

# **Mono BN-Substituted Analogues of Naphthalene: A Theoretical Analysis of the Effect of BN Position on Stability, Aromaticity and Frontier Orbital Energies**

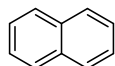
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<sup>b</sup> *University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, P.O.Box 158, 11000 Belgrade, Serbia*

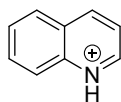
**Supplementary Information**

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



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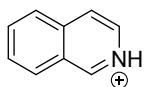
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5	6	0	0.000000	1.243886	-1.400697
6	6	0	0.000000	2.430634	-0.707529
7	1	0	0.000000	-1.243119	2.485975
8	1	0	0.000000	3.373020	1.243931
9	1	0	0.000000	1.243119	2.485975
10	6	0	0.000000	-1.243886	1.400697
11	6	0	0.000000	-1.243886	-1.400697
12	1	0	0.000000	1.243119	-2.485975
13	1	0	0.000000	3.373020	-1.243931
14	6	0	0.000000	-2.430634	-0.707529
15	6	0	0.000000	-2.430634	0.707529
16	1	0	0.000000	-1.243119	-2.485975
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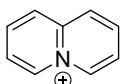
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5	6	0	1.311597	-1.380460	0.000000
6	6	0	2.459501	-0.626439	0.000000
7	1	0	-1.272344	2.293460	0.000000
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9	1	0	1.132666	2.525766	0.000000
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11	1	0	1.357637	-2.463025	0.000000
12	1	0	3.427714	-1.111513	0.000000
13	6	0	-2.391339	-0.786896	0.000000
14	6	0	-2.394102	0.604154	0.000000
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16	1	0	-3.333039	-1.318262	0.000000
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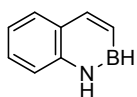
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5	6	0	1.337517	-1.353148	0.000000
6	6	0	2.477731	-0.580300	0.000000
7	1	0	-1.397479	2.376630	0.000000
8	1	0	3.324363	1.412610	0.000000
9	1	0	1.131987	2.553874	0.000000
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11	6	0	-1.148310	-1.468238	0.000000
12	1	0	1.404017	-2.434537	0.000000
13	1	0	3.449486	-1.059915	0.000000
14	6	0	-2.346766	-0.819161	0.000000
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16	1	0	-3.307619	-1.313058	0.000000
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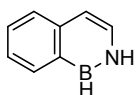
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3	6	0	0.000000	0.000000	-0.728168
4	6	0	0.000000	-1.243741	-1.399443
5	6	0	0.000000	-2.422758	-0.702010
6	1	0	0.000000	1.103597	2.439164
7	1	0	0.000000	-3.302854	1.292426
8	1	0	0.000000	-1.103597	2.439164
9	6	0	0.000000	1.195409	1.362326
10	6	0	0.000000	1.243741	-1.399443
11	1	0	0.000000	-1.229079	-2.481753
12	1	0	0.000000	-3.371456	-1.223666
13	6	0	0.000000	2.422758	-0.702010
14	6	0	0.000000	2.390025	0.711528

15	1	0	0.000000	1.229079	-2.481753
16	1	0	0.000000	3.371456	-1.223666
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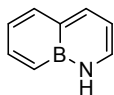
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4	6	0	0.023319	-0.716048	0.000000
5	6	0	-1.207113	-1.406357	0.000000
6	6	0	-2.412653	-0.731229	0.000000
7	1	0	1.115133	2.396990	0.000000
8	1	0	-3.363091	1.209536	0.000000
9	1	0	-1.240926	2.466744	0.000000
10	6	0	1.286921	-1.407695	0.000000
11	1	0	-1.189159	-2.491561	0.000000
12	1	0	-3.347069	-1.279921	0.000000
13	6	0	2.481017	-0.751763	0.000000
14	1	0	1.241861	-2.495486	0.000000
15	1	0	3.392980	-1.341295	0.000000
16	1	0	3.445941	1.477034	0.000000
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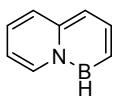
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4	6	0	0.000000	0.683256	0.000000
5	6	0	-1.187057	1.448697	0.000000
6	6	0	-2.422353	0.828619	0.000000
7	1	0	1.285814	-2.737935	0.000000
8	1	0	-3.490517	-1.049878	0.000000
9	1	0	-1.433211	-2.420980	0.000000
10	6	0	1.294765	1.316226	0.000000
11	1	0	-1.121652	2.532214	0.000000
12	1	0	-3.326497	1.428159	0.000000

