Complex pairing of $\text{B}_2\text{H}_4$ with $\text{H}_2\text{O}$, $\text{CH}_3\text{OH}$, $\text{NH}_3$, $\text{NH}_2\text{CH}_3$, $\text{NH}(\text{CH}_3)_2$ and $\text{N}(\text{CH}_3)_3$

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Abstract

Ab initio calculations were carried out to analyze the interactions between a molecule of $\text{B}_2\text{H}_4$ with $\text{H}_2\text{O}$, $\text{CH}_3\text{OH}$, $\text{NH}_3$, $\text{NH}_2\text{CH}_3$, $\text{NH}(\text{CH}_3)_2$, and $\text{N}(\text{CH}_3)_3$ molecules at the MP2/aug-cc-pVDZ computational level. $\text{B}_2\text{H}_4$ through its bridged hydrogens ($\text{H}_b$) could act as a hydrogen bond donor while its B-B act as hydrogen bond acceptor. Thus, interaction of $\text{B}_2\text{H}_4$ with the mentioned molecules resulted in formation of $\text{H}_b...\text{X}$ or B-B...H hydrogen bond complexes. In contrast, $\text{H}_t$ atoms of $\text{B}_2\text{H}_4$ have not enough strength to form $\text{H}_t...\text{H}$ dihydrogen bond complexes with the above molecules. Results showed that the B-B...H interactions are stronger than its $\text{H}_t$...X counterpart. The obtained structures were analyzed by the natural bond orbital (NBO) and Atoms in Molecules (AIMs) methodologies.

Introduction

Borane complexes have been studied extensively and have even been the subject of Nobel Prize work by Brown [1,2]. It has been the subject of proton affinity experiments in chemical ionization mass spectrometers. Among non-covalent interactions which have been known in boron chemistry, both dihydrogen bonding and hydrogen bonding types are particularly significant [4-21].

$\text{B}_2\text{H}_4$, designated as diborane(4), probably is the best known electron-deficient analogue of ethylene [22-26]. The molecule $\text{B}_2\text{H}_4$ bears 10 valence electrons for chemical bonding. There are two standard two electron terminal $\text{B}...\text{H}$ bonds, thus accounting for a total of four electrons. This leaves a total of six electrons to share between the two bridging $\text{H}$ atoms and the two $\text{B}$ atoms. Consequently, there are two 3c-2e curved ‘banana’ $\text{B}...\text{H}$ bridging bonds. According to the above illustrations, $\text{B}_2\text{H}_4$ has two types of terminal ($\text{H}_t$-$\text{B}$) and bridging ($\text{B}...\text{B}$-$\text{H}$) hydrogen atoms which differ in nature and characteristics. The bridging hydrogens of $\text{B}_2\text{H}_4$ are participating in electron deficient ‘three-center, two-electron bonds’ thus, they bear enough partial positive charge to act as hydrogen bond donor (HBD) to form $\text{H}_t...\text{X}$ ($\text{X}=\text{N, O}$) hydrogen bonds with electron donating molecules [13,14,17-21,26]. On other hand, recent studies are showing that $\text{B}_2\text{H}_4$ bond also could act as HBA in the interactions of borane clusters with HBD species to form $\text{H}...\text{B}$-B hydrogen bonds [13,20,26].

From a fundamental point of view, the present work aims to extend the knowledge of the intrinsic activity of $\text{H}_t$, $\text{H}_b$, and $\text{B}...\text{B}$ bond of diborane(4) as hydrogen bond acceptor or hydrogen bond donor towards other molecules. For this propose, we investigated interaction of $\text{B}_2\text{H}_4$ toward $\text{H}_2\text{O}$, $\text{CH}_3\text{OH}$ and $\text{NH}_n(\text{CH}_3)_{3-n}$, $n=0-3$ derivatives thorough theoretical calculation.

Computational methods

Calculations were performed using the Gaussian 03 system of codes [27]. The geometries of the isolated $\text{B}_2\text{H}_4$ and $\text{H}_2\text{O}$, $\text{CH}_3\text{OH}$ and $\text{NH}_n(\text{CH}_3)_{3-n}$ molecules as well as their complexes were fully optimized at the mp2/aug-cc-pVDZ computational level. Harmonic vibrational frequency calculation confirmed the structures as minimal and enabled the evaluation of zero point energy (ZPE). The counterpoise procedure was used to correct the interaction energy for basis set superposition error [28]. The AIM package was used to obtain bond properties and molecular graphs [29,30]. The natural bond orbitals (NBO) method was implemented within the Gaussian 03 set of codes was applied to perform NBO analysis [31].

