

# **STRUCTURE AND** **PROPERTIES OF** **BORANES**

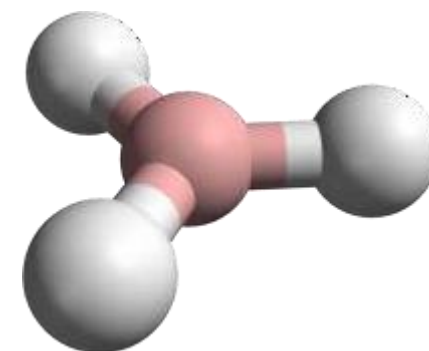
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# CONTENTS

- Introduction
- Boranes
- Diborane
- Types of boranes
- Bonding and structure in boranes
- Carboranes
- Types of carboranes
- Applications

# INTRODUCTION

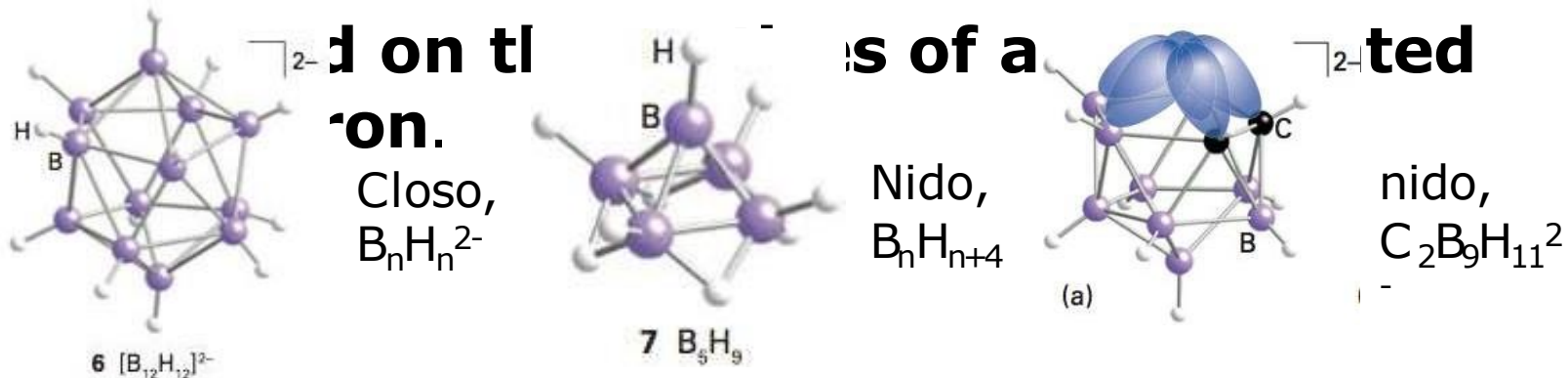
The binary compounds of boron and hydrogen are called boranes. Boranes were first prepared between 1912 and 1936, by Alfred Stock, who developed vacuum line techniques to handle these reactive materials. Boranes are the name to a class of synthetic hydrides of boron. The molecules of these compounds are electron deficient and so reactive with respect to electron donors. Many boranes are synthesised from the thermolysis of  $B_2H_6$ . All boranes are diamagnetic and colourless.



## 1.1 Definitions:

**Borane:** is a chemical compound of boron and hydrogen. Polyhedral boranes are large clusters with more than 6 Boron atoms (usually 6-12).

