

# Does Aromaticity Account for an Enhanced Thermodynamic Stability?

## The Case of Monosubstituted Azaborines and the Stereoelectronic Chameleonism of NH<sub>2</sub> group

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Entry	Compound	$\Delta E_{\text{tot}}$	$\Delta E_{\text{def}}$	$\Delta E_{\text{int}}$	$\Delta E_{\text{elstat}}$	$\Delta E_{\text{Pauli}}$	$\Delta E_{\text{oi}}$	$\Delta E_{\text{disp}}$
		$\Delta E_{\text{iso}}$	$\Delta \Delta E_{\text{def}}$	$\Delta \Delta E_{\text{int}}$	$\Delta \Delta E_{\text{elstat}}$	$\Delta \Delta E_{\text{Pauli}}$	$\Delta \Delta E_{\text{oi}}$	$\Delta \Delta E_{\text{disp}}$
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	<b>2-nitro</b> → <b>3-nitro</b>	<b>19.52</b>	<b>3.05</b>	<b>16.47</b>	<b>10.50</b>	<b>22.00</b>	<b>-16.07</b>	<b>0.04</b>
4	5-nitro-1,2-azaborine	-65.29	13.29	-78.58	-163.81	350.13	-241.48	-23.42
5	<b>2-nitro</b> → <b>5-nitro</b>	<b>21.38</b>	<b>7.00</b>	<b>14.38</b>	<b>10.26</b>	<b>22.54</b>	<b>-17.85</b>	<b>-0.57</b>
6	4-nitro-1,2-azaborine	-64.77	5.72	-70.49	-154.31	327.49	-221.68	-21.99
7	<b>2-nitro</b> → <b>4-nitro</b>	<b>21.90</b>	<b>-0.57</b>	<b>22.47</b>	<b>19.76</b>	<b>-0.10</b>	<b>1.95</b>	<b>0.86</b>
8	6-nitro-1,2-azaborine	-64.71	10.06	-74.77	-162.83	348.78	-237.67	-23.05
9	<b>2-nitro</b> → <b>6-nitro</b>	<b>21.96</b>	<b>3.77</b>	<b>18.19</b>	<b>11.24</b>	<b>21.19</b>	<b>-14.04</b>	<b>-0.20</b>
10	1-nitro-1,2-azaborine	-41.56	10.29	-51.85	-139.20	330.71	-222.09	-21.27
11	<b>2-nitro</b> → <b>1-nitro</b>	<b>45.11</b>	<b>4.00</b>	<b>41.11</b>	<b>34.87</b>	<b>3.12</b>	<b>1.54</b>	<b>1.58</b>
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	<b>2-amino</b> → <b>4-amino</b>	<b>22.92</b>	<b>3.56</b>	<b>19.36</b>	<b>16.33</b>	<b>-20.75</b>	<b>22.72</b>	<b>1.06</b>
15	6-amino-1,2-azaborine	-99.68	8.59	-108.27	-227.57	481.17	-336.99	-24.88
16	<b>2-amino</b> → <b>6-amino</b>	<b>25.26</b>	<b>6.07</b>	<b>19.19</b>	<b>33.18</b>	<b>-73.00</b>	<b>58.17</b>	<b>0.84</b>
17	3-amino-1,2-azaborine	-98.46	7.69	-106.15	-232.62	507.33	-356.05	-24.81
18	<b>2-amino</b> → <b>3-amino</b>	<b>26.49</b>	<b>5.18</b>	<b>21.31</b>	<b>28.13</b>	<b>-46.84</b>	<b>39.11</b>	<b>0.91</b>
19	5-amino-1,2-azaborine	-93.73	10.49	-104.22	-206.89	433.88	-306.42	-24.79
20	<b>2-amino</b> → <b>5-amino</b>	<b>31.22</b>	<b>7.98</b>	<b>23.24</b>	<b>53.86</b>	<b>-120.29</b>	<b>88.74</b>	<b>0.93</b>
21	1-amino-1,2-azaborine	-71.34	8.59	-79.93	-170.25	370.54	-257.86	-22.36
22	<b>2-amino</b> → <b>1-amino</b>	<b>53.62</b>	<b>6.08</b>	<b>47.53</b>	<b>90.50</b>	<b>-183.63</b>	<b>137.30</b>	<b>3.36</b>
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	<b>3-nitro</b> → <b>2-nitro</b>	<b>18.91</b>	<b>4.07</b>	<b>14.84</b>	<b>-4.05</b>	<b>53.78</b>	<b>-34.03</b>	<b>-0.86</b>
26	4-nitro-1,3-azaborine	-65.97	7.97	-73.94	-161.42	345.30	-235.34	-22.48
27	<b>3-nitro</b> → <b>4-nitro</b>	<b>21.34</b>	<b>1.40</b>	<b>19.94</b>	<b>9.93</b>	<b>23.04</b>	<b>-13.17</b>	<b>0.14</b>
28	6-nitro-1,3-azaborine	-65.54	15.97	-81.51	-173.11	372.69	-256.90	-24.19
29	<b>3-nitro</b> → <b>6-nitro</b>	<b>21.78</b>	<b>9.41</b>	<b>12.37</b>	<b>-1.76</b>	<b>50.43</b>	<b>-34.73</b>	<b>-1.57</b>
30	5-nitro-1,3-azaborine	-63.11	8.64	-71.75	-157.35	334.70	-226.90	-22.20
31	<b>3-nitro</b> → <b>5-nitro</b>	<b>24.21</b>	<b>2.08</b>	<b>22.13</b>	<b>14.00</b>	<b>12.44</b>	<b>-4.73</b>	<b>0.42</b>
32	1-nitro-1,3-azaborine	-37.93	2.32	-40.25	-121.29	287.26	-186.95	-19.27
33	<b>3-nitro</b> → <b>1-nitro</b>	<b>49.38</b>	<b>-4.25</b>	<b>53.63</b>	<b>50.06</b>	<b>-35.00</b>	<b>35.22</b>	<b>3.35</b>
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	<b>3-amino</b> → <b>4-amino</b>	<b>18.46</b>	<b>5.52</b>	<b>12.94</b>	<b>-14.95</b>	<b>77.03</b>	<b>-49.55</b>	<b>0.41</b>
37	2-amino-1,3-azaborine	-99.78	7.47	-107.25	-241.38	522.87	-363.93	-24.81
38	<b>3-amino</b> → <b>2-amino</b>	<b>21.34</b>	<b>4.75</b>	<b>16.59</b>	<b>10.37</b>	<b>-6.33</b>	<b>11.91</b>	<b>0.64</b>