Results and discussion

Interaction of $\text{B}_2\text{H}_4$ with $\text{H}_2\text{O}$ and $\text{CH}_3\text{OH}$ molecules gave the $\text{B}_2\text{H}_4...\text{H}_2\text{O}$ and $\text{B}_2\text{H}_4...\text{CH}_3\text{OH}$ complexes which have hydrogen bond interactions between B-B bond as HBA and OH functions of $\text{H}_2\text{O}$ and $\text{CH}_3\text{OH}$ as HBD. Results are demonstrating that later complex has greater stability than the former one. The association of $\text{B}_2\text{H}_4$ and $\text{NH}_n(\text{CH}_3)_{3-n}$ ($n=0-3$) derivatives led to the formation of the 1:1 hydrogen bond complexes which has been denoted as $\text{B}_2\text{H}_4...\text{NH}_n$, $\text{B}_2\text{H}_4...\text{NH}_n\text{Me}$, $\text{B}_2\text{H}_4...\text{NHMe}_2$, and $\text{B}_2\text{H}_4...\text{NMe}_3$. Figure 1. In these complexes hydrogen bond interactions has been found between a bridging proton of the $\text{B}_2\text{H}_4$ as a proton donor and nitrogen atom of amine as a proton acceptor ($\text{H}_{2n}...\text{N}$). According to the data given in Table 1, stabilities of $\text{B}_2\text{H}_4...\text{NH}_n(\text{CH}_3)_{3-n}$ complexes increased with enhancing basicity of amines in the following order: $\text{B}_2\text{H}_4...\text{NMe}_3 > \text{B}_2\text{H}_4...\text{NHMe}_2 > \text{B}_2\text{H}_4...\text{NHMe}_2 > \text{B}_2\text{H}_4...\text{NH}_3$.

The results due to the intermolecular bond lengths are given in the Table 2 and Figure 1. In the $\text{B}_2\text{H}_4...\text{H}_2\text{O}$ and $\text{B}_2\text{H}_4...\text{CH}_3\text{OH}$ complexes, the B1-B4 bond has elongation (0.0015); but, other bonds of $\text{B}_2\text{H}_4$ are shortened (from -0.0009 to -0.0053) upon complex formation. Moreover, a 0.0061 shortening was observed for O-H bond in these complexes.
On the other hand, the N…H distances in the B\(_2\)H\(_4\)-NH\(_n\)(CH\(_3\))\(_{3-n}\) complexes are in the range of 2.6196 to 2.4997 Å. These distances could be considered as weak bonding interactions between the two components. Comparison of the H\(_b\)…N distances showed that the obtained trend was in agreement with the stability of these complexes.

In B\(_2\)H\(_4\)-NH\(_3\), the NH\(_3\) molecule interacts with H\(_2\) atom of B\(_2\)H\(_4\). Data given in Table 2 showed that the bridging B-H-B bond, as well as B1-B4 bond, have contraction (-0.0046, -0.0055, -0.0023, -0.0028 and -0.0024 for B1-H2, B4-H2, B1-H3, B4-H3 and B1-B4 bonds, respectively); while, the terminal B1-H5 and B4-H6 bonds showed small elongation upon complexation.

### Table 1.
The SE\(_{\text{corr}}\), BSSE, ∆ZPE, and SE\(_{\text{corr}}\) (corrected with BSSE and ∆ZPE) in kcal mol\(^{-1}\) calculated at MP2/aug-cc-pVDZ.

| Complex       | SE\(_{\text{corr}}\) | BSSE | ∆ZPE  | SE\(_{\text{corr}}\) |
|---------------|----------------------|------|-------|----------------------|
| B\(_2\)H\(_4\)-H\(_2\)O | -4.02                | 0.96 | 1.66  | -1.40                |
| B\(_2\)H\(_4\)-CH\(_3\)OH | -4.53                | 1.16 | 1.08  | -2.29                |
| B\(_2\)H\(_4\)-NH\(_3\)   | -2.10                | 0.75 | 0.83  | -0.52                |
| B\(_2\)H\(_4\)-NHMe\(_2\) | -4.15                | 1.15 | 0.80  | -1.20                |
| B\(_2\)H\(_4\)-NMe\(_3\)  | -3.96                | 1.47 | 0.71  | -1.78                |

Values of SE\(_{\text{corr}}\) were determined as follows: SE\(_{\text{corr}}\) = E(B\(_2\)H\(_4\) ∙∙∙Y) - [E(B\(_2\)H\(_4\)) + E(Y)] with Y = H\(_2\)O, CH\(_3\)OH, NH\(_3\), NHMe\(_2\), NMe\(_3\), NH(CH\(_3\))\(_2\), and N(CH\(_3\))\(_3\);