**Carborane:** are compounds having as the basic structural unit of C and B atoms



## 1.2 Properties:

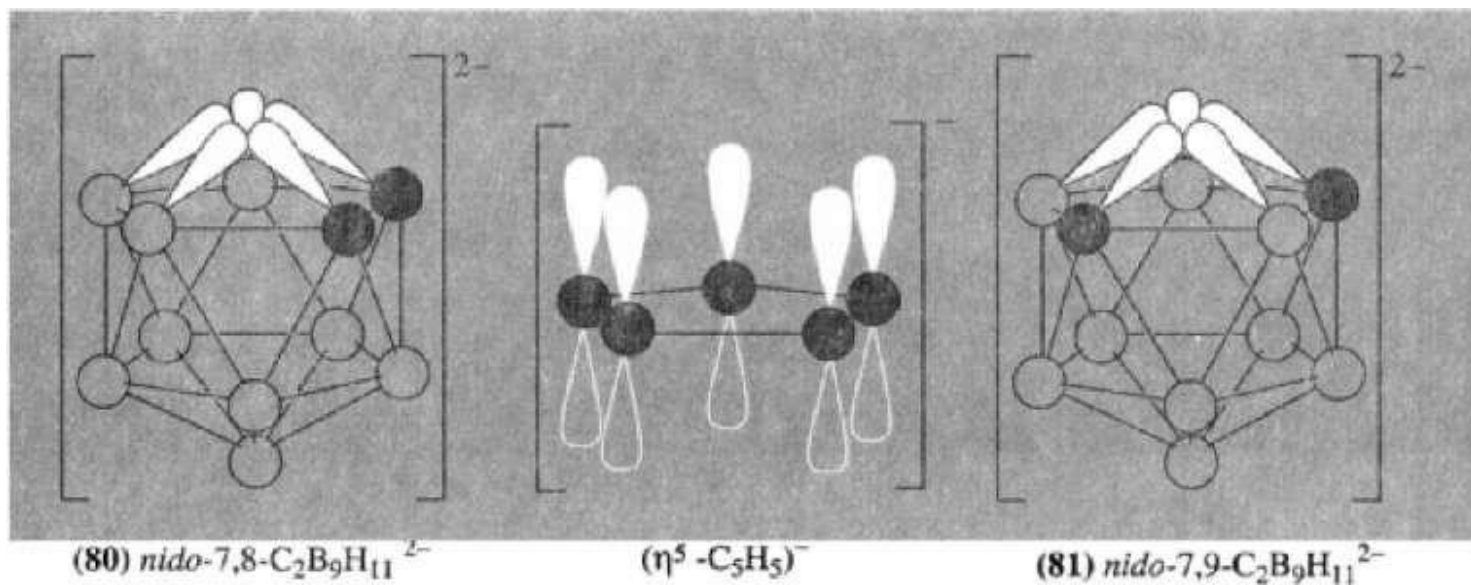
### closo-boranes ( $B_nH_n^{2-}$ ) and closo-carboranes ( $C_2B_{n-2}H_n$ )

their structures resemble their hydrocarbon counterparts (aromatic compounds), 3D aromaticity.

*Stable!*

### nido-boranes and nido-carboranes (nest-like)

without the strict structural limitations, is relatively more reactive

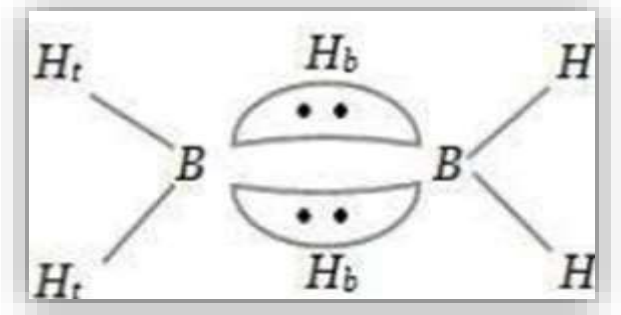
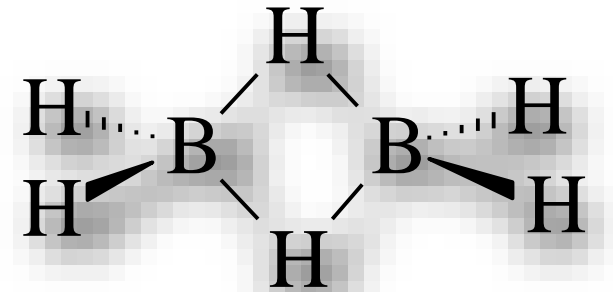