39	5-amino-1,3-azaborine	-96.34	7.74	-104.08	-223.01	475.72	-332.43	-24.36
40	<b>3-amino → 5-amino</b>	<b>24.78</b>	<b>5.02</b>	<b>19.76</b>	<b>28.74</b>	<b>-53.48</b>	<b>43.41</b>	<b>1.09</b>
41	6-amino-1,3-azaborine	-95.59	12.20	-107.79	-207.16	414.54	-290.35	-24.82
42	<b>3-amino → 6-amino</b>	<b>25.53</b>	<b>9.48</b>	<b>16.05</b>	<b>44.59</b>	<b>-114.66</b>	<b>85.49</b>	<b>0.63</b>
43	1-amino-1,3-azaborine	-71.95	3.47	-75.42	-179.26	395.97	-270.31	-21.82
44	<b>3-amino → 1-amino</b>	<b>49.17</b>	<b>0.75</b>	<b>48.42</b>	<b>72.49</b>	<b>-133.23</b>	<b>105.53</b>	<b>3.63</b>
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	<b>4-nitro → 3-nitro</b>	<b>21.64</b>	<b>5.48</b>	<b>16.16</b>	<b>13.95</b>	<b>12.94</b>	<b>-9.99</b>	<b>-0.74</b>
48	2-nitro-1,4-azaborine	-62.65	9.10	-71.75	-162.68	346.18	-232.89	-22.36
49	<b>4-nitro → 2-nitro</b>	<b>23.74</b>	<b>3.60</b>	<b>20.14</b>	<b>14.16</b>	<b>11.15</b>	<b>-4.71</b>	<b>-0.46</b>
50	1-nitro-1,4-azaborine	-39.70	18.16	-57.86	-144.22	342.63	-234.28	-21.99
51	<b>4-nitro → 1-nitro</b>	<b>46.69</b>	<b>12.66</b>	<b>34.03</b>	<b>32.62</b>	<b>7.60</b>	<b>-6.10</b>	<b>-0.09</b>
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	<b>4-amino → 2-amino</b>	<b>29.00</b>	<b>5.29</b>	<b>23.71</b>	<b>35.77</b>	<b>-79.29</b>	<b>66.06</b>	<b>1.17</b>
55	3-amino-1,4-azaborine	-94.86	9.02	-103.88	-224.99	486.46	-340.83	-24.52
56	<b>4-amino → 3-amino</b>	<b>32.25</b>	<b>6.30</b>	<b>25.95</b>	<b>36.98</b>	<b>-67.53</b>	<b>55.49</b>	<b>1.02</b>
57	1-amino-1,4-azaborine	-70.00	16.50	-86.50	-181.58	396.49	-278.60	-22.81
58	<b>4-amino → 1-amino</b>	<b>57.10</b>	<b>13.77</b>	<b>43.33</b>	<b>80.38</b>	<b>-157.50</b>	<b>117.72</b>	<b>2.73</b>


