

SUBJECT - CHEMISTRY
 CLASS - B.Sc (Hons) PART-III
 PAPER - V
 TOPIC - The nmr spectrum
 Dr. Harsi Mohan pd Singh
 Department of Chemistry
 Dr. L.K.V.D College Tarpur Sarmaustapur

Q Discuss The nmr spectrum of
 (i) XeF₂ (ii) XeF₄ (iii) ClF₃

Ans (i) The nmr spectrum of XeF₂:

Total valence electrons = 8 + (7 × 2) = 22

Bonding electron = (3 - 1) × 8 = 16

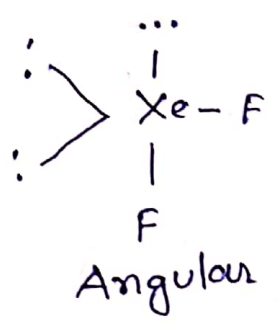
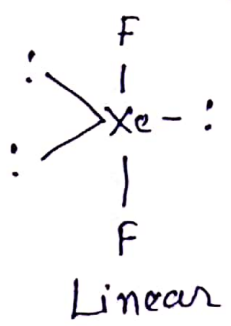
Lone pairs = $\frac{22 - 16}{2} = 3$

Total orbitals mixed = (3 - 1) + 3 = 5

Hybridisation = sp³d

Structure = Trigonal bipyramid

The arrangement of two F atom in trigonal bipyramidal structure can give rise to two shapes of XeF₂ - linear and angular.



The nmr spectrum of XeF₂ shows only one peak. This corresponds to its linear shape. In case of the angular shape of XeF₂, two peaks are expected because the each F-atom is in different environment (or planes).

(ii) The nmr spectrum of XeF_4 :

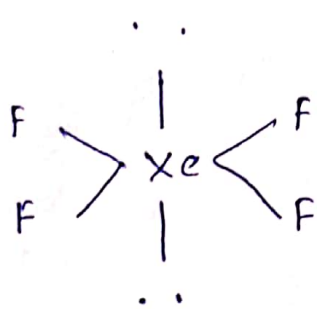
$$\text{Total valence electron} = 8 + (7 \times 4) = 36$$

$$\text{Bonding electron} = (5-1) \times 8 = 32$$

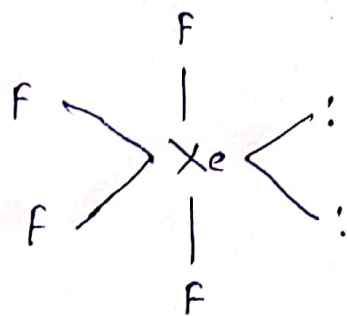
$$\text{Lone pairs} = \frac{36-32}{2} = 2 \quad \text{Total orbitals mixed } (5-1)+2=6$$

Hybridisation = sp^3d^2 Structure = Octahedral

The arrangement of four F atoms in octahedral structure may lead to square planar or other non-square planar shapes. Since the nmr spectrum of XeF_4 shows only one peak, therefore the shape of XeF_4 is square planar.



Square Planar



and other

Non-square planar shapes

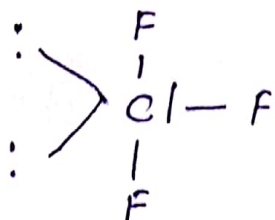
(iii) The nmr spectrum of ClF_3 :

$$\text{Total valence electron} = 7 + (7 \times 3) = 28$$

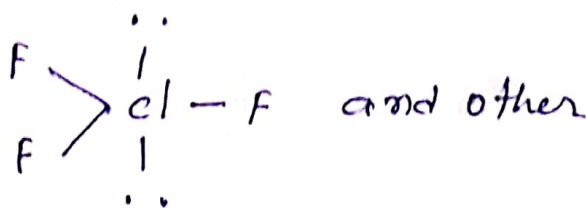
$$\text{Bonding electrons} = (4-1) \times 8 = 24$$

$$\text{Lone pairs} = \frac{28-24}{2} = 2 \quad \text{Total orbitals mixed } (4-1)+2=5$$

Hybridisation = sp^3d Structure = Trigonal bipyramidal



T-shape



Trigonal plane shape