13	6	0	2.440107	0.592277	0.000000
14	1	0	1.357773	2.397864	0.000000
15	1	0	3.414955	1.065070	0.000000
16	1	0	3.321548	-1.243038	0.000000
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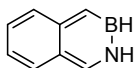
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4	6	0	1.319335	1.515050	0.000000
5	6	0	2.462808	0.759139	0.000000
6	1	0	-1.206087	-2.540452	0.000000
7	1	0	3.412011	-1.191157	0.000000
8	1	0	1.355632	-2.502185	0.000000
9	1	0	1.423463	2.598383	0.000000
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11	1	0	-1.443939	2.360114	0.000000
12	1	0	-3.398821	1.151871	0.000000
13	1	0	-3.351060	-1.307572	0.000000
14	6	0	-1.187680	-1.451451	0.000000
15	6	0	-2.414933	-0.763803	0.000000
16	6	0	-2.455912	0.616989	0.000000
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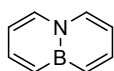
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4	6	0	-1.190683	-1.389223	0.000000
5	6	0	-2.393699	-0.763270	0.000000
6	1	0	1.157783	2.476839	0.000000
7	1	0	-3.388817	1.178454	0.000000
8	1	0	-1.261272	2.442806	0.000000
9	1	0	-1.091644	-2.465587	0.000000
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11	1	0	1.181345	-2.639084	0.000000
12	1	0	3.519701	-1.098748	0.000000
13	1	0	3.338969	1.350349	0.000000
14	6	0	1.205395	1.394906	0.000000
15	6	0	2.441131	0.736519	0.000000
16	6	0	2.532316	-0.648320	0.000000
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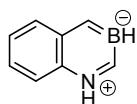
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3	6	0	0.000000	0.681173	0.000000
4	6	0	0.023533	-0.770650	0.000000
5	6	0	-1.249035	-1.438476	0.000000
6	6	0	-2.422295	-0.741430	0.000000
7	1	0	1.208713	2.466180	0.000000
8	1	0	-3.376246	1.217383	0.000000
9	1	0	-1.247372	2.459957	0.000000
10	6	0	1.242122	-1.454849	0.000000
11	1	0	-1.254763	-2.523306	0.000000
12	1	0	-3.367116	-1.274377	0.000000
13	1	0	1.195820	-2.540677	0.000000
14	1	0	3.637465	-1.140400	0.000000
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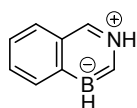
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4	6	0	0.000000	2.396240	0.734491
5	1	0	0.000000	-1.491578	-2.551231
6	1	0	0.000000	3.489358	-1.129399
7	1	0	0.000000	1.491578	-2.551231
8	1	0	0.000000	1.108315	2.445117
9	1	0	0.000000	3.292773	1.342323
10	1	0	0.000000	-1.108315	2.445117
11	1	0	0.000000	-3.292773	1.342323

12	1	0	0.000000	-3.489358	-1.129399
13	6	0	0.000000	-1.371581	-1.471210
14	6	0	0.000000	-2.494694	-0.691241
15	6	0	0.000000	-2.396240	0.734491
16	7	0	0.000000	0.000000	0.661829
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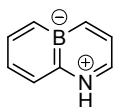
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4	1	0	3.209277	-1.522978	0.000000
5	1	0	1.106801	-2.355261	0.000000
6	1	0	1.213910	2.539318	0.000000
7	1	0	3.657874	1.218621	0.000000
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9	1	0	-3.349991	1.288444	0.000000
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11	6	0	-1.224721	-1.355780	0.000000
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13	6	0	-2.407894	0.752114	0.000000
14	6	0	-1.223222	1.443569	0.000000
15	6	0	0.000000	-0.653001	0.000000
16	6	0	0.039761	0.775491	0.000000
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18	5	0	2.577190	0.714931	0.000000



