b From ref. 8b.

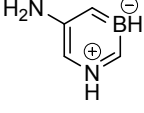
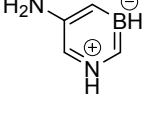
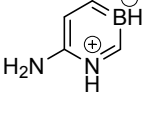
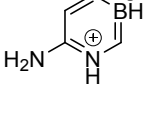
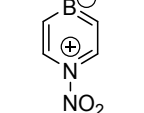
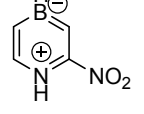
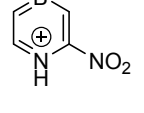
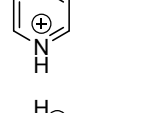
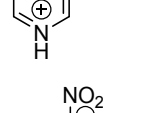
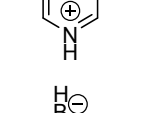
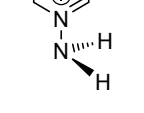
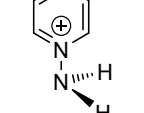
Table S3. Calculated vertical resonance energies of cyclic molecules (VRE_{cyclic}) and acyclic reference molecules (VRE_{acyclic}), extra cyclic resonance energies (ECRE) and extra cyclic resonance energies based on relative weights of the two resonance structure ($ECRE_{\text{rv}}$). All values are in kcal/mol.

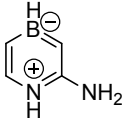
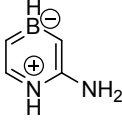
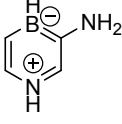
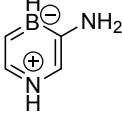
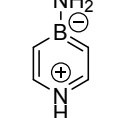
Compound	Resonance weight	VRE_{cyclic}	Reference molecules	VRE_{acyclic}	ECRE	$ECRE_{\text{rv}}$
	a	163.89	$H_2C=CH-CH=CH_2$ $H_2C=CH-CH=CH_2$ $H_2C=CH-CH=CH_2$	23.30 23.30 23.30	93.99	93.99 ^b
	a	156.45	$H_2C=CH-CH=CH_2$ $H_2C=CH-CH=CHNO_2$ $H_2C=CH-C(NO_2)=CH_2$	23.30 23.76 23.67	85.72	85.72
	a	153.33	$H_2C=CH-CH=CH_2$ $H_2C=CH-CH=CHNH_2$ $H_2C=CH-C(NH_2)=CH_2$	23.30 24.02 20.51	85.50	85.50
	0.93	116.4	$H_2C=CH-CH=CH_2$ $H_2N^+=BH^-CH=CH_2$ $H_2B^-=NH^+CH=CH_2$	23.30 16.72 26.98	49.15	55.69 ^b
	0.07	270.50	$H_2N^+=CH-CH=CH_2$ $H_2B^-=CH-CH=CH_2$ $H_2C=BH^-NH^+=CH_2$	45.41 47.48 33.42	144.19	55.69 ^b
	0.49	218.23	$H_2N^+=CH-BH^-CH_2$ $H_2C=NH^+CH=CH_2$ $H_2B^-=CH-CH=CH_2$	62.47 23.19 47.48	85.10	76.66 ^b
	0.51	217.29	$H_2N^+=CH-CH=CH_2$ $H_2C=BH^-CH=CH_2$ $H_2B^-=CH-NH^+=CH_2$	45.41 17.76 85.55	68.56	76.66 ^b
	a	215.10	$H_2N^+=CH-CH=BH^-$ $H_2C=NH^+CH=CH_2$ $H_2C=BH^-CH=CH_2$	140.64 23.19 17.76	33.51	33.51 ^b
	0.88	102.19	$H_2C=CH-CH=CH_2$ $HN(NO_2)^+=BH^-CH=CH_2$ $H_2B^-=N(NO_2)^+CH=CH_2$	23.30 19.32 20.80	38.77	32.25
	0.12	112.89	$HN(NO_2)^+=CH-CH=CH_2$ $H_2B^-=CH-CH=CH_2$ $H_2C=BH^-N(NO_2)^+=CH_2$	47.91 47.48 33.11	-15.61	32.25
	0.70	122.43	$H_2C=CH-CH=CH_2$ $HN^+=B(NO_2)^-CH=CH_2$ $HB(NO_2)^-=NH^+CH=CH_2$	23.30 21.10 23.86	54.17	79.27
	0.30	246.93	$HN^+=CH-CH=CH_2$ $HB(NO_2)^-=CH-CH=CH_2$ $H_2C=B(NO_2)^-NH^+=CH_2$	45.41 36.52 27.16	137.84	79.27
	0.83	120.02	$H_2C=CH-CH=CHNO_2$ $HN^+=BH^-C(NO_2)=CH_2$ $H_2B^-=NH^+CH=CH_2$	23.76 14.48 26.98	54.81	68.45

	0.17	231.68	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{H}_2\text{B}^-=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	30.84	135.05	68.45
			$\text{HC}(\text{NO}_2)=\text{BH}^--\text{NH}^+=\text{CH}_2$	20.38		
	0.74	115.26	$\text{H}_2\text{C}=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	23.67		
			$\text{H}_2\text{N}^+=\text{BH}^--\text{CH}=\text{CHNO}_2$	13.30	51.32	23.39
			$\text{H}_2\text{B}^-=\text{NH}^+-\text{CH}=\text{CH}_2$	26.98		
	0.26	73.53	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CHNO}_2$	37.28		
			$\text{H}_2\text{B}^-=\text{CH}-\text{C}(\text{NO}_2)=\text{CH}_2$	58.92	-56.09	23.39
			$\text{H}_2\text{C}=\text{BH}^--\text{NH}^+=\text{CH}_2$	33.42		
	0.81	114.64	$\text{H}_2\text{C}=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	23.67		
			$\text{H}_2\text{N}^+=\text{BH}^--\text{CH}=\text{CH}_2$	16.72	41.36	59.78
			$\text{H}_2\text{B}^-=\text{NH}^+-\text{CH}=\text{CHNO}_2$	32.90		
	0.19	275.27	$\text{H}_2\text{N}^+=\text{CH}-\text{C}(\text{NO}_2)=\text{CH}_2$	38.78		
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CHNO}_2$	64.77	138.30	59.78
			$\text{H}_2\text{C}=\text{BH}^--\text{NH}^+=\text{CH}_2$	33.42		
	0.74	111.55	$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CHNO}_2$	23.76		
			$\text{H}_2\text{N}^+=\text{BH}^--\text{CH}=\text{CH}_2$	16.72	39.61	42.27
			$\text{H}_2\text{B}^-=\text{NH}^+-\text{C}(\text{NO}_2)=\text{CH}_2$	31.47		
	0.26	208.85	$\text{H}_2\text{N}^+=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	53.02		
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CH}_2$	47.48	49.83	42.27
			$\text{H}_2\text{C}=\text{BH}^--\text{NH}^+=\text{CHNO}_2$	58.53		
	0.72	118.84	$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2$	23.30		
			$\text{HN}(\text{NH}_2)^+=\text{BH}^--\text{CH}=\text{CH}_2$	16.98	54.15	81.12
			$\text{H}_2\text{B}^-=\text{N}(\text{NH}_2)^+-\text{CH}=\text{CH}_2$	24.42		
	0.28	263.95	$\text{HN}(\text{NH}_2)^+=\text{CH}-\text{CH}=\text{CH}_2$	41.55		
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CH}_2$	47.48	150.49	81.12
			$\text{H}_2\text{C}=\text{BH}^--\text{N}(\text{NH}_2)^+=\text{CH}_2$	24.44		
	0.88	103.19	$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2$	23.30		
			$\text{HN}^+=\text{B}(\text{NH}_2)^--\text{CH}=\text{CH}_2$	12.58	35.26	25.64
			$\text{HB}(\text{NH}_2)^-=\text{N}^+-\text{CH}=\text{CH}_2$	32.05		
	0.12	91.75	$\text{HN}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{HB}(\text{NH}_2)^-=\text{CH}-\text{CH}=\text{CH}_2$	60.35	-44.89	25.64
			$\text{H}_2\text{C}=\text{B}(\text{NH}_2)^--\text{N}^+=\text{CH}_2$	30.87		
	0.79	103.07	$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CHNH}_2$	24.02		
			$\text{HN}^+=\text{BH}^--\text{C}(\text{NH}_2)=\text{CH}_2$	15.35	36.72	40.37
			$\text{H}_2\text{B}^-=\text{NH}^+-\text{CH}=\text{CH}_2$	26.98		
	0.21	213.92	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{H}_2\text{B}^-=\text{C}(\text{NH}_2)-\text{CH}=\text{CH}_2$	51.62	54.11	40.37
			$\text{HC}(\text{NH}_2)=\text{BH}^--\text{NH}^+=\text{CH}_2$	62.78		