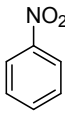
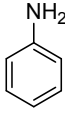
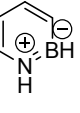
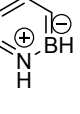
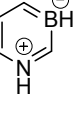
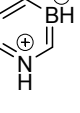
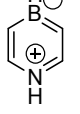
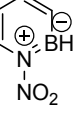
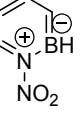
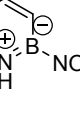
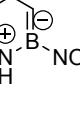
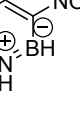
<sup>a</sup>  $\Delta E_{\text{tot}}$  = total binding energy between two fragments,  $\Delta E_{\text{def}}$  = deformation energy,  $\Delta E_{\text{int}}$  = interaction energy,  $\Delta E_{\text{elstat}}$  = electrostatic energy,  $\Delta E_{\text{Pauli}}$  = Pauli repulsion,  $\Delta E_{\text{oi}}$  = orbital interaction energy,  $\Delta E_{\text{disp}}$  = dispersion energy,  $\Delta E_{\text{iso}}$  = isomerization energy.<sup>b</sup>

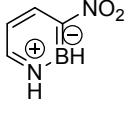
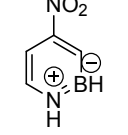
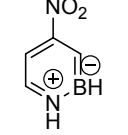
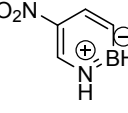
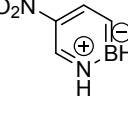
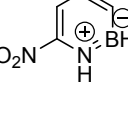
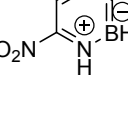
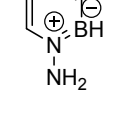
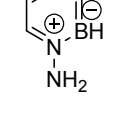
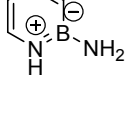
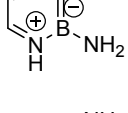
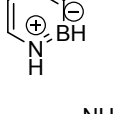
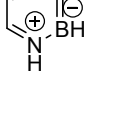
**Table S2.** Contribution of various energy components to the total binding interactions between six radical fragments and energy changes (values in bold) upon constitutional isomerization.<sup>a</sup> Values are in kcal/mol, calculated at the UB3LYP/6-311+G(d,p) level.