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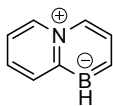
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3	1	0	1.435299	2.447564	0.000000
4	1	0	-3.505394	1.139802	0.000000
5	1	0	-1.240832	2.787299	0.000000
6	1	0	-1.357647	-2.369570	0.000000
7	1	0	-3.251071	-1.114701	0.000000
8	1	0	1.125548	-2.513282	0.000000
9	1	0	3.326648	-1.407090	0.000000

10	1	0	3.481334	1.074923	0.000000
11	6	0	1.360583	1.364929	0.000000
12	6	0	2.506242	0.599946	0.000000
13	6	0	2.419724	-0.812402	0.000000
14	6	0	1.193617	-1.429675	0.000000
15	6	0	0.066507	0.781169	0.000000
16	6	0	0.000000	-0.653284	0.000000
17	5	0	-1.228734	1.594165	0.000000
18	7	0	-2.390028	-0.580675	0.000000



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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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4	1	0	-3.284742	1.279026	0.000000
5	1	0	-1.241798	2.312545	0.000000
6	1	0	-1.461909	-2.602219	0.000000
7	1	0	-3.463400	-1.178355	0.000000
8	1	0	1.619570	-2.542280	0.000000
9	1	0	3.536907	-1.040758	0.000000
10	1	0	3.312325	1.382828	0.000000
11	6	0	1.188794	1.435451	0.000000
12	6	0	2.404414	0.788047	0.000000
13	6	0	2.527438	-0.635829	0.000000
14	6	0	1.435123	-1.469748	0.000000
15	6	0	0.000000	0.671331	0.000000
16	6	0	-2.470450	-0.739469	0.000000
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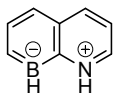


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4	1	0	3.578395	-1.043295	0.000000
5	1	0	1.327695	-2.709656	0.000000
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7	1	0	3.269908	1.392229	0.000000

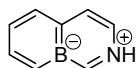


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10	1	0	-3.391267	-1.253305	0.000000
11	6	0	-1.252493	-1.411941	0.000000
12	6	0	-2.442906	-0.731062	0.000000
13	6	0	-2.400978	0.684294	0.000000
14	6	0	-1.204724	1.328845	0.000000
15	6	0	0.009298	-0.769289	0.000000
16	6	0	2.408452	0.729296	0.000000
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18	7	0	0.000000	0.637177	0.000000



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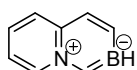
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2	6	0	-1.177882	1.431672	0.000000
3	1	0	1.166811	-2.771919	0.000000
4	1	0	-3.320649	-1.208265	0.000000
5	1	0	-1.270366	-2.296274	0.000000
6	1	0	-1.156090	2.517149	0.000000
7	1	0	-3.332672	1.317624	0.000000
8	1	0	1.333414	2.452406	0.000000
9	1	0	3.414642	1.185561	0.000000
10	1	0	3.505933	-1.232835	0.000000
11	6	0	2.517626	-0.778756	0.000000
12	6	0	2.479793	0.628137	0.000000
13	6	0	1.301323	1.368367	0.000000
14	6	0	0.000000	-0.719205	0.000000
15	6	0	-2.397016	0.774961	0.000000
16	7	0	-1.253081	-1.282165	0.000000
17	6	0	0.046287	0.727873	0.000000
18	5	0	1.258323	-1.573995	0.000000



E = -389.378468 a.u.