	0.73	112.25	$\text{H}_2\text{C}=\text{C}(\text{NH}_2)-\text{CH}=\text{CH}_2$	20.51		
			$\text{H}_2\text{N}^+=\text{BH}^--\text{CH}=\text{CHNH}_2$	21.73	43.04	29.25
			$\text{H}_2\text{B}^-=\text{NH}^+-\text{CH}=\text{CH}_2$	26.98		
	0.27	126.54	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CHNH}_2$	64.99		
			$\text{H}_2\text{B}^-=\text{CH}-\text{C}(\text{NH}_2)=\text{CH}_2$	36.18	-8.05	29.25
			$\text{H}_2\text{C}=\text{BH}^--\text{NH}^+=\text{CH}_2$	33.42		
	0.78	107.36	$\text{H}_2\text{C}=\text{C}(\text{NH}_2)-\text{CH}=\text{CH}_2$	20.51		
			$\text{H}_2\text{N}^+=\text{BH}^--\text{CH}=\text{CH}_2$	16.72	49.28	27.57
			$\text{H}_2\text{B}^-=\text{NH}^+-\text{CH}=\text{CHNH}_2$	20.86		
	0.22	68.33	$\text{H}_2\text{N}^+=\text{CH}-\text{C}(\text{NH}_2)=\text{CH}_2$	48.58		
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CHNH}_2$	35.71	-49.38	27.57
			$\text{H}_2\text{C}=\text{BH}^--\text{NH}^+=\text{CH}_2$	33.42		
	0.71	116.23	$\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CHNH}_2$	24.02		
			$\text{H}_2\text{N}^+=\text{BH}^--\text{CH}=\text{CH}_2$	16.72	52.46	76.17
			$\text{H}_2\text{B}^-=\text{NH}^+-\text{C}(\text{NH}_2)=\text{CH}_2$	23.03 ^c		
	0.29	223.65	$\text{H}_2\text{N}^+=\text{C}(\text{NH}_2)-\text{CH}=\text{CH}_2$	25.50		
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CH}_2$	47.48	134.22	76.17
			$\text{H}_2\text{C}=\text{BH}^--\text{NH}^+=\text{CHNH}_2$	16.46		
	0.50	217.86	$\text{HN}(\text{NO}_2)^+=\text{CH}-\text{BH}^-=\text{CH}_2$	85.58		
			$\text{H}_2\text{C}=\text{N}(\text{NO}_2)^+-\text{CH}=\text{CH}_2$	25.28	59.52	60.14
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CH}_2$	47.48		
	0.50	213.40	$\text{HN}(\text{NO}_2)^+=\text{CH}-\text{CH}=\text{CH}_2$	47.91		
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76	60.75	60.14
			$\text{H}_2\text{B}^-=\text{CH}-\text{N}(\text{NO}_2)^+=\text{CH}_2$	86.99		
	0.20	175.51	$\text{H}_2\text{N}^+=\text{C}(\text{NO}_2)-\text{BH}^-=\text{CH}_2$	78.56		
			$\text{HC}(\text{NO}_2)=\text{NH}^+-\text{CH}=\text{CH}_2$	26.89	22.59	37.38
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CH}_2$	47.48		
	0.80	152.03	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{HC}(\text{NO}_2)=\text{BH}^--\text{CH}=\text{CH}_2$	14.26	41.07	37.38
			$\text{H}_2\text{B}^-=\text{C}(\text{NO}_2)-\text{NH}^+=\text{CH}_2$	51.29		
	0.52	190.86	$\text{H}_2\text{N}^+=\text{CH}-\text{B}(\text{NO}_2)^-=\text{CH}_2$	53.66		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CH}_2$	23.19	104.48	93.06
			$\text{HB}(\text{NO}_2)^-=\text{CH}-\text{CH}=\text{CH}_2$	36.52		
	0.48	203.20	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{H}_2\text{C}=\text{B}(\text{NO}_2)^--\text{CH}=\text{CH}_2$	18.11	81.68	93.06
			$\text{HB}(\text{NO}_2)^-=\text{CH}-\text{NH}^+=\text{CH}_2$	68.19		
	0.57	175.66	$\text{H}_2\text{N}^+=\text{CH}-\text{BH}^-=\text{CHNO}_2$	38.91		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CH}_2$	23.19	82.66	85.74
			$\text{H}_2\text{B}^-=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	30.89		

	0.43	231.35	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CHNO}_2$	37.39		
			$\text{H}_2\text{C}=\text{BH}^--\text{C}(\text{NO}_2)=\text{CH}_2$	18.59	89.82	85.74
			$\text{H}_2\text{B}^--\text{CH}-\text{NH}^+=\text{CH}_2$	85.55		
	0.48	226.83	$\text{H}_2\text{N}^+=\text{CH}-\text{BH}^--\text{CH}_2$	62.47		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CHNO}_2$	21.47	83.97	69.80
			$\text{H}_2\text{B}^--\text{CH}-\text{C}(\text{NO}_2)=\text{CH}_2$	58.92		
	0.52	206.08	$\text{H}_2\text{N}^+=\text{CH}-\text{C}(\text{NO}_2)=\text{CH}_2$	38.78		
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CHNO}_2$	25.03	56.71	69.80
			$\text{H}_2\text{B}^--\text{CH}-\text{NH}^+=\text{CH}_2$	85.55		
	0.40	137.57	$\text{H}_2\text{N}^+=\text{CH}-\text{BH}^--\text{CH}_2$	62.47		
			$\text{H}_2\text{C}=\text{NH}^+-\text{C}(\text{NO}_2)=\text{CH}_2$	22.73	-12.40	-17.20
			$\text{H}_2\text{B}^--\text{CH}-\text{CH}=\text{CHNO}_2$	64.77		
	0.60	184.40	$\text{H}_2\text{N}^+=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	53.02		
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76	-20.40	-17.20
			$\text{H}_2\text{B}^--\text{CH}-\text{NH}^+=\text{CHNO}_2$	134.03		
	0.46	227.08	$\text{HN}(\text{NH}_2)^+=\text{CH}-\text{BH}^--\text{CH}_2$	61.36		
			$\text{H}_2\text{C}=\text{N}(\text{NH}_2)^+-\text{CH}=\text{CH}_2$	21.15	97.09	83.66
			$\text{H}_2\text{B}^--\text{CH}-\text{CH}=\text{CH}_2$	47.48		
	0.54	201.06	$\text{HN}(\text{NH}_2)^+=\text{CH}-\text{CH}=\text{CH}_2$	41.55		
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76	72.22	83.66
			$\text{H}_2\text{B}^--\text{CH}-\text{N}(\text{NH}_2)^+=\text{CH}_2$	69.53		
	0.67	134.33	$\text{H}_2\text{N}^+=\text{C}(\text{NH}_2)-\text{BH}^--\text{CH}_2$	10.58 ^c		
			$\text{HC}(\text{NH}_2)=\text{NH}^+-\text{CH}=\text{CH}_2$	17.71	58.57	30.65
			$\text{H}_2\text{B}^--\text{CH}-\text{CH}=\text{CH}_2$	47.48		
	0.33	136.07	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{HC}(\text{NH}_2)=\text{BH}^--\text{CH}=\text{CH}_2$	23.30	-26.03	30.65
			$\text{H}_2\text{B}^--\text{C}(\text{NH}_2)-\text{NH}^+=\text{CH}_2$	93.38		
	0.44	214.95	$\text{H}_2\text{N}^+=\text{CH}-\text{B}(\text{NH}_2)^--\text{CH}_2$	52.40		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CH}_2$	23.19	79.01	58.07
			$\text{HB}(\text{NH}_2)^--\text{CH}-\text{CH}=\text{CH}_2$	60.35		
	0.56	217.90	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{H}_2\text{C}=\text{B}(\text{NH}_2)^--\text{CH}=\text{CH}_2$	15.08	41.62	58.07
			$\text{HB}(\text{NH}_2)^--\text{CH}-\text{NH}^+=\text{CH}_2$	115.79		
	0.42	231.49	$\text{H}_2\text{N}^+=\text{CH}-\text{BH}^--\text{CHNH}_2$	109.71		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CH}_2$	23.19	46.51	0.94
			$\text{H}_2\text{B}^--\text{C}(\text{NH}_2)-\text{CH}=\text{CH}_2$	52.08		
	0.58	133.54	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CHNH}_2$	66.33		
			$\text{H}_2\text{C}=\text{BH}^--\text{C}(\text{NH}_2)=\text{CH}_2$	13.73	-32.06	0.95
			$\text{H}_2\text{B}^--\text{CH}-\text{NH}^+=\text{CH}_2$	85.55		