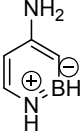
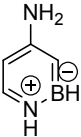
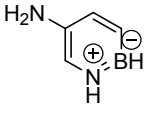
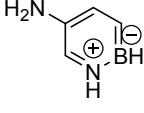
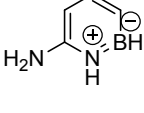
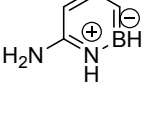
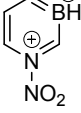
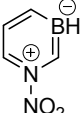
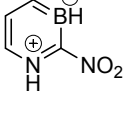
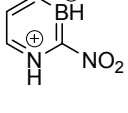
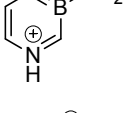
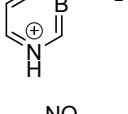
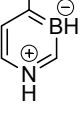
Entry	Compound	$\Delta E_{\text{tot}}$	$\Delta E_{\text{def}}$	$\Delta E_{\text{int}}$	$\Delta E_{\text{elstat}}$	$\Delta E_{\text{Pauli}}$	$\Delta E_{\text{oi}}$	$\Delta E_{\text{disp}}$	Interacting fragments
		$\Delta E_{\text{iso}}$	$\Delta \Delta E_{\text{def}}$	$\Delta \Delta E_{\text{int}}$	$\Delta \Delta E_{\text{elstat}}$	$\Delta \Delta E_{\text{Pauli}}$	$\Delta \Delta E_{\text{oi}}$	$\Delta \Delta E_{\text{disp}}$	
1	1,4-azaborine <sup>b</sup>	-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 <sup>b</sup>	-848.25	205.57	-1053.82	-1215.35	2056.79	-1699.16	-196.09	2×CH(q), C(6)H <sup>+</sup> (t), NH(t), BH(t), C(2) <sup>-</sup> (t)
3	<b>1,4 → 1,3<sup>b</sup></b>	<b>7.88</b>	<b>204.85</b>	<b>-196.97</b>	<b>-161.33</b>	<b>302.62</b>	<b>-361.54</b>	<b>23.28</b>	
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 <sub>2</sub> (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 <sup>+</sup> (t), NH(t), BH(t), CNO <sub>2</sub> <sup>-</sup> (t)
6	<b>2-NO<sub>2</sub>-1,4 → 2-NO<sub>2</sub>-1,3</b>	<b>2.44</b>	<b>152.73</b>	<b>-150.29</b>	<b>-147.07</b>	<b>259.79</b>	<b>-281.21</b>	<b>18.20</b>	
7	1,4-azaborine <sup>b</sup>	-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 <sup>b</sup>	-848.69	205.35	-1054.04	-1174.53	1984.56	-1667.98	-196.09	2×CH(q), C(4)H <sup>+</sup> (t), NH(t), BH(t), C(2) <sup>-</sup> (t)
9	<b>1,4 → 1,3<sup>b</sup></b>	<b>7.43</b>	<b>204.63</b>	<b>-197.20</b>	<b>-120.51</b>	<b>230.39</b>	<b>-330.36</b>	<b>23.28</b>	
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 <sub>2</sub> (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 <sup>-</sup> (t), NH(t), BH(t), CNH <sub>2</sub> <sup>+</sup> (t)
12	<b>3-NH<sub>2</sub>-1,4 → 4-NH<sub>2</sub>-1,3</b>	<b>0.43</b>	<b>124.62</b>	<b>-124.19</b>	<b>-61.59</b>	<b>178.84</b>	<b>-260.55</b>	<b>19.11</b>	
13	1,2-azaborine <sup>b</sup>	-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 <sup>b</sup>	-856.11	0.72	-856.83	-1054.02	1754.17	-1337.62	-219.37	4×CH(q), NH(t), BH(t)
15	<b>1,2 → 1,4<sup>b</sup></b>	<b>21.89</b>	<b>0.05</b>	<b>21.84</b>	<b>-114.67</b>	<b>203.78</b>	<b>-67.79</b>	<b>0.51</b>	
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 <sub>2</sub> (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 <sub>2</sub> (t)
18	<b>2-NO<sub>2</sub>-1,2 → 4-NO<sub>2</sub>-1,4</b>	<b>20.56</b>	<b>-0.31</b>	<b>20.87</b>	<b>-83.11</b>	<b>162.81</b>	<b>-60.12</b>	<b>1.29</b>	
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 <sub>2</sub> (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 <sub>2</sub> (t)
21	<b>2-NH<sub>2</sub>-1,2 → 4-NH<sub>2</sub>-1,4</b>	<b>18.12</b>	<b>-0.09</b>	<b>18.21</b>	<b>3.58</b>	<b>8.23</b>	<b>5.89</b>	<b>0.51</b>	