# **BORANES**

- The parent member  $\text{BH}_3$  is called borane, is found only in the gaseous state, and dimerizes to form diborane,  $\text{B}_2\text{H}_6$ .
- General formula of boranes is  $\text{B}_x\text{H}_y$
- The most important boranes are diborane  $\text{B}_2\text{H}_6$ , pentaborane  $\text{B}_5\text{H}_9$ , and decaborane  $\text{B}_{10}\text{H}_{14}$ .
- Boranes are all colourless and diamagnetic, And some are **pyrophoric**.
- Boranes are highly reactive.
- Common reactions with boranes are: electrophilic substitution, nucleophilic substitution by Lewis bases, deprotonation by strong bases, cluster building reactions with borohydrides, and reaction of a nido-borane with an alkyne to give a carborane cluster.

# DIBORANE

- Diborane is simplest and most studied of boranes. It is an electron deficient molecule .
- It has less number of valence electrons than the number required to form all the electron pair bond in its structure. 2 hydrogen bridges are present.
- The model determined by MOT indicates that the bond between boron & terminal hydrogen atoms are conventional 2c-2e electron bonds.
- Having used 2 electrons in bonding to terminal hydrogen atoms. Each boron has one valence e- remain for additional bonding. The bridging hydrogen provides an electron each. Thus  $B_2H_2$  ring is held together by 4 electrons.



# ❖ BONDING AND STRUCTURE IN DIBORANE

▪ The diborane molecule has 2 type of bonds.

- 1. four terminal (2c-2e) B-H bonds.
- 2. two bridged (3c-2e) B-H-B bonds.

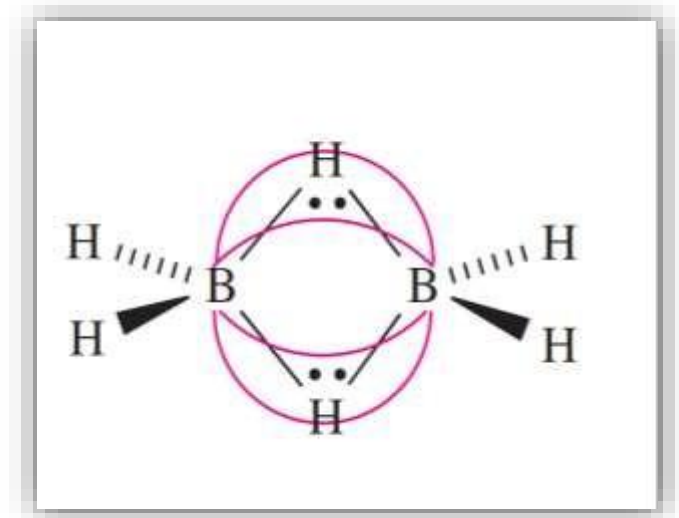
• 1. four terminal (2c-2e) B-H bonds.

Each of these bonds are formed by sharing of 2 electrons between boron and terminal hydrogen atoms. It's a normal  $\sigma$  covalent bond.

• 2. two bridged (3c-2e) B-H-B bonds.

Each of these bond is formed by sharing of 2 electrons between 2 B and 1 H atoms .

• It is also called as **banana bond**

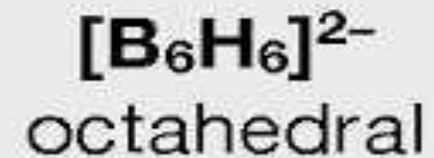
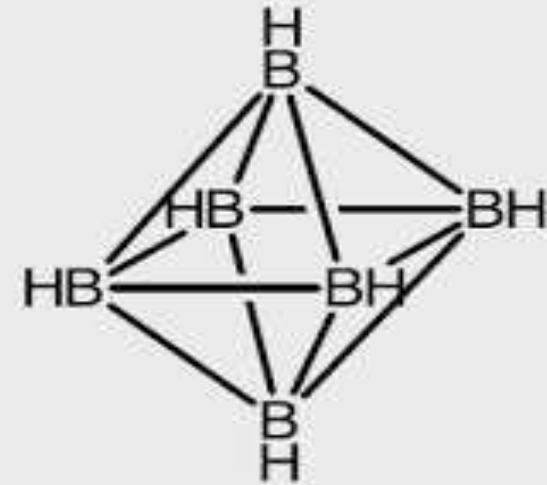