	0.55	171.69	$\text{H}_2\text{N}^+=\text{CH}-\text{BH}^-=\text{CH}_2$	62.47		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CHNH}_2$	33.80	38.71	56.21
			$\text{H}_2\text{B}^-=\text{CH}-\text{C}(\text{NH}_2)=\text{CH}_2$	36.71		
	0.45	226.22	$\text{H}_2\text{N}^+=\text{CH}-\text{C}(\text{NH}_2)=\text{CH}_2$	47.29		
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CHNH}_2$	15.79	77.59	56.21
			$\text{H}_2\text{B}^-=\text{CH}-\text{NH}^+=\text{CH}_2$	85.55		
	0.47	220.41	$\text{H}_2\text{N}^+=\text{CH}-\text{BH}^-=\text{CH}_2$	62.47		
			$\text{H}_2\text{C}=\text{NH}^+-\text{C}(\text{NH}_2)=\text{CH}_2$	20.42	93.33	83.69
			$\text{H}_2\text{B}^-=\text{CH}-\text{CH}=\text{CHNH}_2$	44.19		
	0.53	202.16	$\text{H}_2\text{N}^+=\text{C}(\text{NH}_2)-\text{CH}=\text{CH}_2$	35.53		
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76	75.15	83.69
			$\text{H}_2\text{B}^-=\text{CH}-\text{NH}^+=\text{CHNH}_2$	73.73		
	a	228.17	$\text{HN}(\text{NO}_2)^+=\text{CH}-\text{CH}=\text{BH}^-$	170.61		
			$\text{H}_2\text{C}=\text{N}(\text{NO}_2)^+-\text{CH}=\text{CH}_2$	25.28	14.53	14.53
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76		
	0.48	266.32	$\text{H}_2\text{N}^+=\text{C}(\text{NO}_2)-\text{CH}=\text{BH}^-$	162.30		
			$\text{HC}(\text{NO}_2)=\text{NH}^+-\text{CH}=\text{CH}_2$	23.19	59.38	35.29
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76		
	0.52	201.47	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{BH}^-$	140.64		
			$\text{H}_2\text{C}=\text{NH}^+-\text{C}(\text{NO}_2)=\text{CH}_2$	22.73	13.06	35.29
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CHNO}_2$	25.03		
	0.61	166.02	$\text{H}_2\text{N}^+=\text{CH}-\text{C}(\text{NO}_2)=\text{BH}^-$	101.33		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CH}_2$	23.19	27.24	36.24
			$\text{HC}(\text{NO}_2)=\text{BH}^--\text{CH}=\text{CH}_2$	14.26		
	0.39	231.13	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{BH}^-$	140.64		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CHNO}_2$	21.47	50.32	36.24
			$\text{H}_2\text{C}=\text{BH}^--\text{C}(\text{NO}_2)=\text{CH}_2$	18.70		
	a	199.26	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{BNO}_2^-$	125.51		
			$\text{H}_2\text{C}=\text{NH}^+-\text{CH}=\text{CH}_2$	23.19	32.72	32.72
			$\text{H}_2\text{C}=\text{B}(\text{NO}_2)^--\text{CH}=\text{CH}_2$	17.84		
	0.48	219.96	$\text{HN}(\text{NH}_2)^+=\text{CH}-\text{CH}=\text{BH}^-$	140.00		
			$\text{H}_2\text{C}=\text{N}(\text{NH}_2)^+-\text{CH}=\text{CH}_2$	21.15	41.05	37.87
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76		
	0.52	207.10	$\text{HN}(\text{NH}_2)^+=\text{CH}-\text{CH}=\text{BH}^-$	134.52		
			$\text{H}_2\text{C}=\text{N}(\text{NH}_2)^+-\text{CH}=\text{CH}_2$	19.88	34.94	37.87
			$\text{H}_2\text{C}=\text{BH}^--\text{CH}=\text{CH}_2$	17.76		

	0.59	153.92	$H_2N^+=C(NH_2)-CH=BH^-$ 91.67 $HC(NH_2)=NH^+-CH=CH_2$ 18.01 26.49 37.62 $H_2C=BH^- -CH=CH_2$ 17.76
	0.41	231.86	$H_2N^+=CH-CH=BH^-$ 140.64 $H_2C=NH^+-C(NH_2)=CH_2$ 21.73 53.65 37.62 $H_2C=BH^- -CH=CHNH_2$ 15.84
	0.41	79.98	$H_2N^+=CH-C(NH_2)=BH^-$ 155.38 $H_2C=NH^+-CH=CH_2$ 23.19 -122.04 -56.20 $HC(NH_2)=BH^- -CH=CH_2$ 23.44
	0.51	178.36	$H_2N^+=CH-CH=BH^-$ 140.64 $H_2C=NH^+-CH=CHNH_2$ 34.10 -10.44 -56.20 $H_2C=BH^- -C(NH_2)=CH_2$ 14.07
	^a	212.71	$H_2N^+=CH-CH=BNH_2^-$ 161.79 $H_2C=NH^+-CH=CH_2$ 23.19 12.65 12.65 $H_2C=B(NH_2)^- -CH=CH_2$ 15.08

^a Equal for the two structures. ^b From ref. 8b. ^c Not clear σ/π separation.

Table S4. Correlation between indices used to quantify aromaticity degree of studied compounds.

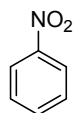
R²	NICS(1)_{zz}	NICS(0)_{πzz}	HOMA	PDI	FLU	ECRE
NICS(1)_{zz}	1	0.899	0.633	0.618	0.561	0.307
NICS(0)_{πzz}	0.899	1	0.675	0.640	0.640	0.250
HOMA	0.633	0.675	1	0.841	0.920	0.412
PDI	0.618	0.640	0.841	1	0.856	0.487
FLU	0.561	0.640	0.920	0.856	1	0.400
ECRE	0.307	0.250	0.412	0.487	0.400	1

Absolute energies and x, y, z coordinates of optimized structures



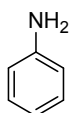
E = -232.3112416 a.u.

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 = -436.8746215 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.218696	-0.429851
2	6	0	0.000000	1.210168	-1.821233
3	6	0	0.000000	0.000000	-2.515597
4	6	0	0.000000	-1.210168	-1.821233
5	6	0	0.000000	-1.218696	-0.429851
6	6	0	0.000000	0.000000	0.241459
7	1	0	0.000000	2.140379	0.135430
8	1	0	0.000000	2.148827	-2.362332
9	1	0	0.000000	0.000000	-3.599542
10	1	0	0.000000	-2.148827	-2.362332
11	1	0	0.000000	-2.140379	0.135430
12	7	0	0.000000	0.000000	1.722390
13	8	0	0.000000	1.084529	2.290903
14	8	0	0.000000	-1.084529	2.290903



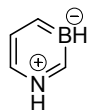
E = -287.6876274 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.003414	-1.170699	1.200908
2	6	0	0.003414	0.220540	1.206239
3	6	0	0.002135	0.937062	0.000000
4	6	0	0.003414	0.220540	-1.206239
5	6	0	0.003414	-1.170699	-1.200908
6	6	0	0.003282	-1.879778	0.000000
7	1	0	0.002797	-1.703708	2.145505
8	1	0	0.008960	0.759784	2.148433
9	1	0	0.008960	0.759784	-2.148433
10	1	0	0.002797	-1.703708	-2.145505
11	1	0	0.002648	-2.963051	0.000000
12	7	0	0.059461	2.334124	0.000000
13	1	0	-0.278412	2.785120	-0.837375
14	1	0	-0.278412	2.785120	0.837375



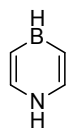
E = -235.7458969 a.u.

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



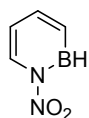
E = -235.6987876 a.u.

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



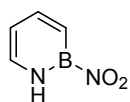
E = -235.7110251 a.u.

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



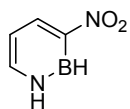
E = -440.2724044 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.737017	-1.994628	0.000000
2	6	0	-1.023017	-0.665990	0.000000
3	6	0	1.665648	-1.584533	0.000000
4	6	0	0.612653	-2.459306	0.000000
5	1	0	-1.560960	-2.696441	0.000000
6	1	0	-2.027285	-0.271844	0.000000
7	1	0	2.674106	-1.985581	0.000000
8	1	0	0.776404	-3.533622	0.000000
9	5	0	1.411445	-0.092794	0.000000
10	1	0	2.222349	0.762297	0.000000
11	7	0	0.000000	0.259142	0.000000
12	7	0	-0.424012	1.668502	0.000000
13	8	0	0.458820	2.489346	0.000000
14	8	0	-1.619240	1.875952	0.000000



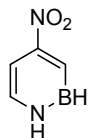
E = -440.3443398 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.922751	-2.365239	0.000000
2	6	0	-0.424297	-2.111397	0.000000
3	6	0	1.467173	0.023088	0.000000
4	6	0	1.860550	-1.299891	0.000000
5	1	0	1.262240	-3.392734	0.000000
6	1	0	-1.163526	-2.902571	0.000000
7	1	0	2.216120	0.805691	0.000000
8	1	0	2.916058	-1.558388	0.000000
9	5	0	0.000000	0.280148	0.000000
10	7	0	-0.882853	-0.829564	0.000000
11	1	0	-1.884405	-0.668874	0.000000
12	7	0	-0.688725	1.667966	0.000000
13	8	0	-1.926360	1.696010	0.000000
14	8	0	0.013547	2.674984	0.000000



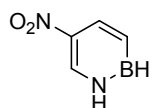
E = -440.3132573 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.023093	-1.898314	0.000000
2	6	0	0.208496	-2.498746	0.000000
3	6	0	0.000000	0.298169	0.000000
4	6	0	-1.127872	-0.488892	0.000000
5	7	0	1.349721	-1.757779	0.000000
6	1	0	2.215374	-2.280145	0.000000
7	5	0	1.382522	-0.318642	0.000000
8	1	0	2.429349	0.228075	0.000000
9	1	0	0.317935	-3.576801	0.000000
10	1	0	-1.913397	-2.512241	0.000000
11	1	0	-2.105670	-0.020342	0.000000
12	7	0	-0.196587	1.758382	0.000000
13	8	0	-1.343347	2.200244	0.000000
14	8	0	0.809182	2.459398	0.000000



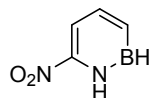
E = -440.3094839 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.040468	-0.711019	0.000000
2	6	0	-0.703475	-2.033290	0.000000
3	6	0	1.331441	-0.049705	0.000000
4	6	0	0.000000	0.252266	0.000000
5	1	0	2.040763	0.768099	0.000000
6	7	0	0.604974	-2.427325	0.000000
7	1	0	0.762299	-3.426005	0.000000
8	5	0	1.713491	-1.518468	0.000000
9	1	0	2.813910	-1.964006	0.000000
10	1	0	-1.457356	-2.810784	0.000000
11	1	0	-2.073695	-0.400757	0.000000
12	7	0	-0.425810	1.695668	0.000000
13	8	0	0.448592	2.547116	0.000000
14	8	0	-1.627656	1.927619	0.000000