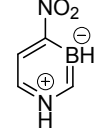
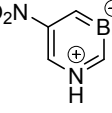
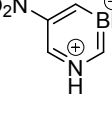
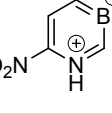
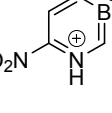
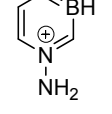
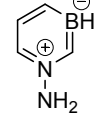
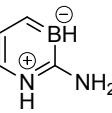
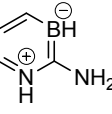
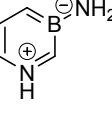
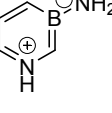
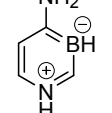
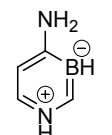
<sup>a</sup> Labeling of various energy terms is the same as in Table S1. <sup>b</sup> From ref. 8b.

**Table S3.** Calculated vertical resonance energies of cyclic molecules ( $VRE_{\text{cyclic}}$ ) and acyclic reference molecules ( $VRE_{\text{acyclic}}$ ), 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.

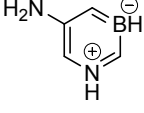
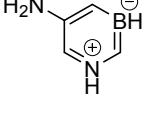
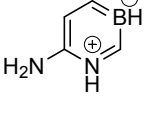
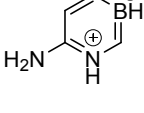
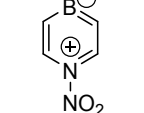
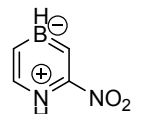
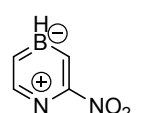
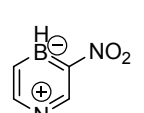
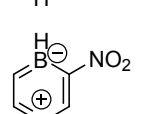
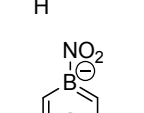
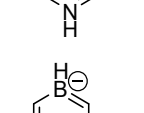
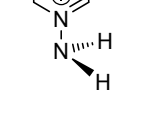
Compound	Resonance weight	$VRE_{\text{cyclic}}$	Reference molecules	$VRE_{\text{acyclic}}$	ECRE	$ECRE_{\text{rv}}$
	a	163.89	$H_2C=CH-CH=CH_2$ $H_2C=CH-CH=CH_2$ $H_2C=CH-CH=CH_2$	23.30 23.30 23.30	93.99	93.99 <sup>b</sup>
	a	156.45	$H_2C=CH-CH=CH_2$ $H_2C=CH-CH=CHNO_2$ $H_2C=CH-C(NO_2)=CH_2$	23.30 23.76 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 <sup>b</sup>
	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 <sup>b</sup>
	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 <sup>b</sup>
	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 <sup>b</sup>
	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 <sup>b</sup>
	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

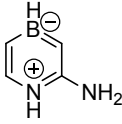
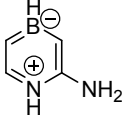
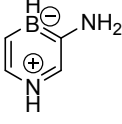
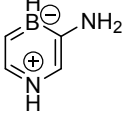
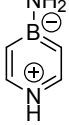
	0.17	231.68	$\text{H}_2\text{N}^+=\text{CH}-\text{CH}=\text{CH}_2$	45.41		
			$\text{H}_2\text{B}^-=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	30.84	135.05	68.45
			$\text{HC}(\text{NO}_2)=\text{BH}^--\text{NH}^+=\text{CH}_2$	20.38		
	0.74	115.26	$\text{H}_2\text{C}=\text{C}(\text{NO}_2)-\text{CH}=\text{CH}_2$	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 <sup>c</sup>
	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 <sup>c</sup>		
			$\text{HC}(\text{NH}_2)=\text{NH}^+-\text{CH}=\text{CH}_2$	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

<sup>a</sup> Equal for the two structures. <sup>b</sup> From ref. 8b. <sup>c</sup> Not clear  $\sigma/\pi$  separation.