# ❖ TYPES OF BORANES

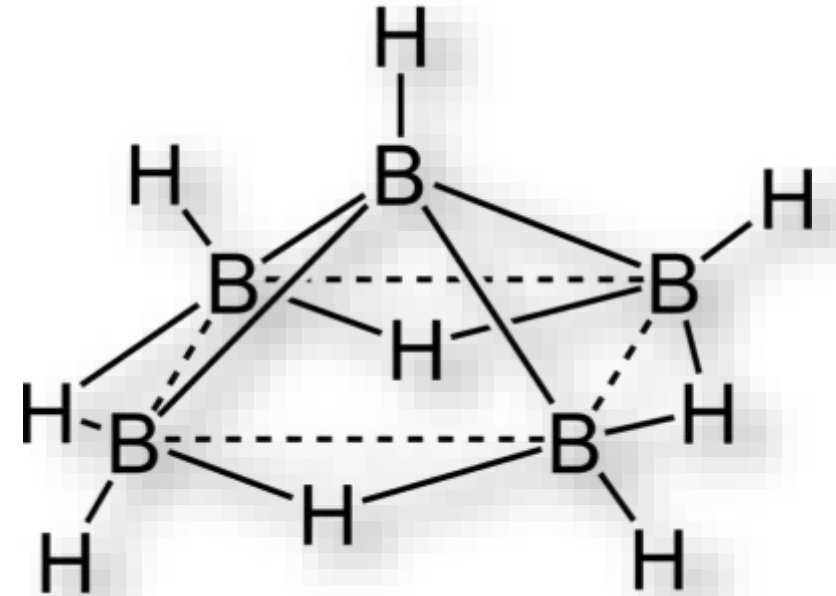
## ➤ CLOSO BORANES

- ❑ Closed, triangulated polyhedra structure.
- ❑ All corners of triangulated polyhedra are occupied.
- ❑ General formula:  $B_nH_{n+2}$ ,
- ❑ Example:  $[B_6H_6]^{2-}$



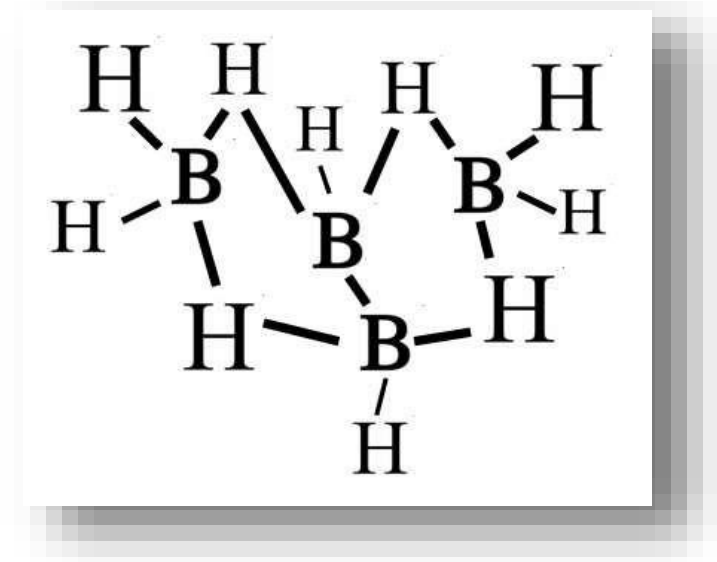
## ➤ NIDO BORANES

- ❑ nido boranes are formed when one corner of the polyhedra is removed.
- ❑ nest like, non-closed structure
- ❑ General formula:  $B_nH_{n+4}$ ,
- ❑ Example:  $B_5H_9$ ,  $B_2H_6$



## ➤ ARACHNO BORANES

- ❑ These boranes are formed when two corners of the polyhedra is removed .
- ❑ Web like ,non-closed polyhedra structure
- ❑ General formula:  $B_nH_{n+6}$ ,
- ❑ Example:  $[B_4H_{10}]$