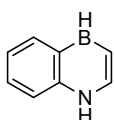
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.266791	-1.362186	0.000000
2	1	0	1.635523	2.507417	0.000000
3	1	0	-3.284872	1.217615	0.000000
4	1	0	-1.450260	2.557586	0.000000
5	1	0	-1.360710	-2.445627	0.000000
6	1	0	-3.413673	-1.065410	0.000000

7	1	0	1.194978	-2.563711	0.000000
8	1	0	3.338871	-1.412096	0.000000
9	1	0	3.558214	1.009097	0.000000
10	6	0	2.549345	0.601936	0.000000
11	6	0	2.426507	-0.823000	0.000000
12	6	0	1.214184	-1.475328	0.000000
13	6	0	-2.426427	-0.625094	0.000000
14	6	0	0.000000	-0.736736	0.000000
15	6	0	1.455811	1.433945	0.000000
16	6	0	-1.262001	1.487680	0.000000
17	7	0	-2.390096	0.744868	0.000000
18	5	0	0.073767	0.794752	0.000000



E = -389.3603588 a.u.

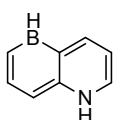
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.199547	1.451504	0.000000
2	1	0	-0.997722	-2.490948	0.000000
3	1	0	3.611147	-1.227104	0.000000
4	1	0	1.146081	-2.436301	0.000000
5	1	0	1.067982	2.530469	0.000000
6	1	0	3.298530	1.553635	0.000000
7	1	0	-1.290212	2.400223	0.000000
8	1	0	-3.402090	1.086221	0.000000
9	1	0	-3.228651	-1.439302	0.000000
10	6	0	-2.342942	-0.816887	0.000000
11	6	0	-2.437588	0.595542	0.000000
12	6	0	-1.274024	1.316962	0.000000
13	6	0	2.447140	0.876805	0.000000
14	6	0	0.000000	0.701187	0.000000
15	6	0	-1.123910	-1.417933	0.000000
16	6	0	1.273541	-1.358821	0.000000
17	5	0	2.575088	-0.636123	0.000000
18	7	0	0.066988	-0.698061	0.000000



E = -389.395154 a.u.

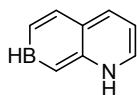
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.403371	-2.460732	0.000000
2	1	0	3.536005	-1.170216	0.000000
3	1	0	1.252672	-2.781594	0.000000
4	1	0	1.242436	2.265514	0.000000

5	1	0	3.290954	1.265863	0.000000
6	1	0	-1.105063	2.492191	0.000000
7	1	0	-3.307827	1.384193	0.000000
8	1	0	-3.466907	-1.097319	0.000000
9	6	0	-2.494039	-0.619322	0.000000
10	6	0	-2.404487	0.784212	0.000000
11	6	0	-1.172418	1.408072	0.000000
12	6	0	2.431947	0.601367	0.000000
13	6	0	0.000000	0.627163	0.000000
14	6	0	-1.338495	-1.377600	0.000000
15	6	0	-0.051592	-0.789166	0.000000
16	6	0	2.530877	-0.761520	0.000000
17	7	0	1.234280	1.256859	0.000000
18	5	0	1.262078	-1.587031	0.000000



E = -389.3657927 a.u.

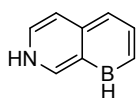
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.479187	-2.685592	0.000000
2	1	0	-3.348314	-1.352572	0.000000
3	1	0	-1.147716	-2.558410	0.000000
4	1	0	-1.294551	2.260961	0.000000
5	1	0	-3.323668	1.154367	0.000000
6	1	0	1.074745	2.510651	0.000000
7	1	0	3.278135	1.472324	0.000000
8	1	0	3.639794	-0.917704	0.000000
9	6	0	2.609969	-0.569365	0.000000
10	6	0	2.416890	0.806015	0.000000
11	6	0	1.147813	1.427220	0.000000
12	6	0	-2.417029	0.563048	0.000000
13	6	0	0.000000	0.655269	0.000000
14	6	0	0.044311	-0.794890	0.000000
15	6	0	-2.411848	-0.812183	0.000000
16	7	0	-1.258173	1.250216	0.000000
17	6	0	-1.167591	-1.472876	0.000000
18	5	0	1.422900	-1.489791	0.000000



E = -389.3691034 a.u.

