A Simple and Precise Interpretation of the Bond Lengths and Angles in Diborane in Terms of Atomic and Ionic Radii

Dedicated to Dmitri Mendeleev (8 Feb.1834- 2 Feb 1907) on his birth anniversary.

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Abstract

Diborane is an unusual molecule with two boron atoms bonded to four terminal hydrogen atoms and two bridging hydrogen atoms. This has puzzled many scientists and gave rise to many theories, with no final definitive explanation. This article brings a simple explanation of the bond lengths and angles in diborane, based on the *additivity* of atomic and Golden ratio based ionic radii, which was found applicable for many other bonds in small as well as small molecules.

Key words: Diborane, BH bonds, HBH angle, Golden ratio based ionic radii, additivity of radii

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Introduction.

Boranes [1a] are boron hydrides of many interesting properties and uses. The studies of these compounds have fetched two Nobel Prizes [2,3]. Diborane, B_2H_6, a colorless highly reactive gas, has been known for more than a century [1b]. This compound has an unusual structure consisting of four terminal and two bridged hydrogen atoms [1-4]. Pauling [4] suggested several resonance forms for this molecule including ionic forms. Fig. 1 is from [2], where the central hydrogens bridging the two boron atoms have been described as 'banana bonds' [1b] and as 'three center two electron bonds' [1a-c].

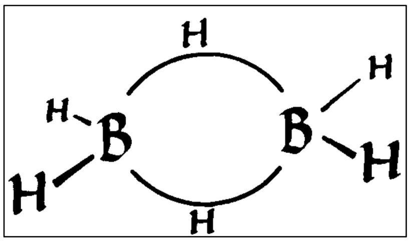

Figure 1. Diborane, from [2]

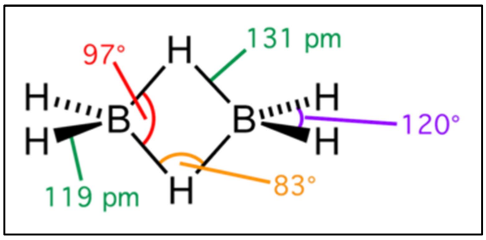

Figure 2. Diborane, from [1b]

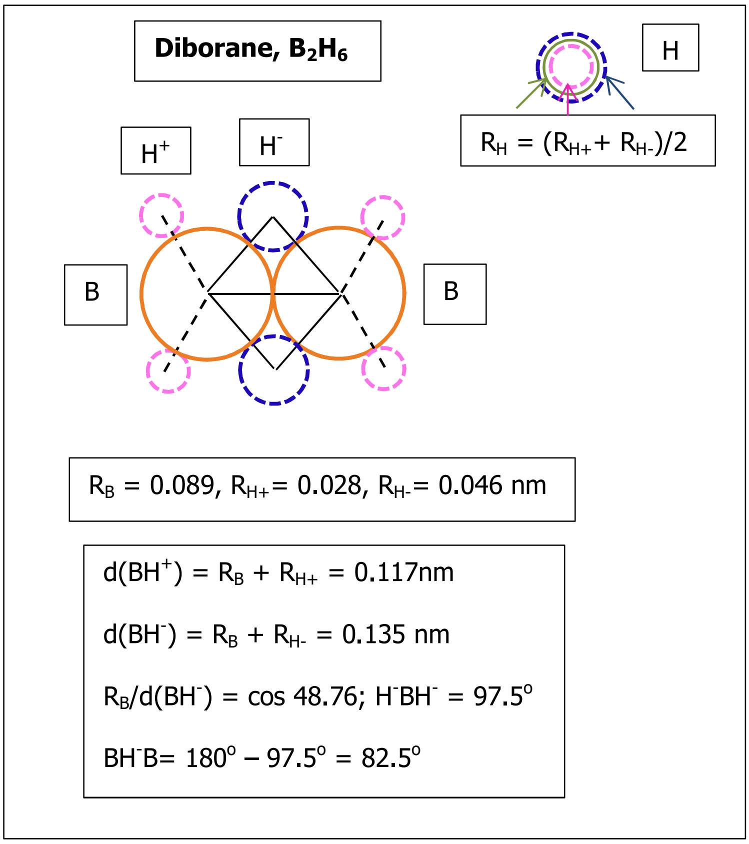

Figure 3. Diborane, this work. See the text for details.

The bond lengths and bond angles in B_2H_6 as given in [1b] can be seen here in Fig. 2. The molecular dimensions as reported by Pauling [4] are four BH bonds of length 0.119 (+/-) 0.003 nm, two BH bonds of length 0.133 (+/-) 0.003 nm and one BB bond of length 0.177 (+/-) 0.001 nm. Although many theoretical attempts have been made, the BH bonds have continued to elude a simple interpretation. Here, the bond lengths and bond angles in Fig. 2, are explained using the covalent single bond radius of boron, $R_B = d(BB)/2$ and the Golden ratio [$\phi = (1 + 5^{1/2})/2$] based radii [5,6] of the cation, R_{H+} (= $d(HH)/\phi^2$) and anion, R_{H-} (= $d(HH)/\phi$) of (the resonance forms[4]) hydrogen [5], where $d(HH) = 2R_H = R_{H+} + R_{H-} = 0.074$ nm is the covalent bond length [4] and $R_H = 0.037$ nm is the covalent radius of H.

Present work.

It was shown earlier [5-8] that chemical bond lengths are exact sums of the appropriate covalent and or ionic radii of the adjacent atoms or ions, in small as well as large molecules. The bond lengths and angles in small molecules like H_{2+}, O_2, O_3, H_2O, SO_2, NO_2 and CO_2 [7] and in those that lead to the formation of ozone [8], as well as in CO_2 related molecules [9], could be interpreted in terms of the atomic and ionic radii. Similarly, this additivity rule shows that the terminal BH bond length is the sum [5,10,11] of the single bond covalent radius, R_B (= 0.089 nm) of B and the Golden ratio based cation radius, R_{H+} (= 0.028 nm) of H^+, and that the length of the BH bridge bond is the sum of the atomic radius, R_B of B and the Golden ratio based anionic radius, R_{H-} (= 0.046 nm) of H^-. The diborane molecule with bond lengths and angles as interpreted here are shown in Fig. 3. The four terminal BH^+ bonds are out of the plane of the paper. Thus, all the six BH bonds are partially ionic The values in the box in Fig. 3 show that their lengths are exact sums of the atomic radius of B atom and the appropriate ionic radii of the adjacent H atom. *Note:* Amongst all the elements in the Periodic Table, boron is the only one, whose covalent single bond radius is equal to its Bohr radius, a_B, obtained from its first ionization potential [12].

The HBH and BHB angles in Fig. 2 are also perfectly accounted for as shown in the box in Fig. 3, as in the case of other molecules [7-9]. Thus, this work gives for the first time, a new, simple and exact interpretation of the bond lengths and angles in diborane.

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