Relaxed Force Constants and QTAIM Analysis for Benzene, Borazine and Azaborines: New Insights into Bonding in the Six Membered Rings

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ABSTRACT

The relaxed force constant (RFC), which is the inverse of the diagonal elements of the compliance matrix, can be used as a measure of bond strength, as has recurrently been suggested in ordinary research-based literature provided that the bonds make a part of the complete basis set in valence internal coordinates. Herein, the RFC values for heterocyclic systems such as azaborine and diazaborine are reported including benzene as well as borazine. The use of RFC as a bond strength parameter has been reinvestigated. The nature of chemical bonding in these prototype systems are analyzed in depth by quantum theory of atoms in molecules (QTAIM). The bond strengths calculated by QTAIM are in accordance with the calculated RFC values. This study not only reveals the mixed ionic and covalent bonding in heterocycles but also advocates the applicability of RFC as a bond strength parameter for a variety of systems.

Keywords: Relaxed force constant; bond strength; topological parameters; chemical bonding; ab initio calculations.
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INTRODUCTION

The compliance constants (CCs) which are the inverse of the force constant matrix elements have more lead over the regular (generalized) force constants were directed by many chemists [1-4]. Although it offers many advantages over regular force constants [1, 5-6], the use of CC as a bond strength parameter is not notably rewarding due to the fact that CC decreases in magnitude as the bond strength increases and its unit is the reciprocal of the unit of regular force constant. As indicated by Wilson *et al.* [7] that the CC of a bond is a measure of bond strength only when the bonds form a part of the complete valence internal coordinates (VICs) basis. The relaxed force constants (RFCs) are obtained by inverting the diagonal elements of the CC matrix. RFC first introduced by Jones [8] who realized as a "more chemical meaningful bond strength parameter than regular (force) constant" [6]. Grunenberg [4] has extensively studied the covalent bonds (bonded pairs) as well as non-covalent bonds (non-bonded pairs) and showed that RFC for bond stretching is a nice parameter for measuring the bond order for a system.

The quantum theory of atoms in molecule (QTAIM) [9] defines the chemical bonding and structure of the chemical system based on the topology of the electron density. In addition to bonding, QTAIM allows the calculation of certain physical properties per atom basis, by dividing space up into atomic volumes containing exactly one nucleus which acts as a local attractor of the electron density (ρ). QTAIM is a very powerful tool for the detection and characterization of non-bonded interaction such as hydrogen bonding [10-13]. In QTAIM, the values of some

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topological parameters at bond critical point (BCP) decide the nature of the chemical interaction. These parameters are Laplacian of electron density ($\nabla^2\rho$), and ratio of eigenvalues of Hessian, $|\lambda_1|/\lambda_3|$. According to the theory, for covalent bonding, $\nabla^2\rho < 0$ and $|\lambda_1|/\lambda_3|$ is greater than unity while ionic bonding is characterized by $\nabla^2\rho > 0$ and $|\lambda_1|/\lambda_3|$ less than unity.　　 In the present investigation, we have calculated RFC values for benzene, borazine, and azaborines. Benzene (C_6H_6) and borazine ($B_3N_3H_6$) are prototype six membered rings containing purely covalent and ionic bonds, respectively. On the contrary, azaborines [14,15] are expected to show a different pattern of bonding due to the presence of B, C and N atoms. Recently we have performed a systematic investigation on these BCN rings [16]. Along with aromaticity and various other molecular properties, we have discussed the lowest energy isomers for 1,2-azaborine (BC_4NH_6) and 1,2,3,4-diazaborine ($B_2C_4N_2H_6$). It seems interesting to analyze the chemical bonding in these heterocycles.