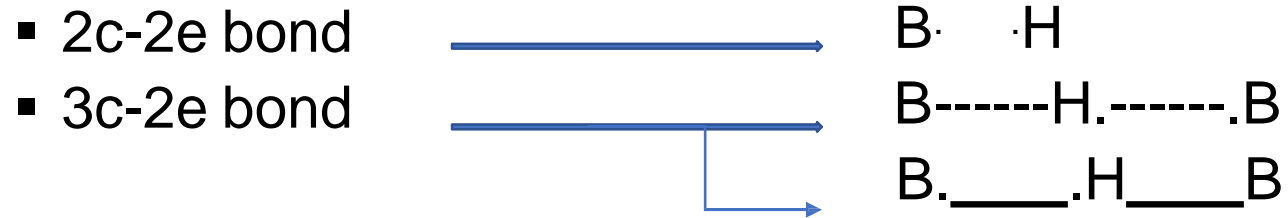
## ➤ HYPOBORANES

- ❑ Hypo- net like
- ❑ These have most open clusters in which Boron atoms occupy n corners of (n+3) polyhedron
- ❑ General formula:  $B_nH_{n+8}$
- ❑ these boranes are having complex structures.
- ❑ Example :  $B_8H_{16}$  and  $B_{10}H_{18}$

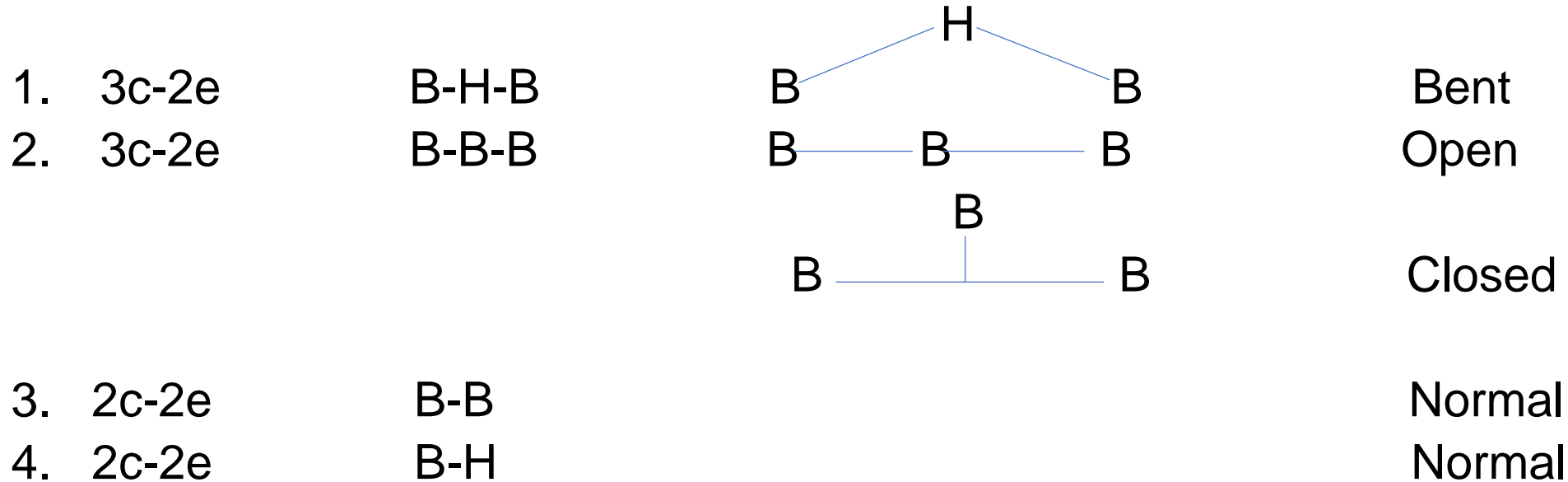
## ➤ CONUCTO BORANES

- ❑ These boranes formed by linking of 2 or more of any other type of boranes.
- ❑ These structures are very complex
- ❑ General formula :  $B_nH_m$
- ❑ Example:  $(B_5H_9)_2$ ,  $(B_4H_{10})_2$

