The Wavefunction Analysis of B_2H_6

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Abstract: B_2H_6, a typical structure with hydrogen bridge bond, has been analyzed. According to the results of computations, the two B-H-B hydrogen bridge bonds formed in B_2H_6 are weaker than other B-H bonds. This is because the 3-center-2-electrons bonds can be structured, the stability, however, has been still weak. Multicenter bond orders are also lower than other bonds. At the same time, it has been supported by other analytical methods, such as ADCH atomic charge, ELF, LOL, and AIM basin analysis, which may explain the reason the molecule is instability.

Computational method:

Geo and wavefunction file: B3LYP/6-311G* by Gaussian 09 D.01 version

Wavefunction analysis: Multiwfn 3.4.1 (dev)

Results and discussions:

Firstly, the ADCH atomic charges can be computed(Table 1). In B_2H_6, two types of hydrogen atoms show different atomic charges. It can be seen that, the charge of hydrogen atom in B-H-B bond, due to stronger covalence property, is greater than the one in B-H bond. Additionally, when the valence electron of H atom has been attracted, the degree electron can be closed to two boron atoms is stronger than one boron atom, which may cause the fact that, the more deflected the valence electron of H atom is, the more positive charge H atom will have.

Table 1. the ADCH atomic charges of all atoms in B_2H_6

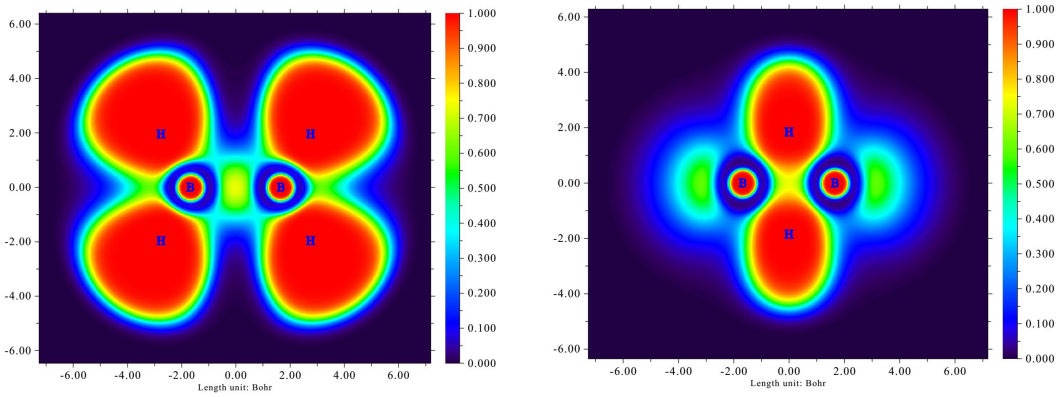
B	-0.127752
H(in B-H bond)	0.005476
H(in B-H-B bond)	0.116735

Table 2. the Mayer bond orders of all bonds in B_2H_6

B-B	0.62262762
B-H(in B-H bond)	0.99266578
B-H(in B-H-B bond)	0.46563980
B-H-B	0.26969303