MATERIALS AND METHODS

Computational Details
The systems considered in this study C_6H_6, $B_3N_3H_6$, BC_4NH_6 and $B_2C_4N_2H_6$ were optimized with MP2/aug-cc-pVDZ level [17] as described in the previous study [16]. The RFC is a measure of the force required to distort a particular internal coordinate with all remaining internal coordinates are allowed to relax to a (new) minimum energy configuration [6]. The standard normal coordinate analysis (NCA) is performed for all these systems by using all complete VIC (bonds, bond angles, out of the plane and torsional angles). Due to more contribution of bonds in VIC basis, we were interested in determining the RFCs for all bonds involved in the system. For electronic structure calculations, Gaussian 09 package [27] was used and the RFCs were calculated through standard NCA method by using a locally developed computer program based on UMAT[28] software. In order to perform QTAIM analysis, the generated wavefunction for the systems is analyzed via AIMAll program [18].

RESULTS AND DISCUSSION

In most of the systems, because of redundancies in the VIC, the number of VIC are commonly more than the number of vibrational degrees of freedom (3N-5/3N-6 for linear/non-linear systems with N number of atoms). Due to these redundancies, usually in bond angles and torsional angles, there is no unique way to select the bond angles and/or torsional angles as part of the VIC basis. A simple example is BF_3 in which three bond angles are dealt in several ways in the literature [19-23]. Similarly, eighteen bond angles in benzene are dealt in various ways [24-26]. In practice, NCA is done in terms of non-redundant symmetric or local coordinates. Therefore, in order to form complete VIC (bonds + angles + out of plane + torsional angles), we have made suitable 3N-6 linear combinations of local coordinates. Now the local coordinates thus formed are converted into symmetric coordinates and the normal mode analysis is done in these symmetric coordinates to find normal mode frequencies.
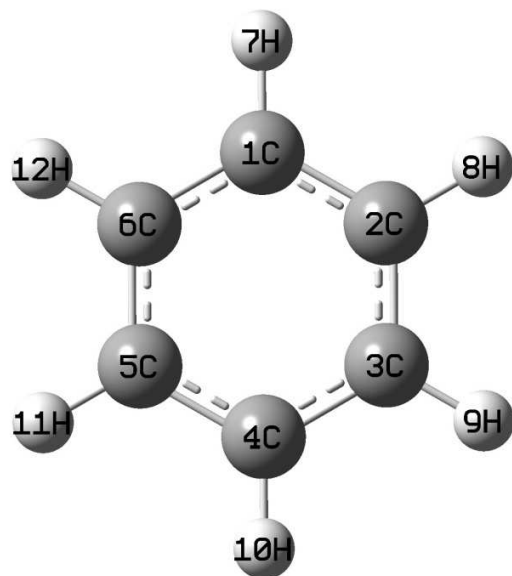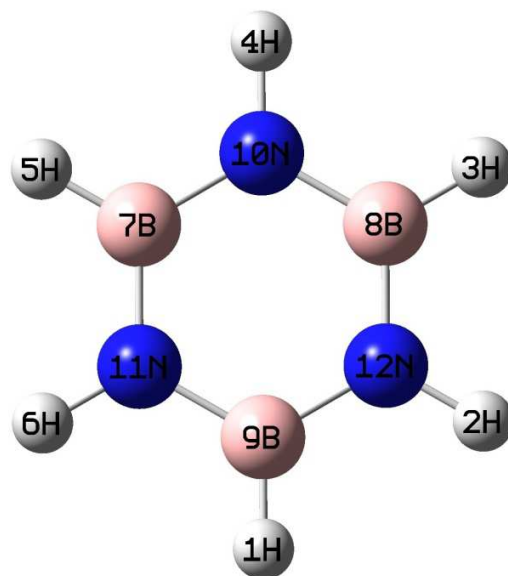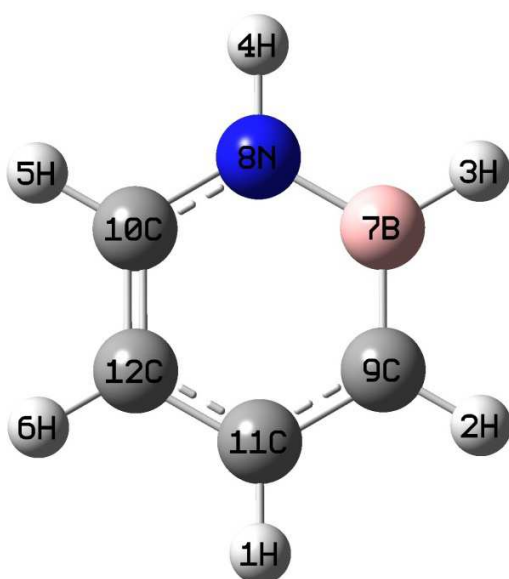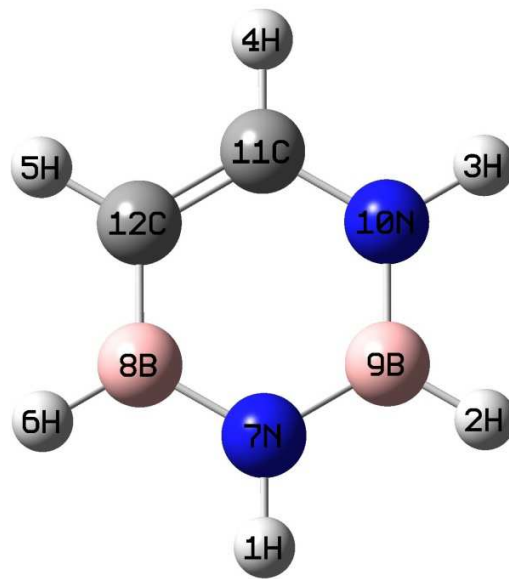
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Fig. 1. Atomic numbering scheme for equilibrium structures of benzene, borazine, azaborine and diazaborine.