# ❖ BONDING IN BORANES



□ In boranes 4 types of bonds are present



## ❖ STYX CODES

The over all boranes bonding can be represented by 4 digital numbers

S = number of B-H-B bonds (1<sup>st</sup> digit)

T = number of B-B-B bonds (2<sup>nd</sup> digit)

Y = number of B-B bond (3<sup>rd</sup> digit)

X = number of B-H<sub>2</sub> groups (4<sup>th</sup> digit)

Ex: B<sub>2</sub>H<sub>6</sub> (Diborane)

S = number of B-H-B bonds = 2

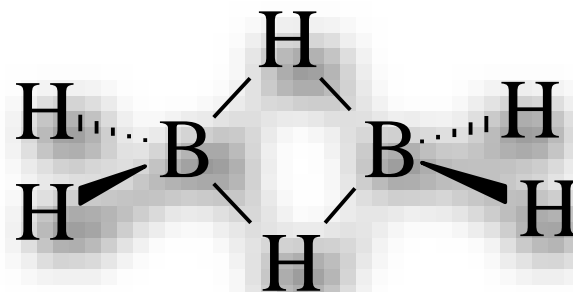
T = number of B-B-B bonds = 0

Y = number of B-B bond = 0

X = number of B-H<sub>2</sub> groups = 2

Hence for diborane styx code is 2002.

Example – B<sub>4</sub>H<sub>10</sub> styx code is 4012



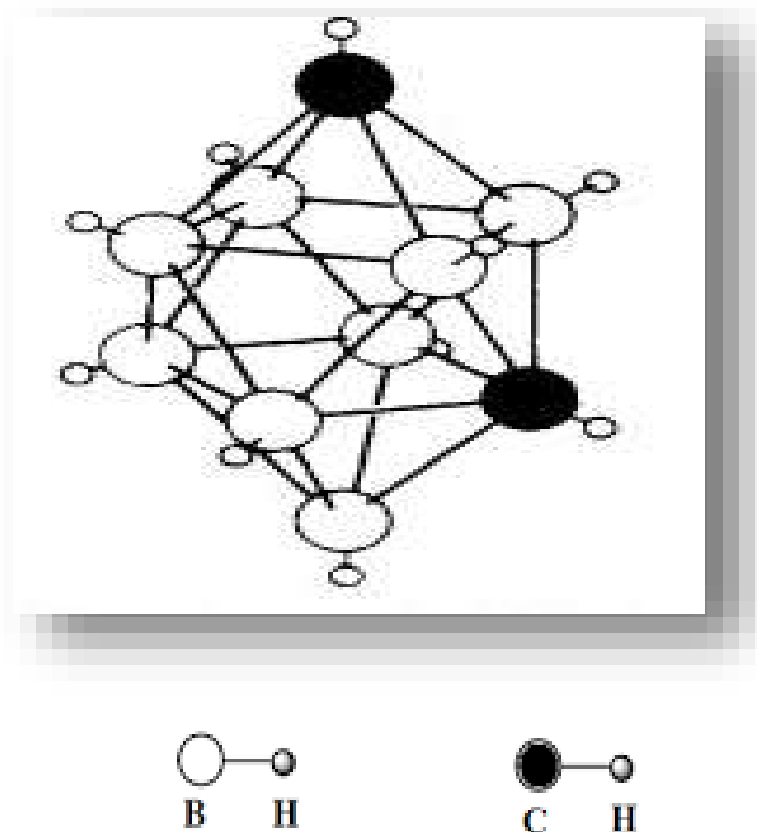
# CARBORANES

- Carboranes are mixed hydrides of boron and carbon in which carbon and boron atoms occupy the vertices of triangulated polyhedron.
- Carboranes are most important heteroboranes.
- Carboranes are member of a class of organometallic compounds containing carbon (C), boron (B), and hydrogen (H).
- General formula of carboranes is  $C_2B_nH_{n+m}$ , where n is an integer
- carboranes with n ranging from 3 to 10 have been characterized.
- Boranes and carboranes have same number of electrons in their bonding framework , will have similar structure.