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

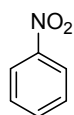
<b>R<sup>2</sup></b>	<b>NICS(1)<sub>zz</sub></b>	<b>NICS(0)<sub>πzz</sub></b>	<b>HOMA</b>	<b>PDI</b>	<b>FLU</b>	<b>ECRE</b>
<b>NICS(1)<sub>zz</sub></b>	1	0.899	0.633	0.618	0.561	0.307
<b>NICS(0)<sub>πzz</sub></b>	0.899	1	0.675	0.640	0.640	0.250
<b>HOMA</b>	0.633	0.675	1	0.841	0.920	0.412
<b>PDI</b>	0.618	0.640	0.841	1	0.856	0.487
<b>FLU</b>	0.561	0.640	0.920	0.856	1	0.400
<b>ECRE</b>	0.307	0.250	0.412	0.487	0.400	1

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



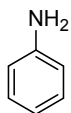
E = -232.3112416 a.u.

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



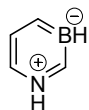
E = -287.6876274 a.u.

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



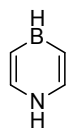
E = -235.7458969 a.u.

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



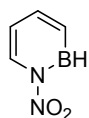
E = -235.6987876 a.u.

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



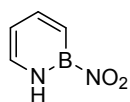
E = -235.7110251 a.u.

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



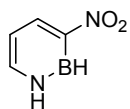
E = -440.2724044 a.u.

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



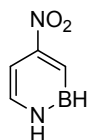
E = -440.3443398 a.u.

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



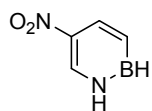
E = -440.3132573 a.u.

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



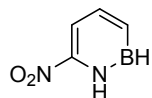
E = -440.3094839 a.u.

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.

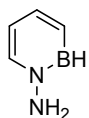
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.235526	0.023359	-0.000001
2	6	0	-0.426742	-1.176546	-0.000001
3	6	0	-1.822365	1.299714	0.000001
4	6	0	-0.451630	1.268134	0.000000
5	1	0	-2.304962	2.271374	0.000002
6	1	0	0.153890	2.166980	-0.000001
7	7	0	-1.780318	-1.191412	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.

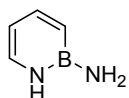
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.286301	-0.229204	0.000000
2	6	0	0.000000	0.224242	0.000000
3	6	0	0.478100	-2.532776	0.000000
4	6	0	1.516164	-1.632549	0.000000
5	1	0	2.096554	0.484740	0.000000
6	1	0	0.722004	-3.590443	0.000000
7	1	0	2.549491	-1.967680	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





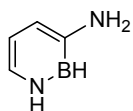
E = -291.0796767 a.u.

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



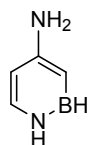
E = -291.1652017 a.u.

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



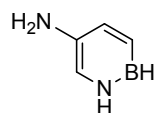
E = -291.1229953 a.u.

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



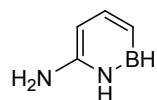
E = -291.1287205 a.u.

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



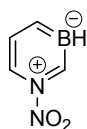
E = -291.1154137 a.u.

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



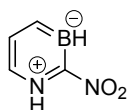
E = -291.1249492 a.u.

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



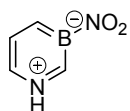
E = -440.2211443 a.u.

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



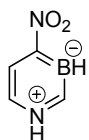
E = -440.2699393 a.u.

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



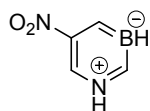
E = -440.3000316 a.u.

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



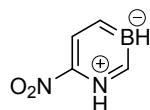
E = -440.2660072 a.u.

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



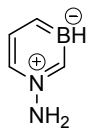
E = -440.2614675 a.u.

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



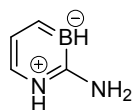
E = -440.2653176 a.u.