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Table 1. Bond Characteristics Parameters for C_6H_6 at MP2/aug-cc-pVDZ level

Bonds	Length	Freq.	RFC	ρ	$\nabla^2\rho$	$|\lambda_1|/\lambda_3|$	δ
C1–C2	1.407	1381	6.7504	0.2954	-0.6981	1.562	1.164
C2–C3	1.407	1381	6.7504	0.2954	-0.6981	1.562	1.164
C3–C4	1.407	1381	6.7504	0.2954	-0.6981	1.562	1.164
C4–C5	1.407	1381	6.7504	0.2954	-0.6981	1.562	1.164
C5–C6	1.407	1381	6.7504	0.2954	-0.6981	1.562	1.164
C6–C1	1.407	1381	6.7504	0.2954	-0.6981	1.562	1.164
C1–H7	1.094	3210	5.6450	0.2730	-0.9970	1.893	0.857
C2–H8	1.094	3210	5.6450	0.2730	-0.9970	1.893	0.857
C3–H9	1.094	3210	5.6450	0.2730	-0.9970	1.893	0.857
C4–H10	1.094	3210	5.6450	0.2730	-0.9970	1.893	0.857
C5–H11	1.094	3210	5.6450	0.2730	-0.9970	1.893	0.857
C6–H12	1.094	3210	5.6450	0.2730	-0.9970	1.893	0.857

Bond-length (in Å), stretching frequency (in cm^{-1}), RFC value (in mdyn/Å) and topological parameters (in a.u.)

Table 2. Bond Characteristics Parameters for $B_3N_3H_6$ at MP2/aug-cc-pVDZ level

Bond	Length	Freq.	RFC	ρ	$\nabla^2\rho$	$|\lambda_1|/\lambda_3|$	δ
B7–N11	1.440	1212	5.3387	0.1869	0.6860	0.290	0.441
N11–B9	1.440	1212	5.3387	0.1869	0.6860	0.290	0.441
B9–N12	1.440	1212	5.3387	0.1869	0.6860	0.290	0.441
N12–B8	1.440	1212	5.3387	0.1869	0.6860	0.290	0.441
B8–N10	1.440	1212	5.3387	0.1869	0.6860	0.290	0.441
N10–B7	1.440	1212	5.3387	0.1869	0.6860	0.290	0.441
B7–H5	1.202	2646	3.8110	0.1720	-0.1404	0.676	0.455
N11–H6	1.013	3640	7.3402	0.3300	-0.1487	0.130	0.716
B9–H1	1.202	2646	3.8110	0.1720	-0.1404	0.676	0.455
N12–H2	1.013	3640	7.3401	0.3300	-0.1487	0.130	0.716
B8–H3	1.202	2646	3.8110	0.1720	-0.1404	0.676	0.455
N10–H4	1.013	3640	7.3402	0.3300	-0.1487	0.130	0.716