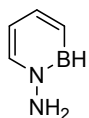
E = -440.3103426 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.235526	0.023359	-0.000001
2	6	0	-0.426742	-1.176546	-0.000001
3	6	0	-1.822365	1.299714	0.000001
4	6	0	-0.451630	1.268134	0.000000
5	1	0	-2.304962	2.271374	0.000002
6	1	0	0.153890	2.166980	-0.000001
7	7	0	-1.780318	-1.191412	0.000000
8	1	0	-2.206184	-2.108599	0.000000
9	5	0	-2.597578	0.000667	0.000001
10	1	0	-3.776797	-0.138594	0.000002
11	1	0	0.113306	-2.113275	-0.000002
12	7	0	1.700163	-0.003673	-0.000004
13	8	0	2.258995	-1.097963	0.000004
14	8	0	2.286129	1.072516	0.000001



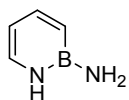
E = -440.3093742 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.286301	-0.229204	0.000000
2	6	0	0.000000	0.224242	0.000000
3	6	0	0.478100	-2.532776	0.000000
4	6	0	1.516164	-1.632549	0.000000
5	1	0	2.096554	0.484740	0.000000
6	1	0	0.722004	-3.590443	0.000000
7	1	0	2.549491	-1.967680	0.000000
8	7	0	-1.079557	-0.596581	0.000000
9	1	0	-1.971350	-0.112290	0.000000
10	5	0	-0.954409	-2.024282	0.000000
11	1	0	-1.947378	-2.674488	0.000000
12	7	0	-0.296173	1.668235	0.000000
13	8	0	0.642093	2.450124	0.000000
14	8	0	-1.483413	1.987590	0.000000



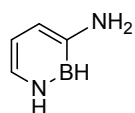
E = -291.0796767 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.167450	-1.171529	0.000000
2	6	0	-1.168097	0.197152	0.000000
3	6	0	1.270059	-1.238551	0.000000
4	6	0	0.056745	-1.889409	0.000000
5	1	0	-2.116028	-1.692932	0.000000
6	1	0	-2.070964	0.793709	0.000000
7	1	0	2.175867	-1.837439	0.000000
8	1	0	0.007307	-2.975725	0.000000
9	5	0	1.293460	0.268513	0.000000
10	1	0	2.252749	0.975821	0.000000
11	7	0	0.000000	0.903111	0.000000
12	7	0	-0.180888	2.327601	0.000000
13	1	0	0.301225	2.696518	0.814921
14	1	0	0.301225	2.696518	-0.814921



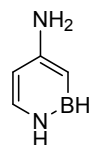
E = -291.1652017 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.053851	-1.872285	0.000000
2	6	0	-1.133242	-1.206265	0.000000
3	6	0	1.317283	0.226158	0.000000
4	6	0	1.285376	-1.139576	0.000000
5	1	0	0.055306	-2.954377	0.000000
6	1	0	-2.082767	-1.729310	0.000000
7	1	0	2.287961	0.715956	0.000000
8	1	0	2.209680	-1.713028	0.000000
9	5	0	0.000000	1.003458	0.000000
10	7	0	-1.185680	0.163551	0.000000
11	1	0	-2.113494	0.563024	0.000000
12	7	0	-0.125194	2.422623	0.000000
13	1	0	-0.999163	2.922209	0.000000
14	1	0	0.678998	3.026820	0.000000



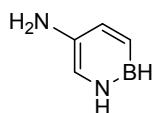
E = -291.1229953 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.099073	1.236690	0.002750
2	6	0	1.857938	0.103177	0.003007
3	6	0	-1.003569	-0.026050	-0.006041
4	6	0	-0.320140	1.176220	0.000408
5	7	0	1.238387	-1.125483	0.002761
6	1	0	1.851811	-1.927908	0.007153
7	5	0	-0.172645	-1.306781	-0.002649
8	1	0	-0.613093	-2.415241	0.002928
9	1	0	2.939910	0.117848	0.005292
10	1	0	1.593520	2.199952	0.005391
11	1	0	-0.869928	2.116161	-0.002012
12	7	0	-2.396233	-0.065008	-0.068072
13	1	0	-2.833612	-0.923721	0.227292
14	1	0	-2.900272	0.760037	0.223627



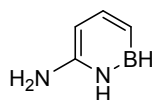
E = -291.1287205 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.208428	-1.177867	-0.005977
2	6	0	-1.154125	-1.163092	0.001689
3	6	0	0.295440	1.264454	-0.003139
4	6	0	0.956779	0.045724	-0.006379
5	1	0	0.899964	2.168357	-0.004918
6	7	0	-1.853989	0.007046	0.006563
7	1	0	-2.859895	-0.073918	0.012858
8	5	0	-1.201563	1.296293	0.003320
9	1	0	-1.893227	2.266837	0.010228
10	1	0	-1.724891	-2.084788	0.003130
11	1	0	0.724545	-2.130596	-0.020099
12	7	0	2.339434	-0.051347	-0.059635
13	1	0	2.862079	0.777147	0.178489
14	1	0	2.761991	-0.909715	0.258049



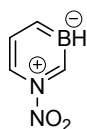
E = -291.1154137 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.917469	-0.014493	-0.004861
2	6	0	0.197244	-1.180484	0.007399
3	6	0	-1.150514	1.307950	0.005431
4	6	0	0.219177	1.231867	-0.010595
5	1	0	-1.600406	2.296248	0.004679
6	1	0	0.827531	2.135029	-0.034273
7	7	0	-1.177231	-1.161482	0.002180
8	1	0	-1.619549	-2.069410	0.001792
9	5	0	-1.964438	0.030241	0.006150
10	1	0	-3.150724	-0.072438	0.008163
11	1	0	0.680056	-2.151244	0.010740
12	7	0	2.329140	-0.010407	-0.087282
13	1	0	2.761428	0.738184	0.438042
14	1	0	2.760228	-0.893392	0.151580



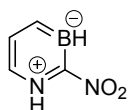
E = -291.1249492 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.155370	-1.213753	0.004188
2	6	0	-0.906871	-0.058614	-0.005347
3	6	0	1.950855	0.045504	0.009080
4	6	0	1.259518	-1.147442	0.001933
5	1	0	-0.661288	-2.171486	0.018185
6	1	0	3.035398	0.013124	0.011428
7	1	0	1.794380	-2.095041	0.003804
8	7	0	-0.277580	1.153338	-0.008558
9	1	0	-0.883168	1.960904	-0.073381
10	5	0	1.157477	1.323039	0.004476
11	1	0	1.568425	2.441357	0.001228
12	7	0	-2.299908	-0.045962	-0.074861
13	1	0	-2.730328	-0.946751	0.075917
14	1	0	-2.757178	0.676896	0.465252



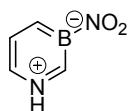
E = -440.2211443 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.726884	-2.054412	0.000000
2	6	0	-1.023351	-0.701019	0.000000
3	6	0	1.318745	-0.104201	0.000000
4	6	0	0.588325	-2.520723	0.000000
5	1	0	-1.574572	-2.732630	0.000000
6	1	0	-2.019741	-0.291891	0.000000
7	1	0	1.959272	0.767340	0.000000
8	1	0	0.718249	-3.599976	0.000000
9	5	0	1.738570	-1.549283	0.000000
10	1	0	2.892180	-1.843015	0.000000
11	7	0	0.000000	0.189995	0.000000
12	7	0	-0.409809	1.671908	0.000000
13	8	0	0.500776	2.451450	0.000000
14	8	0	-1.593349	1.885475	0.000000



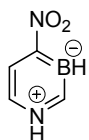
E = -440.2699393 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.091063	-1.050795	0.000000
2	6	0	0.000000	0.319143	0.000000
3	6	0	-0.114140	-2.057932	0.000000
4	6	0	1.281499	-2.172731	0.000000
5	1	0	3.164255	-1.223797	0.000000
6	1	0	-0.781599	-2.908256	0.000000
7	1	0	1.693260	-3.176689	0.000000
8	7	0	-0.688179	-0.852304	0.000000
9	1	0	-1.705089	-0.752522	0.000000
10	5	0	1.499864	0.351555	0.000000
11	1	0	2.128143	1.354054	0.000000
12	7	0	-0.906801	1.460658	0.000000
13	8	0	-0.420764	2.579244	0.000000
14	8	0	-2.127231	1.228862	0.000000



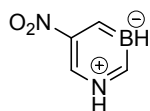
E = -440.3000316 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.489769	-1.676722	0.000000
2	6	0	0.374339	-2.501668	0.000000
3	6	0	-1.146704	-0.642920	0.000000
4	6	0	1.366710	-0.286811	0.000000
5	1	0	2.461951	-2.158361	0.000000
6	1	0	0.431197	-3.580921	0.000000
7	1	0	-2.200506	-0.394650	0.000000
8	1	0	2.273437	0.309478	0.000000
9	5	0	0.000000	0.303322	0.000000
10	7	0	-0.870711	-1.969054	0.000000
11	1	0	-1.646131	-2.621091	0.000000
12	7	0	-0.264435	1.830238	0.000000
13	8	0	-1.436191	2.222432	0.000000
14	8	0	0.701365	2.596239	0.000000