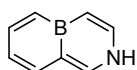
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.457747	-2.402664	0.000000
2	1	0	-3.220615	-1.515054	0.000000

3	1	0	-0.945806	-2.569361	0.000000
4	1	0	-1.403135	2.225676	0.000000
5	1	0	-3.363864	0.990889	0.000000
6	1	0	0.893139	2.644762	0.000000
7	1	0	3.459409	1.662810	0.000000
8	1	0	3.504857	-1.091917	0.000000
9	6	0	2.556583	-0.557987	0.000000
10	6	0	1.091250	1.572916	0.000000
11	6	0	-2.421452	0.459198	0.000000
12	6	0	0.000000	0.730094	0.000000
13	6	0	0.113350	-0.723032	0.000000
14	6	0	-2.325187	-0.909876	0.000000
15	7	0	-1.305111	1.219317	0.000000
16	6	0	-1.040956	-1.488075	0.000000
17	6	0	1.421937	-1.314711	0.000000
18	5	0	2.476178	0.981695	0.000000



E = -389.3676053 a.u.

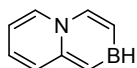
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.396919	2.403580	0.000000
2	1	0	3.307920	1.486052	0.000000
3	1	0	1.117889	2.540597	0.000000
4	1	0	1.476241	-2.657469	0.000000
5	1	0	3.652651	-0.904652	0.000000
6	1	0	-1.151647	-2.517447	0.000000
7	1	0	-3.169798	-1.365041	0.000000
8	1	0	-3.429315	0.971826	0.000000
9	6	0	-2.426892	0.567902	0.000000
10	6	0	-1.122058	-1.433946	0.000000
11	6	0	2.625504	-0.547781	0.000000
12	6	0	0.067478	-0.741727	0.000000
13	6	0	0.000000	0.718881	0.000000
14	6	0	2.440365	0.827564	0.000000
15	6	0	1.173108	1.456728	0.000000
16	6	0	-1.301740	1.323854	0.000000
17	5	0	1.428438	-1.460314	0.000000
18	7	0	-2.326258	-0.812104	0.000000



E = -389.3845742 a.u.

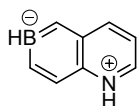
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.426296	-2.613892	0.000000

2	1	0	3.555317	-1.002218	0.000000
3	1	0	1.656856	-2.512736	0.000000
4	1	0	1.180608	2.560500	0.000000
5	1	0	3.335500	1.422832	0.000000
6	1	0	-1.379544	2.398602	0.000000
7	1	0	-3.259499	1.092386	0.000000
8	1	0	-3.435084	-1.189942	0.000000
9	6	0	-2.428493	-0.786350	0.000000
10	6	0	-1.235922	1.321259	0.000000
11	6	0	2.423271	0.834613	0.000000
12	6	0	0.000000	0.710220	0.000000
13	6	0	2.543613	-0.600699	0.000000
14	6	0	1.463344	-1.441775	0.000000
15	6	0	-1.291389	-1.535694	0.000000
16	7	0	-2.382680	0.593818	0.000000
17	6	0	1.215726	1.472561	0.000000
18	5	0	0.062000	-0.831412	0.000000



E = -389.36597 a.u.

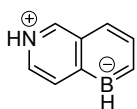
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.935325	2.491899	0.000000
2	1	0	-3.336977	1.129587	0.000000
3	1	0	-1.193298	2.355874	0.000000
4	1	0	-1.100604	-2.553305	0.000000
5	1	0	-3.288999	-1.406107	0.000000
6	1	0	1.280860	-2.472721	0.000000
7	1	0	3.686929	-1.109615	0.000000
8	1	0	3.208029	1.638292	0.000000
9	6	0	2.401810	0.909941	0.000000
10	6	0	1.325053	-1.386852	0.000000
11	6	0	-2.365569	-0.839782	0.000000
12	6	0	0.087854	-0.764079	0.000000
13	6	0	-2.401046	0.587473	0.000000
14	6	0	-1.235991	1.275420	0.000000
15	6	0	1.147799	1.428208	0.000000
16	6	0	-1.163412	-1.472200	0.000000
17	5	0	2.605950	-0.603308	0.000000
18	7	0	0.000000	0.644837	0.000000



E = -389.3562329 a.u.