Bond-length (in Å), stretching frequency (in cm^{-1}), RFC value (in mdyn/Å) and topological parameters (in a.u.)

Fig. 1 depicts the atomic labeling of the equilibrium structures. Table 1 and 2 lists the bond-lengths, normal mode stretching frequencies, RFC values as well as topological parameters for C_6H_6 and $B_3N_3H_6$, respectively. The calculated RFC value for C-C bonds in C_6H_6 is 6.7504 mdyn/Å (1.407 Å) whereas 5.6450 mdyn/Å (1.094 Å) for C-H bonds. One can see that for all C-C and C-H bonds, $\nabla^2\rho < 0$ and $|\lambda_1|/\lambda_3| > 1$. Therefore, all these bonds are purely covalent in nature. The QTAIM calculated bond orders (δ) for C-C and C-H bonds are 1.164 and 0.857, respectively (see Table 1). In $B_3N_3H_6$, however, the situation is slightly different (see Table 2). One can notice that $\nabla^2\rho > 0$ and $|\lambda_1|/\lambda_3| < 1$ for B-N bonds but $\nabla^2\rho < 0$ and $|\lambda_1|/\lambda_3| > 1$ for B-H and N-H bonds. Hence, all B-N bonds in the ring are purely ionic which can be expected due to large electrongativity difference between B and N atoms. On the contrary, all B-H and N-H bonds are of covalent character. The RFC values for B-N, B-H, and N-H bonds are calculated 5.3387, 3.8110 and 7.3402 mdyn/Å whereas the calculated δ values are 0.441, 0.455 and 0.716, respectively.

Table 3. Bond Characteristics Parameters for BC_4NH_6 at MP2/aug-cc-pVDZ level

Bond	Length	Freq.	RFC	ρ	$\nabla^2\rho$	$|\lambda_1|/\lambda_3|$	δ
B7–N8	1.444	1188	5.1334	0.1759	0.8162	0.2551	0.462
N8–C10	1.373	1328	6.7197	0.3039	-0.8731	2.0757	0.982
C10–C12	1.383	1462	7.5652	0.3091	-0.7516	1.6964	1.228
C12–C11	1.428	1311	6.0816	0.2852	-0.6702	1.5229	1.086
C11–C9	1.394	1422	7.1486	0.3006	-0.7078	1.5812	1.303
C9–B7	1.522	1176	4.6810	0.1878	0.0982	0.4470	0.513
B7–H3	1.202	2648	3.8153	0.1690	-0.1143	0.6474	0.483
N8–H4	1.016	3601	7.1865	0.3325	-1.5256	1.2959	0.691
C10–H5	1.092	3224	5.6940	0.2766	-1.0321	1.9608	0.836
C12–H6	1.092	3233	5.7284	0.2729	-0.9959	1.9115	0.857
C11–H1	1.097	3178	5.5333	0.2725	-0.9905	1.8669	0.852
C9–H2	1.095	3199	5.6074	0.2700	-0.9671	1.8500	0.883

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Bond-length (in Å), stretching frequency (in cm⁻¹), RFC value (in mdyn/Å) and topological parameters (in a.u.)