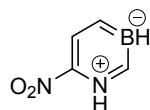
E = -440.2660072 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.295831	0.082098	0.003891
2	6	0	1.945774	1.177121	0.057883
3	6	0	1.732445	-1.210659	-0.061411
4	6	0	0.352810	-1.149572	-0.051523
5	1	0	2.288074	-2.135401	-0.110889
6	1	0	-0.217123	-2.069169	-0.087497
7	7	0	2.461380	-0.066393	-0.006395
8	1	0	3.469538	-0.171934	-0.015403
9	5	0	0.449217	1.387211	0.067183
10	1	0	-0.034684	2.464787	0.129060
11	1	0	2.700773	1.955061	0.095082
12	7	0	-1.778499	0.019525	0.001258
13	8	0	-2.319213	-1.075369	0.151639
14	8	0	-2.386290	1.069714	-0.152058



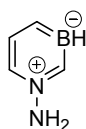
E = -440.2614675 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.393469	1.311543	0.000004
2	6	0	2.549900	0.002658	-0.000004
3	6	0	0.433059	-1.134729	0.000004
4	6	0	-0.239842	0.080872	0.000007
5	1	0	-0.068256	-2.088803	0.000006
6	7	0	1.779588	-1.116553	-0.000001
7	1	0	2.238526	-2.020102	-0.000003
8	5	0	1.903594	1.357646	-0.000002
9	1	0	2.542050	2.361015	-0.000004
10	1	0	3.612210	-0.216084	-0.000009
11	1	0	-0.250326	2.184236	0.000007
12	7	0	-1.731347	-0.007132	0.000013
13	8	0	-2.234136	-1.125929	-0.000008
14	8	0	-2.359536	1.037834	-0.000009



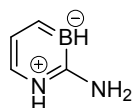
E = -440.2653176 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.890625	1.250680	-0.000009
2	6	0	1.726989	-1.280337	-0.000002
3	6	0	-0.216128	0.088919	0.000021
4	6	0	0.503236	1.280580	0.000011
5	7	0	0.395760	-1.117595	0.000017
6	1	0	-0.247548	-1.909401	0.000027
7	5	0	2.634529	-0.062515	-0.000016
8	1	0	3.817983	-0.176623	-0.000031
9	1	0	2.029093	-2.322206	-0.000005
10	1	0	2.391374	2.214895	-0.000017
11	1	0	-0.070245	2.199268	0.000017
12	7	0	-1.659653	0.028208	0.000030
13	8	0	-2.280779	1.082524	-0.000016
14	8	0	-2.178519	-1.095861	-0.000029



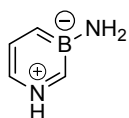
E = -291.0352447 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.169316	-1.215020	0.000000
2	6	0	-1.167986	0.175556	0.000000
3	6	0	1.223400	0.263233	0.000000
4	6	0	0.013688	-1.947231	0.000000
5	1	0	-2.141724	-1.698837	0.000000
6	1	0	-2.055501	0.788876	0.000000
7	1	0	2.038872	0.979969	0.000000
8	1	0	-0.083756	-3.030511	0.000000
9	5	0	1.342124	-1.232950	0.000000
10	1	0	2.408607	-1.767421	0.000000
11	7	0	0.000000	0.856889	0.000000
12	7	0	-0.138387	2.281084	0.000000
13	1	0	0.346440	2.633815	0.821359
14	1	0	0.346440	2.633815	-0.821359



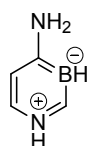
E = -291.0797748 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.327194	1.196464	0.006629
2	6	0	0.952596	0.114885	-0.009041
3	6	0	-1.068612	-1.214464	-0.000346
4	6	0	-1.873870	-0.102992	0.012011
5	1	0	-2.038019	2.019155	0.025439
6	1	0	-1.430448	-2.232281	0.000601
7	1	0	-2.946961	-0.267291	0.026770
8	7	0	0.298114	-1.070561	-0.013695
9	1	0	0.843419	-1.923617	-0.055892
10	5	0	0.144180	1.403951	-0.009492
11	1	0	0.712062	2.456937	-0.003722
12	7	0	2.336639	0.039034	-0.058459
13	1	0	2.799129	0.920361	0.104431
14	1	0	2.799122	-0.735690	0.399396



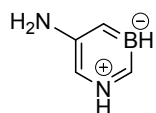
E = -291.1137403 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.259305	-1.138181	0.000000
2	6	0	0.057128	-1.850319	0.000000
3	6	0	-1.243956	0.176228	0.000000
4	6	0	1.292695	0.245038	0.000000
5	1	0	2.174440	-1.723459	0.000000
6	1	0	-0.010193	-2.928070	0.000000
7	1	0	-2.279570	0.503381	0.000000
8	1	0	2.279263	0.706685	0.000000
9	5	0	0.000000	1.054436	0.000000
10	7	0	-1.111363	-1.168854	0.000000
11	1	0	-1.955938	-1.727252	0.000000
12	7	0	-0.064484	2.486318	0.000000
13	1	0	-0.924128	3.009065	0.000000
14	1	0	0.756022	3.068626	0.000000



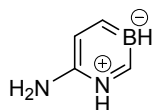
E = -291.0843334 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.010987	0.055609	-0.004057
2	6	0	1.247455	1.194995	0.002182
3	6	0	1.078483	-1.197994	0.000815
4	6	0	-0.302734	-1.161940	-0.001311
5	1	0	1.633559	-2.126260	0.002398
6	1	0	-0.827907	-2.114009	-0.004199
7	7	0	1.804942	-0.062458	0.002243
8	1	0	2.811052	-0.154234	0.005070
9	5	0	-0.221223	1.363558	-0.002262
10	1	0	-0.756209	2.433551	0.000962
11	1	0	1.990039	1.985590	0.007209
12	7	0	-2.381902	0.027193	-0.033567
13	1	0	-2.886245	0.886593	0.104140
14	1	0	-2.892754	-0.826187	0.129224



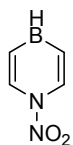
E = -291.0742045 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.287707	1.273015	-0.005026
2	6	0	1.907951	0.031138	0.009516
3	6	0	-0.191903	-1.145197	-0.007730
4	6	0	-0.941964	0.035934	-0.008220
5	1	0	-0.636047	-2.130781	-0.029229
6	7	0	1.161715	-1.094410	0.001995
7	1	0	1.636889	-1.988603	0.002152
8	5	0	1.208883	1.366575	0.004724
9	1	0	1.817714	2.392893	0.013002
10	1	0	2.975425	-0.162137	0.018321
11	1	0	-0.931587	2.152289	-0.009523
12	7	0	-2.340471	-0.067265	-0.073698
13	1	0	-2.743038	-0.899399	0.333257
14	1	0	-2.830735	0.765251	0.219082



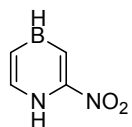
E = -291.0730029 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.240631	1.252789	0.001176
2	6	0	1.139818	-1.258679	0.002191
3	6	0	-0.880151	0.061778	-0.006076
4	6	0	-0.152868	1.249560	0.001305
5	7	0	-0.210252	-1.114931	-0.017556
6	1	0	-0.812618	-1.930846	-0.054539
7	5	0	2.016490	-0.041514	0.011394
8	1	0	3.206637	-0.120983	0.020414
9	1	0	1.452604	-2.297841	-0.003900
10	1	0	1.717365	2.230855	0.002212
11	1	0	-0.725009	2.173694	0.012914
12	7	0	-2.297919	-0.074211	-0.015815
13	1	0	-2.712853	0.097852	0.894629
14	1	0	-2.735958	0.546153	-0.686676



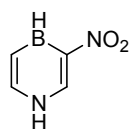
E = -440.2371908 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.805181	1.282369	0.000000
2	6	0	-0.449400	1.223069	0.000000
3	6	0	-0.449400	-1.223079	0.000000
4	6	0	-1.805182	-1.282378	0.000000
5	1	0	-2.226958	2.282489	0.000000
6	1	0	0.216139	2.073548	0.000000
7	1	0	0.216138	-2.073558	0.000000
8	1	0	-2.226959	-2.282498	0.000000
9	5	0	-2.634267	-0.000004	0.000000
10	1	0	-3.824780	-0.000004	0.000000
11	7	0	0.203289	-0.000004	0.000000
12	7	0	1.654861	0.000004	0.000000
13	8	0	2.191592	1.086154	0.000000
14	8	0	2.191619	-1.086134	0.000000



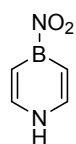
E = -440.2738155 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.215507	0.138152	-0.000001
2	6	0	-1.773797	-1.170439	-0.000003
3	6	0	-2.576362	-0.062663	0.000003
4	1	0	-2.138606	-2.191624	-0.000007
5	1	0	-3.645225	-0.249422	0.000005
6	7	0	-0.412467	-1.069094	-0.000006
7	1	0	0.181740	-1.889657	-0.000012
8	6	0	-0.423843	1.335548	0.000001
9	1	0	0.201008	2.219966	0.000003
10	5	0	-1.954246	1.321639	0.000006
11	1	0	-2.592553	2.326395	0.000012
12	7	0	1.697965	0.008305	-0.000016
13	8	0	2.155994	-1.134177	0.000018
14	8	0	2.358675	1.028937	-0.000002