Values of SE\(_{\text{corr}}\) were determined as follows: SE\(_{\text{corr}}\) = SE\(_{\text{corr}}\) + ∆ZPE + BSSE
In B$_2$H$_4$-NH$_2$CH$_3$, interaction occurred between NH$_2$CH$_3$ molecule and the bridging H$_3$ atom of B$_2$H$_4$. In this complex, B$_1$-H$_2$, B$_1$-H$_3$, B$_4$-H$_3$ and B$_1$-B$_4$ bonds showed contraction (-0.0077, -0.0069, -0.0023, and -0.0015, respectively); while, the terminal B$_1$-H$_5$ bond and the bridging B$_4$-H$_2$ bond revealed elongation after complexation.

The unsymmetric stretching frequencies (cm$^{-1}$) with the corresponding intensities (km mol$^{-1}$) for the studied complexes are listed in Table 3. The unsymmetric stretching frequencies of B$_1$-H$_5$ and B$_4$-H$_6$ showed a 5 cm$^{-1}$ blue shift in B$_2$H$_4$-H$_2$O and in B$_2$H$_4$-CH$_3$OH complexes, respectively. These charge transfers indicated that electron fraction is outweighed by the kinetic, the positive profile of $\nabla$\(2\rho\) indicates a depletion of charge density along the inter-nuclear connecting bond path (BP) [33]. Furthermore, the atomic connection is recognized as close-shell interaction, which is often designated to H-bonds or other intermolecular weakly bound contacts, such as halogen bonds, dihydrogen bonds, and π-staking [34-40]. Regarding the values gathered in Table 4, it should be highlighted that the positive values of V$^\alpha$\(\nabla_\alpha\) ensure that all H-bonds are closed-shell interactions due to the low charge density concentration. The inter-atomic and inter-molecular interactions are also studied in terms of local electron energy density (H) and its components, the local kinetic electron energy density (G), and local potential electron energy density (V) at the BCPs. The relation between these energetic parameters is given in Equation 1.

Also it has been suggested that both V$^\alpha$\(\nabla_\alpha\) and the H should be used for characterizing hydrogen bond [41]. The weak hydrogen-bonds means that both V$^\alpha$\(\nabla_\alpha\) and H are positive, medium hydrogen-bonds show that V$^\alpha$\(\nabla_\alpha\)>0 and H<0; while, strong hydrogen-bonds bearing both V$^\alpha$\(\nabla_\alpha\)>0 and H>0. For the investigated complexes (Table 4), V$^\alpha$\(\nabla_\alpha\) and H at BCP for H...N and H...B interactions are positive. This means that these interactions belong to close shell weak HB interactions.

The balance between G and V could be used to show the nature of interactions [42]. If $\nabla$\(2\rho\)>1, then, the nature of the interaction is purely non-covalent. For all the examined complexes, this ratio was greater than 1, which confirmed the existence of weak interactions between the two systems and nature of the interaction was purely non-covalent.

### Natural bond orbital analysis

Natural bond orbital (NBO) analysis was performed for the minima found on the studied B$_2$H$_4$ complexes. These complex formations are associated with an orbital interaction between the bonding pairs in the electron donor and the antibonding orbital in the electron acceptor. The quantity of charge transferred from donor to acceptor (AQ) due to the interaction of donor and acceptor orbitals were 0.0060, 0.0085, 0.0039, 0.0072, 0.0082 and 0.0085 for B$_2$H$_4$-H$_2$O, B$_2$H$_4$-CH$_3$OH, B$_2$H$_4$-NH$_3$, B$_2$H$_4$-NH$_2$CH$_3$, B$_2$H$_4$-NH(CH$_3$)$_2$ and B$_2$H$_4$-N(CH$_3$)$_3$ complexes, respectively. These charge transfers indicated that electron fraction is...
Table 3. Unscaled vibrational frequencies (cm\(^{-1}\)) with corresponding intensities (values given in parenthesis, km mol\(^{-1}\)) for B\(_2\)H\(_4\) and its complexes at MP2/aug-cc-pVDZ.