Table 4. Bond Characteristics Parameters for $B_2C_2N_2H_6$ at MP2/aug-cc-pVDZ level

Bond	Length	Freq.	RFC	ρ	$\nabla^2\rho$	$\lvert\lambda_1\rvert/\lvert\lambda_3\rvert$	δ
N7–B9	1.434	1232	5.5162	0.1906	0.7094	0.2832	0.461
B9–N10	1.437	1216	5.3697	0.1843	0.7680	0.2689	0.460
N10–C11	1.387	1284	6.2834	0.2960	-0.8842	2.1986	0.948
C11–C12	1.376	1494	7.8925	0.3105	-0.7537	1.7383	1.349
C12–B8	1.536	1142	4.4153	0.1832	0.0634	0.4818	0.474
B8–N7	1.445	1196	5.1975	0.1812	0.7265	0.2819	0.441
B9–H2	1.200	2660	3.8508	0.1721	-0.1351	0.6620	0.466
N10–H3	1.013	3641	7.3447	0.3331	-1.5227	1.2975	0.696
C11–H4	1.095	3192	5.5832	0.2763	-1.0291	1.9332	0.832
C12–H5	1.093	3223	5.6937	0.2694	-0.9594	1.8500	0.884
B8–H6	1.204	2632	3.7687	0.1697	-0.1318	0.6796	0.468
N7–H1	1.015	3615	7.2400	0.3299	-1.4899	1.2959	0.713

Bond-length (in Å), stretching frequency (in cm⁻¹), RFC value (in mdyn/Å) and topological parameters (in a.u.)

Table 3 and 4 lists the RFC values as well as topological parameters for azaborines, BC_4NH_6 and $B_2C_2N_2H_6$, respectively. As displayed in Fig. 1, BC_4NH_6, ring system has three C-C covalent bonds and one ionic B-N bond. In the $B_2C_2N_2H_6$ ring, on the contrary, there is only one C-C covalent bond while three ionic B-N bonds. Therefore, it seems interesting to compare the strengths of purely covalent and ionic bonds of azaborines with those of benzene and borazine. Furthermore, it provides an opportunity to analyze other bonds in these heterocycles. Let's first discuss the nature of chemical bonding in BC_4NH_6. From Table 3, one can note that for all C-C bonds, $\nabla^2\rho < 0$ and $\lvert\lambda_1\rvert/\lambda_3 > 1$ and $\nabla^2\rho > 0$ and $\lvert\lambda_1\rvert/\lambda_3 < 1$ for B-N bond. Therefore, all C-C bonds are covalent and B-N is ionic as mentioned earlier. $\nabla^2\rho$ and $\lvert\lambda_1\rvert/\lambda_3$ values further suggest that N-C bond in the ring is covalent but C-B is found to be ionic in nature. In BC_4NH_6 ring, the RFC value for C10-C12 and C11-C9 bonds is 7.5652 mdyn/Å (1.383 Å) and 7.1486 mdyn/Å (1.394 Å) respectively which is much greater than the RFC value of C12-C11 bond (6.0816 mdyn/Å with bond length 1.428Å) in the same ring while more than the RFC value of C-C bond (6.7504 mdyn/Å with bond length 1.407Å) in C_6H_6 (see Table 1). Therefore, these C-C bonds in the BC_4NH_6 ring are much stronger than those in C_6H_6. This fact is also consistent with our calculated bond order of C10-C12 (1.228) and C11-C9 (1.303) which are larger than those of   C-C bonds in C_6H_6 (1.164). The RFC value for B-N bond in BC_4NH_6 is 5.1334 mdyn/Å (1.444 Å) which is slightly smaller than (~ 0.2) that of B-N bond in $B_3N_3H_6$ (see Table 2) and therefore, B-N bond of BC_4NH_6 is only slightly weaker than that of $B_3N_3H_6$. However, δ value of B7-N8 bond of the BC_4NH_6 ring is slightly larger than (~ 0.2) that of B-N bond in $B_3N_3H_6$ which suggests the stronger nature of B-N bond in the former. The RFC values for N8-C10 and C9-B7 bonds are calculated 6.7197 and 4.6810 mdyn/Å with δ value of 0.982 and 0.513 respectively. Furthermore, the RFC and δ values of C12-H16 and C12-H6 bonds in BC_4NH_6 suggest its strength comparable to C-H bonds in C_6H_6. Moreover, N8-H4 and B7-H3 bonds are found to be slightly stronger and weaker than those in $B_3N_3H_6$, respectively.