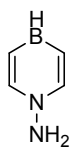
E = -440.2771988 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.347918	-1.104677	0.000003
2	6	0	-2.513331	-0.053910	-0.000002
3	6	0	-1.993714	1.202564	-0.000002
4	1	0	-3.573447	-0.281636	-0.000003
5	1	0	-2.709219	2.018288	-0.000004
6	7	0	-1.700868	-1.166133	0.000001
7	1	0	-2.133621	-2.077710	0.000001
8	6	0	0.294000	0.105341	0.000003
9	5	0	-0.481916	1.413046	0.000000
10	1	0	0.030497	2.480367	0.000000
11	1	0	0.183842	-2.047177	0.000004
12	7	0	1.768717	0.025499	0.000006
13	8	0	2.388720	1.078169	-0.000001
14	8	0	2.299076	-1.086774	-0.000006



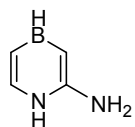
E = -440.3116447 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	-1.290550	0.464486
2	6	0	0.004346	-1.206268	1.826663
3	6	0	-0.004346	1.206268	1.826663
4	6	0	0.000000	1.290550	0.464486
5	1	0	-0.007022	-2.280815	0.024118
6	1	0	0.004537	-2.067476	2.485301
7	1	0	-0.004537	2.067476	2.485301
8	1	0	0.007022	2.280815	0.024118
9	5	0	0.000000	0.000000	-0.307020
10	7	0	0.000000	0.000000	2.473513
11	1	0	0.000000	0.000000	3.482193
12	7	0	0.000000	0.000000	-1.848973
13	8	0	-0.970883	-0.488414	-2.426969
14	8	0	0.970883	0.488414	-2.426969



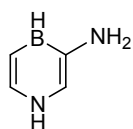
E = -291.0452819 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.299409	-1.169482	0.000000
2	6	0	-1.209359	0.193561	0.000000
3	6	0	1.195263	0.161320	0.000000
4	6	0	1.254107	-1.201731	0.000000
5	1	0	-2.307239	-1.573803	0.000000
6	1	0	-2.049579	0.877080	0.000000
7	1	0	2.065428	0.810628	0.000000
8	1	0	2.251449	-1.631725	0.000000
9	5	0	-0.035519	-2.011413	0.000000
10	1	0	-0.047588	-3.205222	0.000000
11	7	0	0.000000	0.840676	0.000000
12	7	0	-0.037092	2.255214	0.000000
13	1	0	0.440576	2.603436	0.826426
14	1	0	0.440576	2.603436	-0.826426



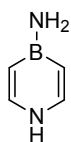
E = -291.0901848 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.906324	0.092479	-0.007167
2	6	0	-1.174774	-1.153097	0.001701
3	6	0	-1.945295	-0.034913	0.015754
4	1	0	-1.559694	-2.167741	-0.000832
5	1	0	-3.019650	-0.189192	0.033477
6	7	0	0.202043	-1.085855	-0.012775
7	1	0	0.720577	-1.942360	-0.136451
8	6	0	0.248785	1.297768	-0.003745
9	1	0	0.876764	2.184881	0.021888
10	5	0	-1.261996	1.332446	0.001823
11	1	0	-1.876043	2.357518	0.012725
12	7	0	2.295681	-0.078303	-0.067005
13	1	0	2.799644	0.794149	0.004080
14	1	0	2.674070	-0.763803	0.575200



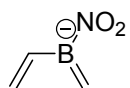
E = -291.0850244 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.297077	-1.123552	-0.002535
2	6	0	-1.854895	-0.029669	0.005030
3	6	0	-1.292523	1.222524	0.004165
4	1	0	-2.922316	-0.222940	0.010144
5	1	0	-1.983236	2.059849	0.010837
6	7	0	-1.079363	-1.145046	0.002115
7	1	0	-1.532343	-2.045071	0.002983
8	6	0	1.001227	0.055870	-0.008137
9	5	0	0.206321	1.366911	-0.003801
10	1	0	0.771214	2.422526	0.003013
11	1	0	0.762635	-2.104115	-0.010380
12	7	0	2.400578	0.031669	-0.072341
13	1	0	2.847763	0.887053	0.219960
14	1	0	2.870852	-0.789254	0.282885



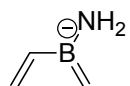
E = -291.1363811 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	-1.291064	0.218354
2	6	0	0.000000	-1.208291	-1.135396
3	6	0	0.000000	1.208291	-1.135396
4	6	0	0.000000	1.291064	0.218354
5	1	0	0.000000	-2.294670	0.636307
6	1	0	0.000000	-2.071669	-1.793062
7	1	0	0.000000	2.071669	-1.793062
8	1	0	0.000000	2.294670	0.636307
9	5	0	0.000000	0.000000	1.057435
10	7	0	0.000000	0.000000	-1.797500
11	1	0	0.000000	0.000000	-2.803868
12	7	0	0.000000	0.000000	2.479167
13	1	0	0.000000	0.841895	3.031521
14	1	0	0.000000	-0.841895	3.031521



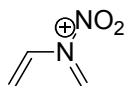
E = -347.4442489 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.366096	1.842565	-0.328588
2	6	0	-2.696838	-0.489640	0.154294
3	6	0	-1.363771	-0.655075	0.194032
4	1	0	0.495032	2.492965	-0.465681
5	1	0	-3.390693	-1.310100	0.328485
6	1	0	-1.020724	-1.673155	0.397080
7	5	0	-0.258733	0.438132	-0.030401
8	7	0	1.194631	-0.190549	0.001493
9	8	0	2.032791	0.184423	0.832943
10	8	0	1.451970	-1.106190	-0.797767
11	1	0	-3.145413	0.479432	-0.052175
12	1	0	-1.324814	2.341082	-0.465986



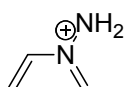
E = -198.2153646 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.331321	-2.100224	0.000000
2	1	0	1.417367	-2.034689	0.000000
3	1	0	-0.088670	-3.106309	0.000000
4	6	0	-0.431281	-0.992895	0.000000
5	1	0	-1.514012	-1.193286	0.000000
6	6	0	1.391296	1.015905	0.000000
7	1	0	2.248440	0.342176	0.000000
8	1	0	1.675984	2.071722	0.000000
9	5	0	0.000000	0.543352	0.000000
10	7	0	-1.179939	1.443655	0.000000
11	1	0	-1.096625	2.446710	0.000000
12	1	0	-2.130930	1.114615	0.000000



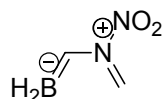
E = -376.931532 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.795256	1.482615	0.000000
2	1	0	-0.415380	2.501399	0.000000
3	1	0	-1.866731	1.297745	0.000000
4	6	0	1.414334	0.398754	0.000000
5	1	0	1.766089	-0.623744	0.000000
6	6	0	2.231876	1.450001	0.000000
7	1	0	1.901718	2.482077	0.000000
8	1	0	3.300716	1.277012	0.000000
9	7	0	0.000000	0.492478	0.000000
10	7	0	-0.809172	-1.059047	0.000000
11	8	0	-0.039915	-1.943862	0.000000
12	8	0	-1.976076	-0.925729	0.000000



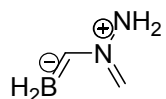
E = -227.7615493 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.223114	0.831209	0.000000
2	1	0	2.025380	0.102958	0.000000
3	1	0	1.442917	1.891788	0.000000
4	6	0	-0.464256	-0.930368	0.000000
5	1	0	-1.543437	-0.959740	0.000000
6	6	0	0.320528	-2.001858	0.000000
7	1	0	1.403819	-1.982851	0.000000
8	1	0	-0.145288	-2.979261	0.000000
9	7	0	0.000000	0.438584	0.000000
10	7	0	-1.084975	1.367868	0.000000
11	1	0	-1.032441	1.944022	0.836577
12	1	0	-1.032441	1.944022	-0.836577



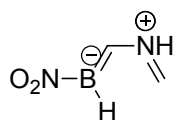
E = -363.9286158 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.938904	1.386148	0.000000
2	1	0	-0.630510	2.420968	0.000000
3	1	0	-1.970794	1.080891	0.000000
4	6	0	1.361058	0.514394	0.000000
5	1	0	1.800172	-0.472758	0.000000
6	5	0	2.161645	1.771212	0.000000
7	1	0	1.648316	2.851186	0.000000
8	1	0	3.349289	1.682428	0.000000
9	7	0	0.000000	0.482577	0.000000
10	7	0	-0.629653	-1.036409	0.000000
11	8	0	0.182878	-1.905774	0.000000
12	8	0	-1.824134	-1.087377	0.000000



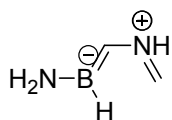
E = -214.7471197 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.216210	0.867550	0.000000
2	1	0	-2.039888	0.171070	0.000000
3	1	0	-1.337524	1.936912	0.000000
4	6	0	0.435865	-0.932356	0.000000
5	1	0	1.518692	-0.978426	0.000000
6	5	0	-0.427565	-2.132870	0.000000
7	1	0	-1.623637	-2.069149	0.000000
8	1	0	0.090540	-3.208129	0.000000
9	7	0	0.000000	0.390802	0.000000
10	7	0	1.005337	1.425032	0.000000
11	1	0	1.587178	1.245034	0.816338
12	1	0	1.587178	1.245034	-0.816338



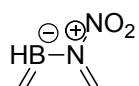
E = -364.0076818 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.011741	-0.284456	0.000000
2	1	0	2.870545	0.785622	0.000000
3	1	0	3.995885	-0.726639	0.000000
4	6	0	0.608993	-0.819615	0.000000
5	1	0	0.020865	-1.727544	0.000000
6	5	0	0.000000	0.511003	0.000000
7	1	0	0.538427	1.565368	0.000000
8	7	0	1.970916	-1.073462	0.000000
9	1	0	2.200461	-2.064016	0.000000
10	7	0	-1.553558	0.574002	0.000000
11	8	0	-2.076976	1.691246	0.000000
12	8	0	-2.207036	-0.474641	0.000000