# ❖ TYPES OF CARBORANES

## ➤ CLOSO CARBORANES

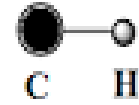
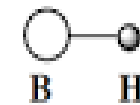
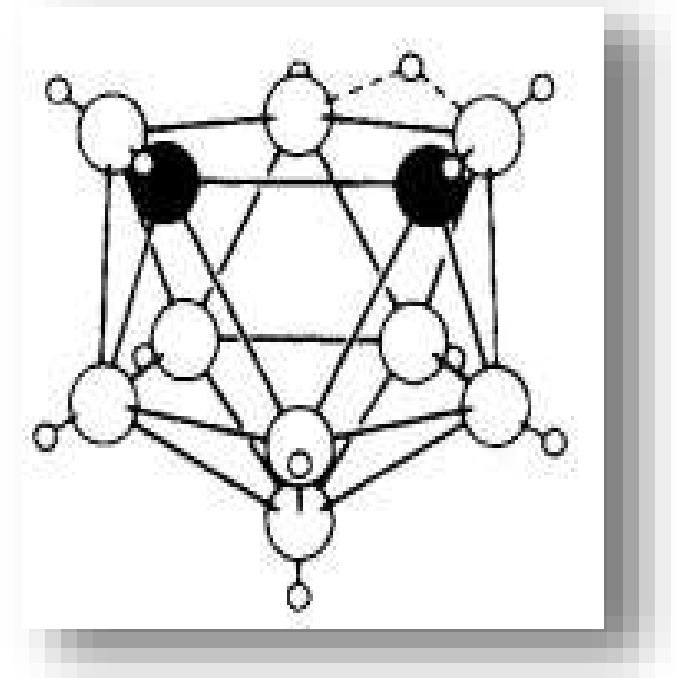
- ❑ Closed, triangulated polyhedra structure.
- ❑ General formula:  $C_2B_nH_{n+2}$ ,
- ❑ Total number of electron in bonding framework is  $(2n+2)e^-$ . i.e.  $(n+1)$  e pairs.
- ❑ Example-1,6- $C_2B_8H_{10}$





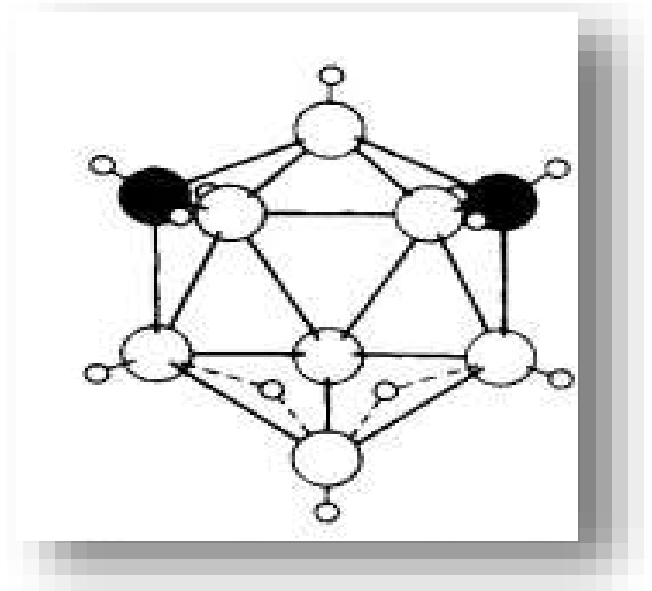
## ➤ NIDO CARBORANES

- ❑ One corner of triangulated polyhedra is removed
- ❑ General formula:  $C_2B_nH_{n+4}$ ,
- ❑ Total number of electron in bonding framework is  $(2n+4)e^-$ . i.e.  $(n+2) e^-$  pairs.
- ❑ Example-  $C_2B_4H_8$ ,  $[1,7-C_2B_9H_{12}]^-$