The RFC values and topological parameters of the $B_2C_2N_2H_6$ ring are collected in Table 4. Like BC_4NH_6, the $B_2C_2N_2H_6$ ring also contains purely covalent C-C bond, purely ionic B-N bonds, partially covalent N-C bond and partially ionic C-B bond. The RFC value 7.8925 mdyn/Å with bond length 1.376 Å for C-C bond in $B_2C_2N_2H_6$ ring clearly shows that this C-C bond is much stronger than the C-C bond in benzene ring and slightly stronger than the C-C bond in BC_4NH_6 ring. The calculated bond order of C11-C12 bond (1.349) also supports this fact (see Table 4). In the $B_2C_2N_2H_6$ ring, there are three B-N bonds, first B9-N10 bond which is adjacent to C10-N11 bond, the second B8-N7 bond which is adjacent to C12-B8 bond and the third B7-N9 bond which is between two B-N bonds B8-N7 and B9-N10 bond as clearly shown in Fig. 1. The RFC values calculated for B9-N10, B7-N9 and B8-N7 bonds are 5.3697 mdyn/Å (1.437 Å), 5.5162 mdyn/Å (1.434 Å) and 5.1975 mdyn/Å (1.445 Å) respectively. These values suggest that the B9-N10 bond is slightly weaker than the B7-N9 bond while slightly stronger than the B8-N7 bond. Furthermore, B9-N10 and B7-N9 bonds are moderately stronger than the B-N bond in $B_3N_3H_6$ but B8-N7 bond is somewhat weaker. The calculated bond orders of B9-N10 (0.460) and B7-N9 (0.461) are also greater than those B-N bonds $B_3N_3H_6$ (0.441) in accordance with their RFC values. The calculated RFC (δ values) for N-C and C-B bonds in $B_2C_2N_2H_6$ are 6.2834 mdyn/Å (0.948) and 4.4153 mdyn/Å (0.474), respectively. These values are smaller than RFC and δ values of corresponding bonds in BC_4NH_6 ring system (see Table 3). Therefore, both N-C and   C-B

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bonds in diazaborine are slightly lower in strength than those in azaborine. The larger N-C and C-B bond lengths in $B_2C_2N_2H_6$ are in accordance with their bond strength. The strengths of C-H, B-H and N-H bonds also vary due to change in the proportion of electropositive B, electroneutral C and electronegative N atoms in azaborines which affect the charge transfer within these heterocyclic ring systems and hence their bond strengths.

CONCLUSION

Using normal coordinate analysis, we have calculated the relaxed force constant (RFC) values for all valence internal coordinate basis in six-membered rings formed by B, C and N atoms at MP2/aug-cc-pVDZ method. The RFC values suggest that the C-C bond in the $B_2C_2N_2H_6$ ring (which has only one covalent C-C bond) is much stronger than the C-C bond in benzene ring(having six C-C covalent bonds) but stronger than that in the BC_4NH_6 ring (having three C-C covalent bonds). The B-C and C-N bond in the BC_4NH_6 ring are observed stronger than that in the $B_2C_2N_2H_6$ ring. The B-N bond is observed weaker in the BC_4NH_6 ring in comparison to both $B_2C_2N_2H_6$ and borazine ring. In addition, to this, the detailed study of chemical bonding in above -tested systems has also been performed well with the aid of quantum theory of atoms in molecules (QTAIM). The calculated RFC values for the systems are consistent with QTAIM calculated bond order δ. Therefore, the use of RFC as a bond strength parameter is also recommended for heterocyclic systems. The nature of chemical bonding in benzene, borazine and azaborines has been analyzed by QTAIM analysis in which $\nabla^2\rho$ and $|\lambda_1|/\lambda_3$ descriptors show that all C-C and C-H bonds are pure covalent bonds in benzene, BC_4NH_6 and $B_2C_2N_2H_6$ rings. All B-N bonds in the borazine, BC_4NH_6 and $B_2C_2N_2H_6$ rings are pure ionic bonds and all B-H, N-H bonds are pure covalent bonds while all N-C and C-B bonds are found as partially covalent and partially ionic, respectively in BC_4NH_6 and $B_2C_2N_2H_6$ rings.