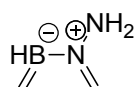
E = -214.8393273 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.129835	-0.585061	0.000000
2	1	0	-1.689042	-1.567908	0.000000
3	1	0	-3.196810	-0.435555	0.000000
4	6	0	0.000000	0.670009	0.000000
5	1	0	0.261418	1.723402	0.000000
6	5	0	1.032042	-0.438595	0.000000
7	1	0	0.720479	-1.594687	0.000000
8	7	0	-1.349984	0.486279	0.000000
9	1	0	-1.874825	1.355364	0.000000
10	7	0	2.418174	-0.157065	0.000000
11	1	0	2.800175	0.776292	0.000000
12	1	0	3.120081	-0.878118	0.000000



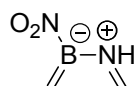
E = -363.9462222 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.859598	1.376315	0.000000
2	1	0	-0.472262	2.386535	0.000000
3	1	0	-1.919930	1.170186	0.000000
4	6	0	2.215631	1.674148	0.000000
5	1	0	1.765953	2.664993	0.000000
6	1	0	3.300858	1.702113	0.000000
7	5	0	1.523232	0.406557	0.000000
8	1	0	2.005142	-0.671605	0.000000
9	7	0	0.000000	0.413940	0.000000
10	7	0	-0.724720	-1.012410	0.000000
11	8	0	0.006864	-1.950192	0.000000
12	8	0	-1.926750	-0.974619	0.000000



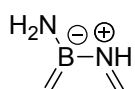
E = -214.7687076 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.217608	0.874020	0.000000
2	1	0	-2.013440	0.141611	0.000000
3	1	0	-1.410515	1.937826	0.000000
4	6	0	-0.355968	-2.119496	0.000000
5	1	0	-1.444234	-2.085344	0.000000
6	1	0	0.032933	-3.133474	0.000000
7	5	0	0.530583	-0.989194	0.000000
8	1	0	1.725789	-0.999260	0.000000
9	7	0	0.000000	0.453376	0.000000
10	7	0	0.967123	1.527282	0.000000
11	1	0	1.564072	1.346431	0.806519
12	1	0	1.564072	1.346431	-0.806519



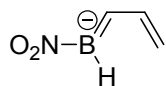
E = -364.0407052 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.547448	0.490185	0.000000
2	1	0	2.646647	1.569156	0.000000
3	1	0	3.432476	-0.134382	0.000000
4	6	0	-0.368469	1.920227	0.000000
5	1	0	0.339849	2.743866	0.000000
6	1	0	-1.408747	2.224193	0.000000
7	5	0	0.000000	0.541490	0.000000
8	7	0	1.378323	-0.043206	0.000000
9	1	0	1.316078	-1.070687	0.000000
10	7	0	-1.008559	-0.636725	0.000000
11	8	0	-0.536219	-1.797144	0.000000
12	8	0	-2.212346	-0.420675	0.000000



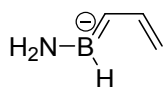
E = -214.8342276 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.312732	-1.997848	0.000000
2	1	0	1.392512	-1.939564	0.000000
3	1	0	-0.182782	-2.959772	0.000000
4	6	0	1.409506	0.941654	0.000000
5	1	0	2.229273	0.229213	0.000000
6	1	0	1.745378	1.974538	0.000000
7	5	0	0.000000	0.572923	0.000000
8	7	0	-0.381681	-0.900941	0.000000
9	1	0	-1.386717	-1.065350	0.000000
10	7	0	-1.176642	1.427248	0.000000
11	1	0	-1.088255	2.428462	0.000000
12	1	0	-2.134572	1.120867	0.000000



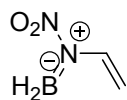
E = -347.4463 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.149868	-0.185331	0.000000
2	1	0	2.994931	0.888718	0.000000
3	1	0	4.176622	-0.537674	0.000000
4	6	0	2.113506	-1.058085	0.000000
5	1	0	2.397275	-2.114897	0.000000
6	6	0	0.686879	-0.805162	0.000000
7	1	0	0.075726	-1.706651	0.000000
8	5	0	0.000000	0.473916	0.000000
9	1	0	0.455684	1.576042	0.000000
10	7	0	-1.560202	0.493140	0.000000
11	8	0	-2.132540	1.603000	0.000000
12	8	0	-2.227503	-0.557454	0.000000



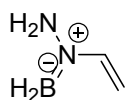
E = -198.2251168 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.271155	-0.538414	0.000000
2	1	0	-1.904710	-1.560771	0.000000
3	1	0	-3.348429	-0.399335	0.000000
4	6	0	-1.426091	0.544032	0.000000
5	1	0	-1.952483	1.507574	0.000000
6	6	0	0.000000	0.654852	0.000000
7	1	0	0.353397	1.693615	0.000000
8	5	0	1.019726	-0.429358	0.000000
9	1	0	0.744689	-1.609974	0.000000
10	7	0	2.456915	-0.182679	0.000000
11	1	0	3.145350	-0.915011	0.000000
12	1	0	2.848627	0.746625	0.000000



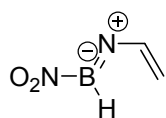
E = -364.0089554 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.392606	0.111923	0.000000
2	1	0	1.591146	-0.948554	0.000000
3	6	0	2.381989	1.000676	0.000000
4	1	0	2.234260	2.071299	0.000000
5	1	0	3.399858	0.634427	0.000000
6	7	0	0.000000	0.421643	0.000000
7	5	0	-0.589060	1.715356	0.000000
8	1	0	0.158521	2.631995	0.000000
9	1	0	-1.758549	1.841044	0.000000
10	7	0	-0.876450	-0.758249	0.000000
11	8	0	-0.333032	-1.843769	0.000000
12	8	0	-2.066012	-0.547024	0.000000



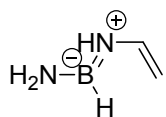
E = -214.8124763 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.393365	-0.915908	0.000000
2	1	0	-1.471840	-1.016494	0.000000
3	6	0	0.400587	-1.986093	0.000000
4	1	0	1.480714	-1.926870	0.000000
5	1	0	-0.049434	-2.969773	0.000000
6	7	0	0.000000	0.448482	0.000000
7	5	0	1.306520	0.953786	0.000000
8	1	0	2.228687	0.206146	0.000000
9	1	0	1.452389	2.135656	0.000000
10	7	0	-1.148027	1.319712	0.000000
11	1	0	-1.090129	1.918524	0.817900
12	1	0	-1.090129	1.918524	-0.817900



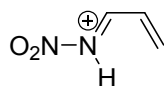
E = -364.0762307 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.053092	-0.935961	0.000000
2	1	0	2.272046	-1.997602	0.000000
3	6	0	3.039986	-0.042143	0.000000
4	1	0	2.866786	1.026568	0.000000
5	1	0	4.066216	-0.383088	0.000000
6	7	0	0.668411	-0.654203	0.000000
7	5	0	0.000000	0.552108	0.000000
8	1	0	0.455354	1.636374	0.000000
9	1	0	0.065345	-1.472701	0.000000
10	7	0	-1.553064	0.419158	0.000000
11	8	0	-2.211297	1.455428	0.000000
12	8	0	-2.050159	-0.712447	0.000000



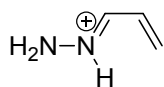
E = -214.9115907 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.397266	0.516667	0.000000
2	1	0	-1.892579	1.483662	0.000000
3	6	0	-2.145585	-0.590993	0.000000
4	1	0	-1.724987	-1.587771	0.000000
5	1	0	-3.223268	-0.500182	0.000000
6	7	0	0.000000	0.616781	0.000000
7	5	0	0.972931	-0.431147	0.000000
8	1	0	0.626258	-1.568099	0.000000
9	1	0	0.325585	1.572653	0.000000
10	7	0	2.354859	-0.145870	0.000000
11	1	0	2.751068	0.781464	0.000000
12	1	0	3.046358	-0.876415	0.000000



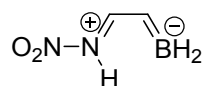
E = -376.9522313 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.626858	-0.775338	0.000000
2	1	0	-0.036990	-1.641086	0.000000
3	6	0	2.046856	-0.994258	0.000000
4	1	0	2.341920	-2.036799	0.000000
5	6	0	2.981846	-0.023850	0.000000
6	1	0	2.751912	1.037173	0.000000
7	1	0	4.035329	-0.279709	0.000000
8	7	0	0.000000	0.357062	0.000000
9	1	0	0.399544	1.294690	0.000000
10	7	0	-1.571215	0.411020	0.000000
11	8	0	-1.961769	1.531028	0.000000
12	8	0	-2.091552	-0.654798	0.000000



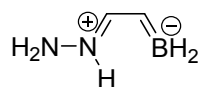
E = -227.788073 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.657547	0.000000
2	1	0	-0.445770	1.648601	0.000000
3	6	0	1.435715	0.528175	0.000000
4	1	0	1.968158	1.471881	0.000000
5	6	0	2.122923	-0.627078	0.000000
6	1	0	1.660277	-1.609349	0.000000
7	1	0	3.206587	-0.619222	0.000000
8	7	0	-0.870857	-0.305633	0.000000
9	1	0	-0.571102	-1.280834	0.000000
10	7	0	-2.245475	-0.003171	0.000000
11	1	0	-2.677826	-0.400654	-0.831413
12	1	0	-2.677826	-0.400654	0.831413