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



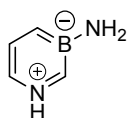
E = -291.0352447 a.u.

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



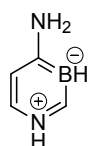
E = -291.0797748 a.u.

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.

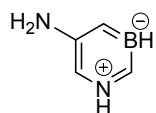
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.259305	-1.138181	0.000000
2	6	0	0.057128	-1.850319	0.000000
3	6	0	-1.243956	0.176228	0.000000
4	6	0	1.292695	0.245038	0.000000
5	1	0	2.174440	-1.723459	0.000000
6	1	0	-0.010193	-2.928070	0.000000
7	1	0	-2.279570	0.503381	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.

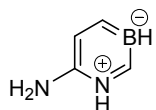
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.010987	0.055609	-0.004057
2	6	0	1.247455	1.194995	0.002182
3	6	0	1.078483	-1.197994	0.000815
4	6	0	-0.302734	-1.161940	-0.001311
5	1	0	1.633559	-2.126260	0.002398
6	1	0	-0.827907	-2.114009	-0.004199
7	7	0	1.804942	-0.062458	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





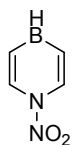
E = -291.0742045 a.u.

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



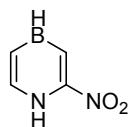
E = -291.0730029 a.u.

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



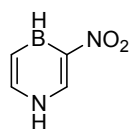
E = -440.2371908 a.u.

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



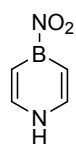
E = -440.2738155 a.u.

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



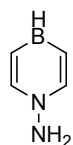
E = -440.2771988 a.u.

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



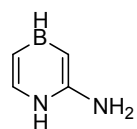
E = -440.3116447 a.u.

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



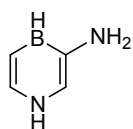
E = -291.0452819 a.u.

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



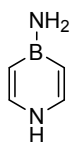
E = -291.0901848 a.u.

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



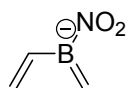
E = -291.0850244 a.u.

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



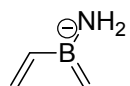
E = -291.1363811 a.u.

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



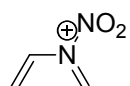
E = -347.4442489 a.u.

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



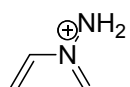
E = -198.2153646 a.u.

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



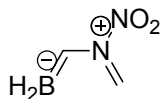
E = -376.931532 a.u.

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



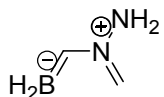
E = -227.7615493 a.u.

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.

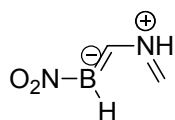
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.938904	1.386148	0.000000
2	1	0	-0.630510	2.420968	0.000000
3	1	0	-1.970794	1.080891	0.000000
4	6	0	1.361058	0.514394	0.000000
5	1	0	1.800172	-0.472758	0.000000
6	5	0	2.161645	1.771212	0.000000
7	1	0	1.648316	2.851186	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.

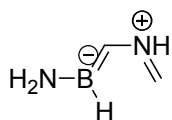
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.216210	0.867550	0.000000
2	1	0	-2.039888	0.171070	0.000000
3	1	0	-1.337524	1.936912	0.000000
4	6	0	0.435865	-0.932356	0.000000
5	1	0	1.518692	-0.978426	0.000000
6	5	0	-0.427565	-2.132870	0.000000
7	1	0	-1.623637	-2.069149	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





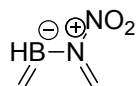
E = -364.0076818 a.u.

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



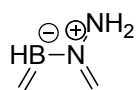
E = -214.8393273 a.u.

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



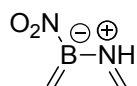
E = -363.9462222 a.u.

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



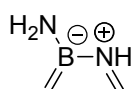
E = -214.7687076 a.u.

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



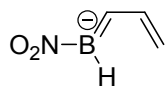
E = -364.0407052 a.u.

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



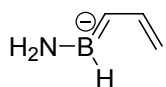
E = -214.8342276 a.u.