CONFLICT OF INTEREST
The authors state that this paper or part of it has not been published elsewhere. The authors also state that there is no conflict of interests regarding the publication of this paper.

CONTRIBUTION OF THE AUTHORS
SKP and AKS performed all calculations and prepared the draft. SKP and AKS designed the research and NM finalized the draft. SKP, AKS and NM revised the draft paper. All authors read and approved the final version.

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APPENDIX
It should be noted that coordinates are given in **Å**.

Benzene (C₆H₆)
  Cartesian Coordinates

1	C	0.00000000	1.40795800	0.00000000
2	C	1.21932740	0.70397900	0.00000000
3	C	1.21932740	-0.70397900	0.00000000
4	C	0.00000000	-1.40795800	0.00000000
5	C	-1.21932740	-0.70397900	0.00000000
6	C	-1.21932740	0.70397900	0.00000000
7	H	0.00000000	2.50216700	0.00000000
8	H	2.16694019	1.25108350	0.00000000
9	H	2.16694019	-1.25108350	0.00000000
10	H	0.00000000	-2.50216700	0.00000000
11	H	-2.16694019	-1.25108350	0.00000000
12	H	-2.16694019	1.25108350	0.00000000

Borazine (B₃N₃H₆)
  Cartesian Coordinates

1	H	0.00000000	-2.66552100	0.00000000
2	H	2.10581600	-1.21579400	0.00000000
3	H	2.30840890	1.33276050	0.00000000
4	H	0.00000049	2.43158715	0.00000000
5	H	-2.30840890	1.33276050	0.00000000
6	H	-2.10581649	-1.21579315	0.00000000
7	B	-1.26718700	0.73161100	0.00000000
8	B	1.26718721	0.73161063	0.00000000
9	B	-0.00000021	-1.46322163	0.00000000
10	N	0.00000000	1.41762800	0.00000000
11	N	-1.22770186	-0.70881400	0.00000000
12	N	1.22770186	-0.70881400	0.00000000

_____

Azaborine (BC₄NH₆)
  Cartesian Coordinates

```
   1   H    -2.11837500    -1.24915800     0.00000000
   2   H    -2.28817600     1.32305600     0.00000000
   3   H     0.04459200     2.36601700     0.00000000
   4   H     2.10340300     1.32929200     0.00000000
   5   H     2.29465900    -1.12184800     0.00000000
   6   H    -0.05795600    -2.71578200     0.00000000
   7   N    -1.23369200    -0.75022900     0.00000000
   8   B    -0.00566900    -1.51203700     0.00000000
   9   B    -1.27189100     0.68363900     0.00000000
  10   N     0.00000000     1.35353900     0.00000000
  11   C     1.21633300     0.68600700     0.00000000
  12   C     1.29125000    -0.68813300     0.00000000
```

Diazaborine (B₂C₂N₂H₆)
  Cartesian Coordinates

```
   1   H    -0.02483400    -2.52346600     0.00000000
   2   H     2.16431100    -1.40125700     0.00000000
   3   H     2.26856100     1.45966400     0.00000000
   4   H    -0.08154100     2.38600200     0.00000000
   5   H    -2.11079800     1.27339900     0.00000000
   6   H    -2.15922500    -1.21703200     0.00000000
   7   B     1.30119500     0.74459200     0.00000000
   8   N     0.00000000     1.37285700     0.00000000
   9   C     1.26388900    -0.77764100     0.00000000
  10   C    -1.18957500     0.68546800     0.00000000
  11   C     0.02987700    -1.42775400     0.00000000
  12   C    -1.19793200    -0.69845000     0.00000000
```