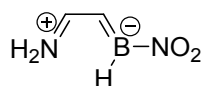
E = -363.9891355 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.997076	-1.056395	0.000000
2	1	0	2.328853	-2.090346	0.000000
3	6	0	0.645041	-0.912257	0.000000
4	1	0	-0.046478	-1.746924	0.000000
5	7	0	0.000000	0.299315	0.000000
6	1	0	0.477708	1.191757	0.000000
7	5	0	3.002684	0.086101	0.000000
8	1	0	2.637502	1.227577	0.000000
9	1	0	4.173724	-0.123017	0.000000
10	7	0	-1.385694	0.425778	0.000000
11	8	0	-1.793299	1.576557	0.000000
12	8	0	-2.048899	-0.595719	0.000000



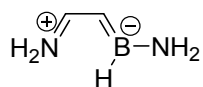
E = -214.7853237 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.374075	0.715812	0.000000
2	1	0	1.780931	1.723210	0.000000
3	6	0	0.000000	0.672812	0.000000
4	1	0	-0.584499	1.592533	0.000000
5	7	0	-0.779839	-0.430614	0.000000
6	1	0	-0.356638	-1.346391	0.000000
7	5	0	2.282683	-0.484426	0.000000
8	1	0	1.840682	-1.601719	0.000000
9	1	0	3.470200	-0.364014	0.000000
10	7	0	-2.181192	-0.424388	0.000000
11	1	0	-2.540662	0.035893	0.830577
12	1	0	-2.540662	0.035893	-0.830577



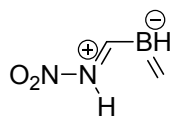
E = -364.0539412 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.184994	0.473126	0.294926
2	6	0	0.818106	0.608158	0.363953
3	1	0	2.821956	1.235281	0.737755
4	1	0	0.469730	1.486105	0.897555
5	5	0	-0.151455	-0.330638	-0.256033
6	7	0	2.880607	-0.528318	-0.274550
7	1	0	3.885140	-0.510907	-0.303810
8	7	0	-1.655160	-0.084958	-0.067088
9	8	0	-2.279273	-0.951182	0.545191
10	8	0	-2.159496	0.930044	-0.540708
11	1	0	2.411287	-1.301934	-0.719372
12	1	0	0.082579	-1.281024	-0.929640



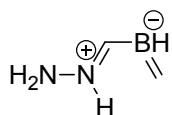
E = -214.890585 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.733719	0.000000
2	1	0	0.328355	1.771485	0.000000
3	6	0	-1.349194	0.574656	0.000000
4	1	0	-2.003185	1.444115	0.000000
5	7	0	-2.043641	-0.602883	0.000000
6	1	0	-1.559841	-1.484978	0.000000
7	5	0	1.029660	-0.399651	0.000000
8	1	0	0.701185	-1.555929	0.000000
9	1	0	-3.046549	-0.612885	0.000000
10	7	0	2.416216	-0.154348	0.000000
11	1	0	3.106911	-0.886944	0.000000
12	1	0	2.811958	0.773762	0.000000



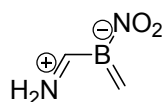
E = -363.9551773 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.486880	-0.981876	0.000000
2	1	0	-0.315091	-1.717218	0.000000
3	6	0	2.991077	-0.315255	0.000000
4	1	0	2.801793	0.759190	0.000000
5	1	0	4.055892	-0.534984	0.000000
6	7	0	0.000000	0.262342	0.000000
7	1	0	0.567290	1.102669	0.000000
8	5	0	1.963044	-1.363458	0.000000
9	1	0	2.205556	-2.530757	0.000000
10	7	0	-1.385731	0.586092	0.000000
11	8	0	-1.614713	1.782714	0.000000
12	8	0	-2.172572	-0.334947	0.000000



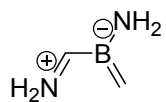
E = -214.7582547 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	-0.703847	0.000000
2	1	0	-0.510492	-1.669728	0.000000
3	6	0	2.213375	0.668631	0.000000
4	1	0	1.717322	1.641096	0.000000
5	1	0	3.296204	0.769783	0.000000
6	7	0	-0.860679	0.300818	0.000000
7	1	0	-0.518977	1.252793	0.000000
8	5	0	1.538337	-0.623432	0.000000
9	1	0	2.106534	-1.677020	0.000000
10	7	0	-2.268583	0.211778	0.000000
11	1	0	-2.578846	-0.288320	-0.828264
12	1	0	-2.578846	-0.288320	0.828264



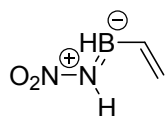
E = -364.0304976 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.448932	-0.041306	0.000000
2	1	0	1.651454	-1.110619	0.000000
3	6	0	-0.419167	1.824621	0.000000
4	1	0	0.264812	2.671302	0.000000
5	1	0	-1.465913	2.110874	0.000000
6	7	0	2.529740	0.712548	0.000000
7	1	0	2.459046	1.721588	0.000000
8	5	0	0.000000	0.445989	0.000000
9	1	0	3.459867	0.319834	0.000000
10	7	0	-1.045335	-0.713928	0.000000
11	8	0	-0.622836	-1.881827	0.000000
12	8	0	-2.244501	-0.447317	0.000000



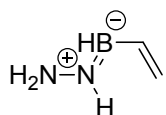
E = -214.8282599 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.556696	-0.848183	0.000000
2	1	0	-1.634272	-1.031510	0.000000
3	6	0	1.464152	0.751148	0.000000
4	1	0	2.165797	-0.081417	0.000000
5	1	0	1.977412	1.710539	0.000000
6	7	0	0.132794	-1.982730	0.000000
7	1	0	1.143148	-1.956467	0.000000
8	5	0	0.000000	0.594997	0.000000
9	1	0	-0.307969	-2.888864	0.000000
10	7	0	-0.997275	1.656797	0.000000
11	1	0	-0.746172	2.630492	0.000000
12	1	0	-1.991309	1.505992	0.000000



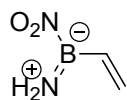
E = -364.0371204 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.697086	-1.678347	0.000000
2	1	0	1.820510	-2.759709	0.000000
3	6	0	2.817400	-0.943002	0.000000
4	1	0	2.809066	0.144568	0.000000
5	1	0	3.805352	-1.393386	0.000000
6	7	0	0.000000	0.259162	0.000000
7	1	0	0.704626	0.985414	0.000000
8	5	0	0.238170	-1.142994	0.000000
9	1	0	-0.702154	-1.858739	0.000000
10	7	0	-1.264890	0.884788	0.000000
11	8	0	-2.252164	0.183221	0.000000
12	8	0	-1.230453	2.106437	0.000000



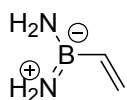
E = -214.8317599 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.545254	0.510638	0.000000
2	1	0	2.187289	1.391200	0.000000
3	6	0	2.164136	-0.676929	0.000000
4	1	0	1.620895	-1.619212	0.000000
5	1	0	3.246559	-0.768555	0.000000
6	7	0	-0.927417	-0.282106	0.000000
7	1	0	-0.659198	-1.255711	0.000000
8	5	0	0.000000	0.760621	0.000000
9	1	0	-0.439289	1.873125	0.000000
10	7	0	-2.350020	-0.167538	0.000000
11	1	0	-2.635270	0.360651	0.818945
12	1	0	-2.635270	0.360651	-0.818945



E = -364.099892 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.542708	0.391333	0.000000
2	1	0	2.036979	-0.575841	0.000000
3	6	0	2.304199	1.492690	0.000000
4	1	0	1.882960	2.495081	0.000000
5	1	0	3.388630	1.444046	0.000000
6	7	0	-0.863581	1.479436	0.000000
7	1	0	-0.569438	2.443279	0.000000
8	5	0	0.000000	0.403822	0.000000
9	1	0	-1.863747	1.327802	0.000000
10	7	0	-0.757275	-0.985059	0.000000
11	8	0	-0.085965	-2.013620	0.000000
12	8	0	-1.990388	-0.976161	0.000000



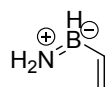
E = -214.9287013 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.663412	-0.920591	0.000000
2	1	0	-1.754268	-0.963204	0.000000
3	6	0	-0.025051	-2.094739	0.000000
4	1	0	1.060301	-2.165468	0.000000
5	1	0	-0.550910	-3.045150	0.000000
6	7	0	1.411372	0.667188	0.000000
7	1	0	2.048360	-0.110846	0.000000
8	5	0	0.000000	0.505840	0.000000
9	1	0	1.874327	1.561242	0.000000
10	7	0	-0.860216	1.638711	0.000000
11	1	0	-0.542732	2.594646	0.000000
12	1	0	-1.862398	1.550265	0.000000



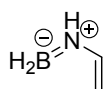
E = -156.0344785 a.u.

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



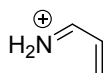
E = -159.5025744 a.u.

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



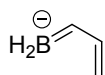
E = -159.481795 a.u.

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



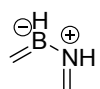
E = -172.4490176 a.u.

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



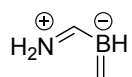
E = -142.811853 a.u.

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



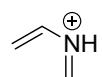
E = -159.4301881 a.u.

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.

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



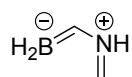
E = -172.4256625 a.u.

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



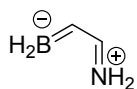
E = -142.8095564 a.u.

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