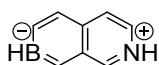
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	1	0	0.941828	2.587054	0.000000
2	1	0	-3.325739	1.049943	0.000000
3	1	0	-1.318525	2.203147	0.000000
4	1	0	-1.036626	-2.602529	0.000000
5	1	0	-3.248427	-1.478433	0.000000
6	1	0	1.413357	-2.466847	0.000000
7	1	0	3.740308	-0.986529	0.000000
8	1	0	3.210453	1.707426	0.000000
9	6	0	2.394030	0.987176	0.000000
10	6	0	1.399199	-1.378283	0.000000
11	6	0	-2.332416	-0.902759	0.000000
12	6	0	0.126798	-0.791597	0.000000
13	6	0	-2.403436	0.487397	0.000000
14	6	0	1.121487	1.511475	0.000000
15	6	0	-1.093622	-1.518996	0.000000
16	5	0	2.633318	-0.532097	0.000000
17	6	0	0.000000	0.656504	0.000000
18	7	0	-1.259351	1.191679	0.000000



E = -389.355044 a.u.

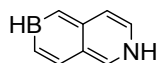
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.135274	-2.573863	0.000000
2	1	0	3.648025	-0.862519	0.000000
3	1	0	1.536427	-2.657496	0.000000
4	1	0	1.071263	2.546267	0.000000
5	1	0	3.287978	1.531154	0.000000
6	1	0	-1.402318	2.338896	0.000000
7	1	0	-3.272363	0.995503	0.000000
8	1	0	-3.327293	-1.344395	0.000000
9	6	0	-2.365028	-0.854597	0.000000
10	6	0	-1.263606	1.264228	0.000000
11	6	0	2.423649	0.869332	0.000000
12	6	0	0.000000	0.669613	0.000000
13	6	0	2.614355	-0.522121	0.000000
14	6	0	-1.150216	-1.489756	0.000000
15	6	0	1.166870	1.465328	0.000000
16	6	0	0.076563	-0.788695	0.000000
17	7	0	-2.379489	0.522585	0.000000
18	5	0	1.446892	-1.462327	0.000000



E = -389.35401 a.u.

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

1	1	0	-1.414837	2.354832	0.000000
2	1	0	3.254945	1.691166	0.000000
3	1	0	1.012576	2.611789	0.000000
4	1	0	1.392094	-2.448725	0.000000
5	1	0	3.745871	-1.009009	0.000000
6	1	0	-1.057847	-2.549962	0.000000
7	1	0	-3.081915	-1.454374	0.000000
8	1	0	-3.433881	0.860002	0.000000
9	6	0	-2.419553	0.491681	0.000000
10	6	0	-1.055576	-1.467157	0.000000
11	6	0	0.141786	-0.733569	0.000000
12	6	0	2.425673	0.984787	0.000000
13	6	0	-1.295784	1.277455	0.000000
14	6	0	1.399519	-1.359375	0.000000
15	6	0	0.000000	0.724060	0.000000
16	7	0	-2.256696	-0.871033	0.000000
17	6	0	1.161038	1.533147	0.000000
18	5	0	2.647449	-0.532933	0.000000



E = -389.3640394 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.031469	-2.612494	0.000000
2	1	0	3.751807	-0.960026	0.000000
3	1	0	1.436335	-2.444306	0.000000
4	1	0	0.969007	2.610903	0.000000
5	1	0	3.239091	1.745651	0.000000
6	1	0	-1.427917	2.294099	0.000000
7	1	0	-3.284049	0.888781	0.000000
8	1	0	-3.232974	-1.463102	0.000000
9	6	0	-2.292998	-0.929201	0.000000
10	6	0	-1.263159	1.223338	0.000000
11	6	0	0.000000	0.681124	0.000000
12	6	0	-1.078763	-1.530012	0.000000
13	6	0	1.154431	1.537294	0.000000
14	6	0	0.150067	-0.777373	0.000000
15	7	0	-2.377291	0.448679	0.000000
16	6	0	1.406807	-1.355630	0.000000
17	6	0	2.419669	1.029010	0.000000
18	5	0	2.648977	-0.494313	0.000000