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Class — B.Sc. part III
Subject - chemistry
Paper - VI
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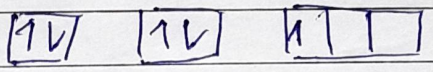
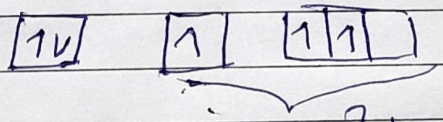
Inorganic chains, Rings, cages and clusters continued.

STRUCTURE OF DIBORANE — Diborane is an electron deficient compound, there is not enough valence electrons to form the expected number of covalent bonds. The atomic number of boron is five and hence its electronic configuration is:

B_5 — $1s^2\ 2s^2\ 2p^1$



B^* —



sp^3 hybridisation.

In diborane molecule each boron atom in the excited state has initial uncoupling of the paired 2S electrons and promotion of one of the 2S electrons to 2py orbitals. Then there are three unpaired electrons. Boron shows sp^3 hybridisation, due

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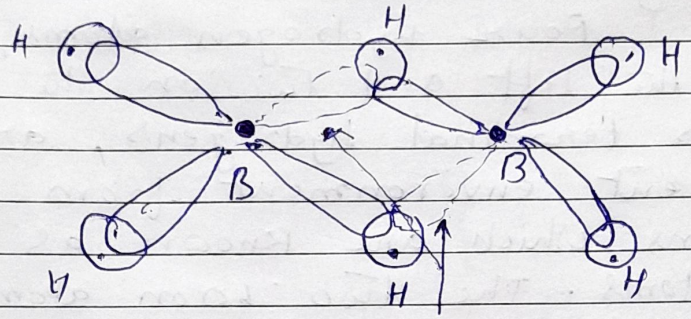
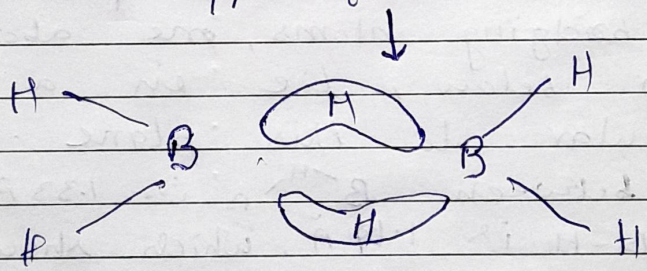
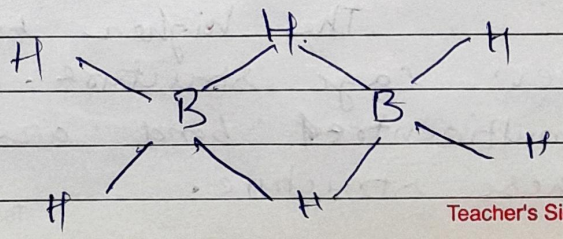
to availability of only three electrons out four sp^3 hybrid orbitals one sp^3 hybrid orbital is empty.

In diborane formation, 1S orbital of a bridging hydrogen atom is overlapping with two sp^3 hybrid orbitals, one from each boron atom to form a three centre bond containg one pair of electrons but hold all the three nuclei, i.e B – H – B.



Overlappin of atomic orbitals.





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In diborane there are six hydrogen atoms. Two hydrogen atoms are used for the formation of two three centred bonds whereas remaining four hydrogen atoms are joined two boron atoms. Two sp^3 hybrid orbitals of each boron atom overlap with 1s orbitals of two hydrogen atoms forming two sigma (σ) bonds. The orientation of four hydrogen atoms about each boron atom is approximetly tetrahedral.

Four hydrogen atoms, two on the left and two on the right, known as terminal hydrogens, are in different environment from other two atoms which are known as the bridging atoms. The two boron atoms and the four terminal hydrogen atoms lie in the same plane while the two bridging atoms, one above and the other below, lie in a plane perpendicular to this plane. Bond length between B-H-B is 1.33 Å and between B-H is 1.19 Å which shows that electron deficiency is associated with the bridge atoms.

The higher boran have an open cage structure. Both normal and multicentred bond are present in these structure.

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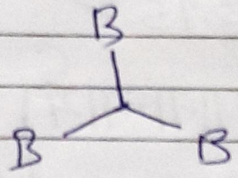
i) ~~one~~ Terminal B-H bonds i.e (2c-2e) bonds or two centre two electron bonds.

ii) B-B bonds - Normal covalent bond two centre two electron bond.

iii) B···H···B bond - Three centre bridge bonds including 3c-2e bonds.

iv) B···B···B - Three centre bridging bonds, similar to hydrogen bond. These are called open boron bridge bonds and are the type 3c-2e

v) Closed 3c-2e bonds between three Boron atoms.



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