| Compound Bond | \(B\_2\)H\(_4\) | \(B\_2\)H\(_4\)-H\(_2\)O | \(B\_2\)H\(_4\)-MeOH | \(B\_2\)H\(_4\)-NH\(_3\) | \(B\_2\)H\(_4\)-NH\(_2\)Me | \(B\_2\)H\(_4\)-HMe\(_2\) | \(B\_2\)H\(_4\)-NMe\(_3\) |
|---------------|----------------|---------------------|--------------------|----------------|----------------|----------------|----------------|
| \(v\)          | \(\Delta v\)    | \(v\)               | \(\Delta v\)       | \(v\)          | \(\Delta v\)   | \(v\)          | \(\Delta v\)   |
| B1 - B4       | 1343(3)        | -8                  | 1335(2)            | 1345(2)        | 2               | 1342(2)        | 0              | 1342(2)       |
| sym-B1-H2-B4  | 2129(18)       | 15                  | 2144(15)           | 2136(27)       | 7               | 2134(34)       | 5              | 2123(13)      |
| unsy-B1-H2-B4 | 2136(44)       | 15                  | 2149(29)           | 2147(13)       | 11              | 2147(21)       | 11             | 2141(40)      |
| sym-B1-H5,B4-H6 | 2811(36) | 5                  | 2816(23)           | 2805(42)       | -6              | 2805(37)       | -6             | 2803(35)      |
| unsy-B1-H5,B4-H6 | 2851(0.2) | 4                  | 2855(0)            | 2847(0)        | -4              | 2846(0.2)      | -5             | 2844(0)       |

Table 4. Topological parameters for the fully optimized complexes at MP2/aug-cc-pVDZ.

| Complex | H-bond | \(\rho\) | \(\nabla^2\) | \(V\) | \(G/V\) | \(H_e\) |
|---------|--------|----------|-------------|-------|--------|--------|
| \(B\_2\)H\(_4\)-H\(_2\)O | B5...H9 | 0.0153   | 0.0344      | 1.1122 | 0.0088 |
| \(B\_2\)H\(_4\)-CH\(_3\)OH | B8...B4 | 0.0164   | 0.0345      | 1.0735 | 0.0066 |
| \(B\_2\)H\(_4\)-NH\(_3\) | N7...H2 | 0.0094   | 0.0242      | 1.0629 | 0.0003 |
| \(B\_2\)H\(_4\)-NH\(_2\)Me | N7...H3 | 0.0097   | 0.0270      | 1.0931 | 0.0005 |
| \(B\_2\)H\(_4\)-HMe\(_2\) | H3...N7 | 0.0118   | 0.0300      | 1.0257 | 0.0002 |
| \(B\_2\)H\(_4\)-NMe\(_3\) | H3...N7 | 0.0126   | 0.0308      | 0.9945 | 0.0001 |

Table 5. The NBO analysis of studied complexes at MP2/aug-cc-pVDZ.

| complexes | donor→ acceptor | qCT* | \(E\) (2) |
|-----------|----------------|------|----------|
| \(B\_2\)H\(_4\)-H\(_2\)O | bd(B1-B4)→σ*(O-H) | 0.0060 | 3.85    |
| \(B\_2\)H\(_4\)-CH\(_3\)OH | bd(B1-B4)→σ*(O-H) | 0.0085 | 5.54    |
| \(B\_2\)H\(_4\)-NH\(_3\) | lp(N)→σ*(B1-H2-B4) | 0.0039 | 2.15    |
| \(B\_2\)H\(_4\)-NH\(_2\)Me | lp(N)→σ*(B1-H3-B4) | 0.0072 | 1.27    |
| \(B\_2\)H\(_4\)-HMe\(_2\) | lp(N)→σ*(B1-H3-B4) | 0.0082 | 2.09    |
| \(B\_2\)H\(_4\)-NMe\(_3\) | lp(N)→σ*(B1-H3-B4) | 0.0085 | 2.15    |

transferred from HBA to HBD molecules. Thus, charge transfer is not concentrated on the interacting atoms; but, is mostly dispersed among the molecules. Therefore, interpretation of the bond variations and frequency shifts in \(B\_2\)H\(_4\) could not be carried out simply.

A useful quantity which might be derived from the results of natural bond orbital analysis is NBO binding energy (\(E\)\(^2\)). The second-order perturbation energy can be taken as an index to judge the strength of the intermolecular bonds.

Table 5, lists the quantity of charge transfer from the donor to the acceptor qCT and the second-order perturbation energy due to the interaction of donor and acceptor orbitals. \(E\)\(^2\) allow us to quantitatively evaluate the charge transfer involving the formation of the \(B\_2\)H\(_4\) complexes. According to results, the \(E\)\(^2\) value of \(B\_2\)H\(_4\)-CH\(_3\)OH was greater than \(B\_2\)H\(_4\)-H\(_2\)O, confirming the order obtained for the interaction energies of these complexes. Whereas, for the amine complexes some controversies were seen between the order obtained for their \(E\)\(^2\) and the interaction energies.
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