## ➤ ARACHNO CARBORANES

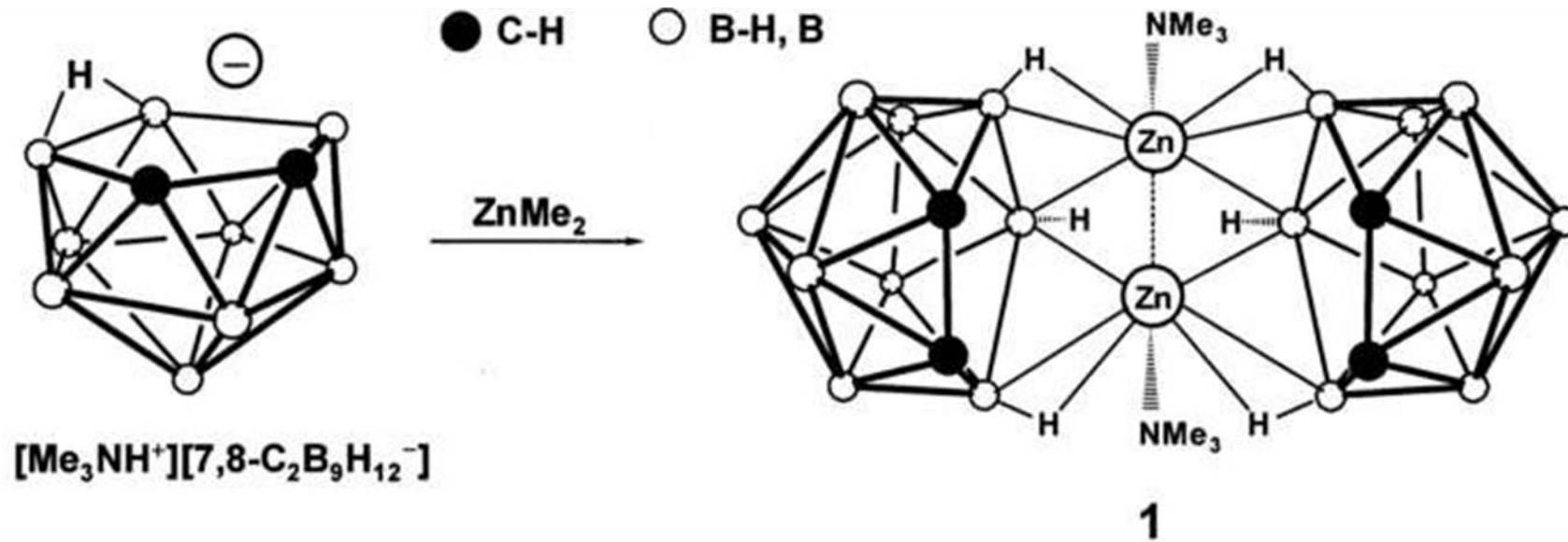
- Two corners of triangulated polyhedra is removed.
- General formula:  $C_2B_nH_{n+6}$ ,
- Total number of electron in bonding framework is  $(2n+6)e^-$ . i.e.  $(n+4) e^-$  pairs.
- Example- 1,3- $C_2B_7H_{13}$



# ❖ APPLICATIONS OF BORANES AND CARBORANES

- Boranes are used as rocket fuels in supersonic aeroplanes.
- Used as catalyst in polymerisation reaction
- Used as reducing agent in organic reactions
- Boranes can be used as vulcanising agent for natural and synthetic rubber.
- Used in borane coating

## 2.3 some good examples



1. Highly planar
2. Zn<sub>2</sub>B<sub>2</sub> diamond-like structure
- 3. Weak Zn-Zn bond**

## ❖ CONCLUSION

- Boranes are colourless and gaseous at room temperatures.
- Boranes are highly reactive and reacts violently with water.
- In boranes 3c-2e bonds are present; It is unique type of bond present in boranes only.
- Carboranes are mixed hydrides of boron and carbon. And have same structure like boranes.
- Carboranes derived from pyrolysis of boranes

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THANK YOU

