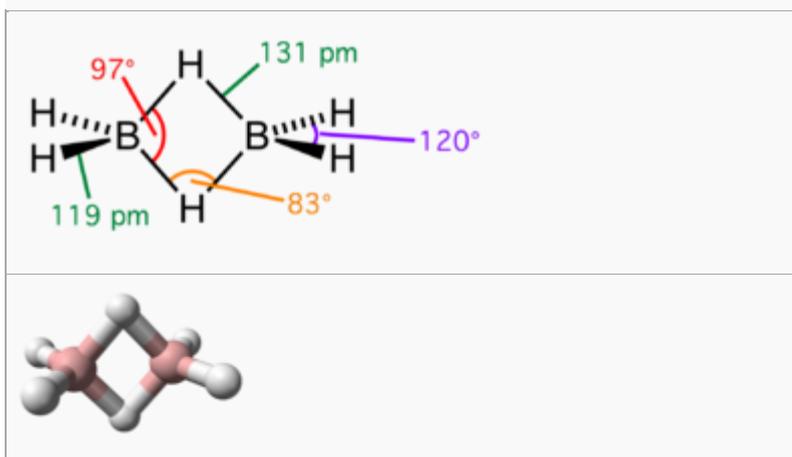


# Diborane

**Diborane** is the chemical compound consisting of boron and hydrogen with the formula  $B_2H_6$ . It is a colourless and highly unstable gas at room temperature with a repulsively sweet odour. Diborane mixes well with air, easily forming explosive mixtures. Diborane will ignite spontaneously in moist air at room temperature. Synonyms include boroethane, boron hydride, and diboron hexahydride.

Diborane is a key boron compound with a variety of applications. The compound is classified as "endothermic", meaning that its heat of formation,  $\Delta H_f^\circ$  is positive (36 kJ/mol). Despite a high thermodynamic instability, diborane is surprisingly nonreactive for kinetic reasons, and it is known to take part in an extensive range of chemical transformations, many of them entailing loss of dihydrogen.

## Diborane

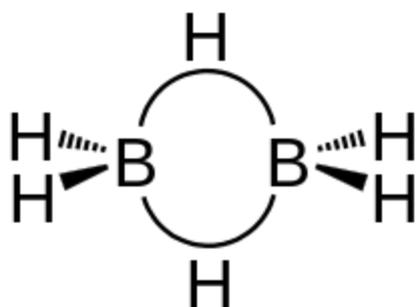


## Structure and bonding

Diborane adopts a  $D_{2h}$  structure containing four terminal and two bridging hydrogen atoms. The model determined by molecular orbital theory indicates that the bonds between boron and the terminal hydrogen atoms are conventional 2-center, 2-electron covalent bonds. The bonding between the boron atoms and the bridging hydrogen atoms is, however, different from that in molecules such as hydrocarbons. Having used two electrons in bonding to the terminal hydrogen atoms, each boron has one valence electron remaining for additional bonding. The bridging hydrogen atoms provide one electron each. Thus the  $B_2H_2$  ring is held together by four electrons, an example of 3-center 2-electron bonding. This type of bond is

sometimes called a 'banana bond'. The lengths of the B-H<sub>bridge</sub> bonds and the B-H<sub>terminal</sub> bonds are 1.33 and 1.19 Å respectively, and this difference in the lengths of these bonds reflects the difference in their strengths, the B-H<sub>bridge</sub> bonds being relatively weaker. The weakness of the B-H<sub>bridge</sub> vs B-H<sub>terminal</sub> bonds is indicated by their vibrational signatures in their infrared spectrum, being ~2100 and 2500 cm<sup>-1</sup>, respectively.<sup>[4]</sup> The structure is isoelectronic with C<sub>2</sub>H<sub>6</sub><sup>2+</sup>, which would arise from the diprotonation of the planar molecule ethene. Diborane is one of many compounds with such unusual bonding.

Of the other elements in Group IIIA, gallium is known to form a similar compound, digallane, Ga<sub>2</sub>H<sub>6</sub>. Aluminium forms a polymeric hydride, (AlH<sub>3</sub>)<sub>n</sub>, although unstable Al<sub>2</sub>H<sub>6</sub> has been isolated in solid hydrogen and is isostructural with diborane.



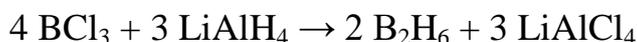
Bonding diagram of **diborane**(B<sub>2</sub>H<sub>6</sub>) showing with curved lines a pair of three-center two-electron bonds, each of which consists of a pair of electrons bonding three atoms, two boron atoms and a hydrogen atom in the middle.

## Production and synthesis[edit]

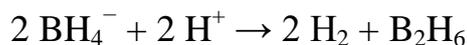
Extensive studies of diborane have led to the development of multiple syntheses. Most preparations entail reactions of hydride donors with boron halides or alkoxides. The industrial synthesis of diborane involves the reduction of BF<sub>3</sub> by sodium hydride, lithium hydride or lithium aluminium hydride



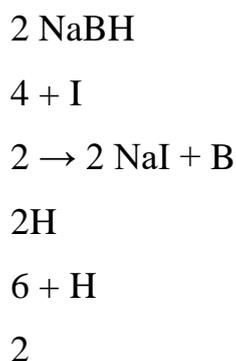
Two laboratory methods start from boron trichloride with lithium aluminium hydride or from boron trifluoride ether solution with sodium borohydride. Both methods result in as much as 30% yield:



Older methods entail the direct reaction of borohydride salts with a non-oxidizing acid, such as phosphoric acid or dilute sulfuric acid.



Similarly, oxidation of borohydride salts has been demonstrated and remains convenient for small scale preparations. For example, using iodine as an oxidizer:

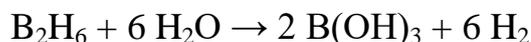


Another small-scale synthesis uses potassium hydroborate and phosphoric

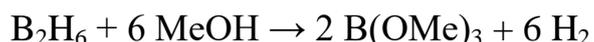
## Reactions

Diborane is a highly reactive and versatile reagent that has a large number of applications. Its dominating reaction pattern involves formation of adducts with Lewis bases. Often such initial adducts proceed rapidly to give other products. It reacts with ammonia to form the diammoniate of diborane, DADB, with lesser quantities of ammonia borane depending on the conditions used. Diborane also reacts readily with alkynes to form substituted alkene products which will readily undergo further addition reactions.

Diborane reacts with water to form hydrogen and boric acid:



Diborane also reacts with methanol to give hydrogen and trimethoxyborate ester:



Treating diborane with sodium amalgam gives  $\text{NaBH}_4$  and  $\text{Na}[\text{B}_3\text{H}_8]$  When diborane is treated with lithium hydride in diethyl ether, Lithium borohydride is formed:



Diborane reacts with anhydrous hydrogen chloride or hydrogen bromide gas to give a boron halohydride:



Reacting diborane with carbon monoxide at 470K and 20bar gives  $\text{H}_3\text{BCO}$ .<sup>[11]</sup>

## Reagent in organic synthesis.

---

Diborane and its variants are central organic synthesis reagents for hydroboration, whereby alkenes add across the B-H bonds to give trialkylboranes. Diborane is used as a reducing agent roughly complementary to the reactivity of lithium aluminium hydride. The compound readily reduces carboxylic acids to the corresponding alcohols, whereas ketones react only sluggishly as starting materials