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



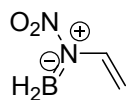
E = -347.4463 a.u.

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



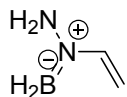
E = -198.2251168 a.u.

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



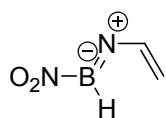
E = -364.0089554 a.u.

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



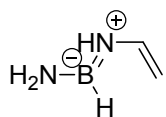
E = -214.8124763 a.u.

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



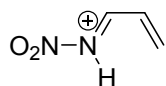
E = -364.0762307 a.u.

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



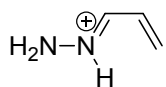
E = -214.9115907 a.u.

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



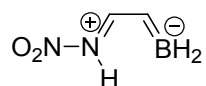
E = -376.9522313 a.u.

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



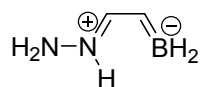
E = -227.788073 a.u.

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.

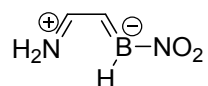
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.997076	-1.056395	0.000000
2	1	0	2.328853	-2.090346	0.000000
3	6	0	0.645041	-0.912257	0.000000
4	1	0	-0.046478	-1.746924	0.000000
5	7	0	0.000000	0.299315	0.000000
6	1	0	0.477708	1.191757	0.000000
7	5	0	3.002684	0.086101	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.

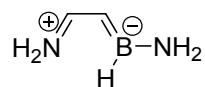
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.374075	0.715812	0.000000
2	1	0	1.780931	1.723210	0.000000
3	6	0	0.000000	0.672812	0.000000
4	1	0	-0.584499	1.592533	0.000000
5	7	0	-0.779839	-0.430614	0.000000
6	1	0	-0.356638	-1.346391	0.000000
7	5	0	2.282683	-0.484426	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





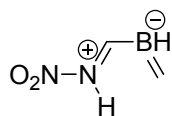
E = -364.0539412 a.u.

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



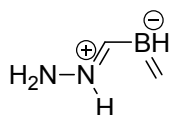
E = -214.890585 a.u.

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



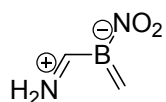
E = -363.9551773 a.u.

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



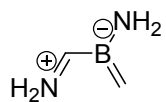
E = -214.7582547 a.u.

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



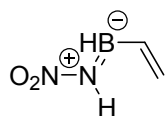
E = -364.0304976 a.u.

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



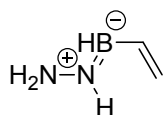
E = -214.8282599 a.u.

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



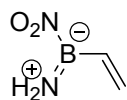
E = -364.0371204 a.u.

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



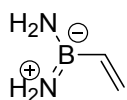
E = -214.8317599 a.u.

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



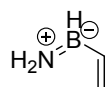
E = -214.9287013 a.u.

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



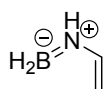
E = -156.0344785 a.u.

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



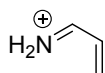
E = -159.5025744 a.u.

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



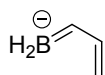
E = -159.481795 a.u.

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.

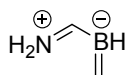
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.360922	0.922471	0.000000
2	1	0	1.966563	0.021528	0.000000
3	1	0	1.885437	1.873835	0.000000
4	6	0	0.000000	0.874101	0.000000
5	1	0	-0.483531	1.859153	0.000000
6	6	0	-0.912118	-0.248900	0.000000
7	1	0	-1.960743	0.065090	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.

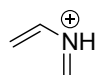
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.293388	0.942568	0.000000
2	1	0	1.864953	0.023853	0.000000
3	1	0	1.801781	1.898413	0.000000
4	6	0	-0.534319	-1.644370	0.000000
5	1	0	0.503175	-1.975095	0.000000
6	1	0	-1.239015	-2.470715	0.000000
7	5	0	-0.984581	-0.273997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



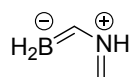
E = -172.4256625 a.u.

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



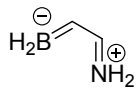
E = -142.8095564 a.u.

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