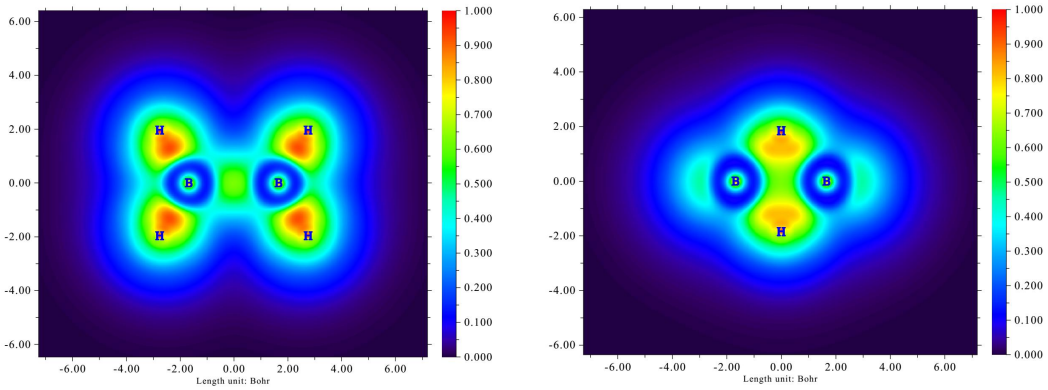
From the results of Mayer bond orders analysis(Table 2), it can be seen that, the acting force of B-H bond at the edge of B_2H_6 is strongest. Relatively, other types of bonds are weaker, such as the B-H bond in B-H-B bond. This is because the valence electron of H atom is much closed to B atoms, which may cause the H atom can be ionized and easier to separate for a dissociative proton. The B-B bond, further, failed to be more stable. A credible explanation is supposed to be that, as the element with strong electron deficiency property, B-B bond failed to be formed without any other atoms. The configuration of extra-nuclear electron of boron atom is $1s^2 2s^2 2p^1$, if three hydrogen atoms formed B-H bond with same single B atom, there are no free electrons of boron atoms to form the B-B bond. Under the help of hydrogen atoms, B-B bond can be structured, but the interatomic force is weak. It must be the reason that, H atom has no p-orbital electrons, which may lead to the failure of forming multicenter bond with conjugacy. Another reason is that, based on the instability of B-H bond in B-H-B bond, the H atom can be ionized and easier to separate for a dissociative proton, which may break the formed structure down. To sum up, the bond order of multicenter bond, B-H-B bond, is low, which may indicate the instability of molecule.

To visualize the electrons distribution in B_2H_6 molecule, the ELF(Electron Localization Function) and LOL(Localized Orbital Locator) plots have been applied(Figure 1 and 2). In the subfigure (a) of figure 1 and 2, the B-H bond at the edge of molecule is stronger, and B-B bond is weaker. On the other hand, obviously, in the subfigure (b) of figure 1 and 2, the multicenter bond, B-H-B bond, is much lower than B-H bond, which is a symbol of instability.



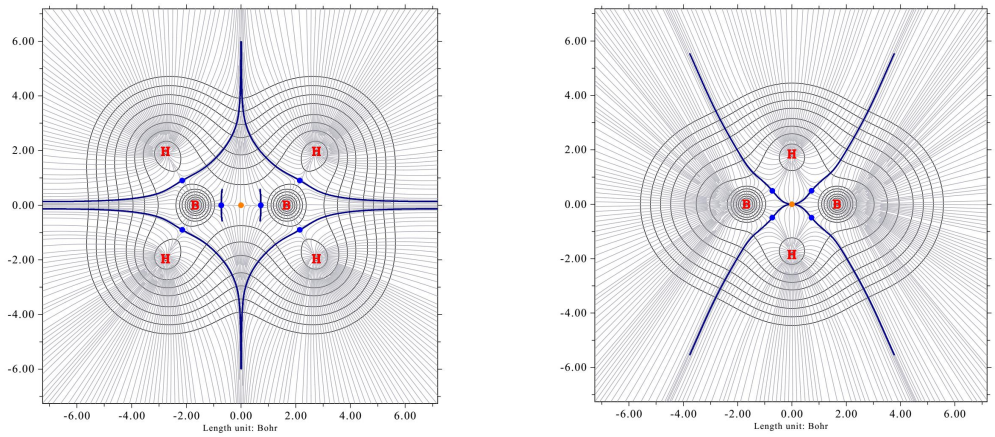
(a) (b)

Figure 1. XY plane(a) and XZ plane(b) ELF plots of B_2H_6



(a) (b)

Figure 2. XY plane(a) and XZ plane(b) LOL plots of B_2H_6



(a) (b)

Figure 3. XY plane(a) and XZ plane(b) of AIM interbasin surface plots of B_2H_6

Figure 3 is a plot of AIM interbasin surface. According to the partition of electron density by AIM basin analysis method, a bold and novel conjecture can be said that, due to the B-H interaction in B-H-B multicenter bond is weak, H atom can be easier to separate. When the H atoms escape from the molecule, the fission will be continued in the unstable surplus structure, until the all of B_2H_6 have been disappeared and the simple hydroboron such as BH_3 and hydroboron compound such as $(BH_3)_n$ will be formed. It is a type of *Jahn-Teller* effect. Notwithstanding, due to the 3-center-2-electron bond is weak, the thermodynamic stability of B_2H_6 has been still maintained. After a long time of storage, B_2H_6 will be changed to H_2 and other hydroboron. It can be studied by dynamics analysis.