class – U.G. Semester – V

Subject – chemistry

Paper – MIC-V

unit – II

Topic – Structure of Borazine

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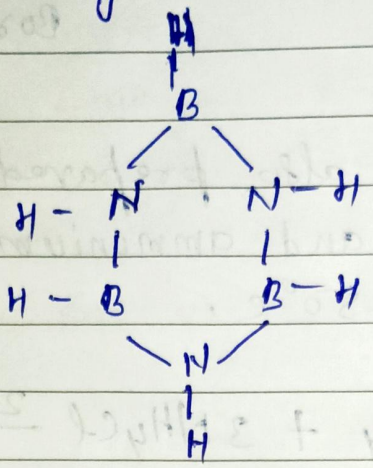
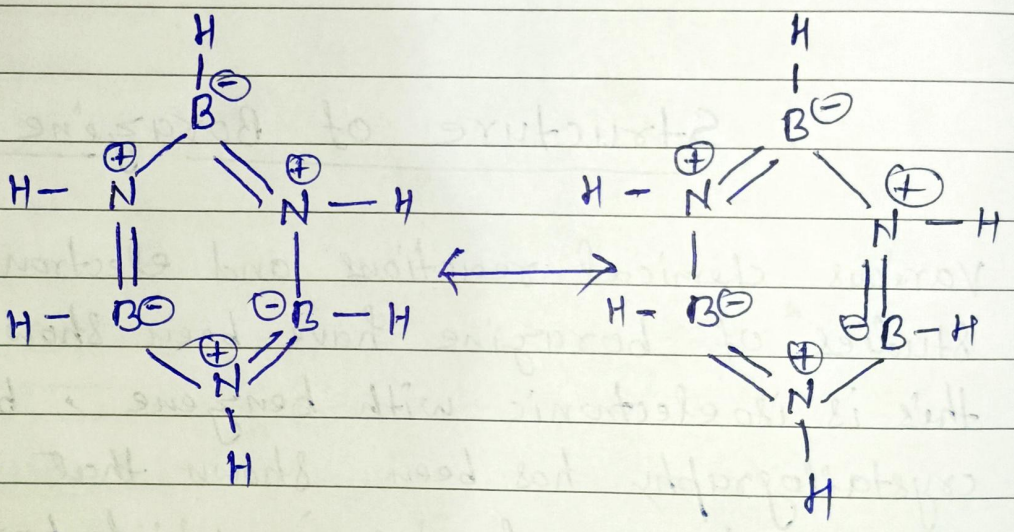
Structure of Borazine

Various chemical reactions and electron diffraction studies of borazine have been shown that this is isoelectronic with benzene, but X-ray crystallography has been shown that this is a planar, hexagonal ring in which boron and nitrogen atoms are arranged alternatively. The Boron-nitrogen bond length is $1.47 \pm 0.0007\ A^\circ$, while the calculated single B-N and double B=N bond lengths are $1.54\ A^\circ$ and $1.36\ A^\circ$ respectively. The bond angles are equal to 120°. These facts are in accordance with the

hexagonal ring structure :



The resonating structures of borazine may be represented as given below :-



Since borazine is isoelectronic with benzene hence both borazine and benzene have aromatic π-clouds of electron density which is de-localized over the atoms of the ring. In borazine B-N bond is polar ($B^{+\delta}-N^{-\delta}$) due to the difference in electronegativity between

boron and nitrogen while in benzene C-C bond is non-polar due to same carbon atoms. In borazine π-cloud is more concentrated or localised on nitrogen atom. Due to this π-bonding becomes weaker in the ring and polar species like HCl can attack this double bond between nitrogen and boron. All the B and N atoms in borazine exhibit sp^2 hybridisation to form six B-N σ bonds. Three B-N π bonds are formed by the sidewise overlaping of the unhybridised p-orbital of B and N atoms which are perpendicular to the plane of the ring. Molecular orbital calculation indicate the partially delocalization of π-electrons. These calculation have been shown that N to B π-electron drift is largely counterbalanced by B to N σ-electrons drift due to greater electronegativity of N. The π bonding stabelizes the planar structure of borazine ring.