

### 4.6.1. Types of hybridisation

There are many types of hybridisations. The three major types of hybridisation are  $sp^3$ ,  $sp^2$  and  $sp$ . The process of mixing up of one 's' orbital and three 'p' orbitals to get four orbitals of equivalent energy, which are directed to the four corners of a regular tetrahedron is called  $sp^3$  hybridisation. The process of mixing up of one 's' orbital with two 'p' orbital to form three equivalent orbitals which are coplanar is called  $sp^2$  hybrid orbitals. The bond angle is  $120^\circ$ . The process of mixing up of one 's' orbital and one p orbital to get two orbitals of same energy which are directed along a line is called  $sp$  hybridisation. The bond angle is  $180^\circ$ .

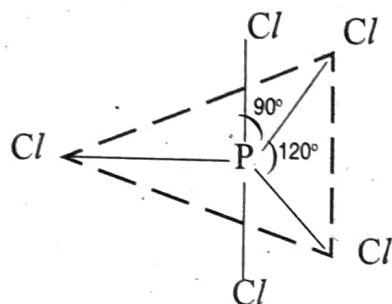
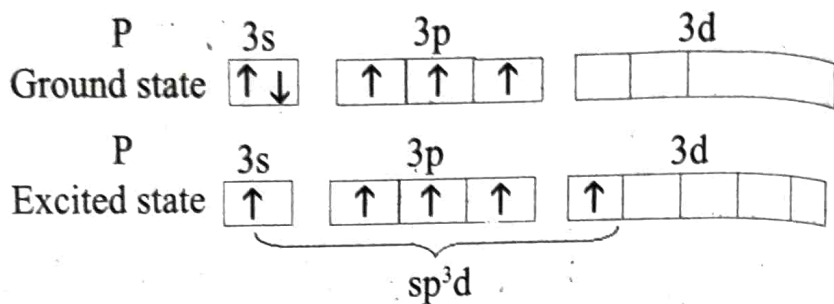
### 4.6.2. Other examples of $sp^3$ , $sp^2$ and $sp$ hybridisation

- **$sp^3$  Hybridisation in  $C_2H_6$  molecule:** In ethane molecule both the carbon atoms assume  $sp^3$  hybrid state. One of the four  $sp^3$  hybrid orbitals of carbon atom overlaps axially with similar orbitals of other atom to form  $sp^3-sp^3$  sigma bond while the other three hybrid orbitals of each carbon atom are used in forming  $sp^3-s$  sigma bonds with hydrogen atoms.
- **$sp^2$  Hybridisation in  $C_2H_4$ :** In the formation of ethene molecule, one of the  $sp^2$  hybrid orbitals of carbon atom overlaps axially with  $sp^2$  hybridised orbital of another carbon atom to form C-C sigma bond.
- **$sp$  Hybridisation in  $C_2H_2$ :** In the formation of ethyne molecule, both the carbon atoms undergo  $sp$ -hybridisation having two unhybridised orbital i.e.,  $2p_y$  and  $2p_x$ .

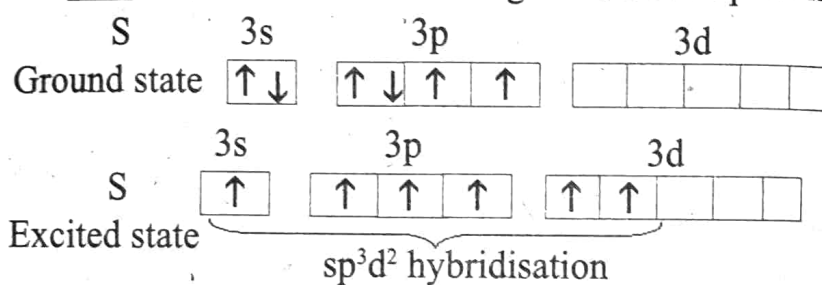
### 4.6.3. Hybridisation of elements involving d-orbitals

**$sp^3d$  hybridisation:** In  $PCl_5$ , the hybridisation of P is  $sp^3d$ . It involves the intermixing of one s - orbital,

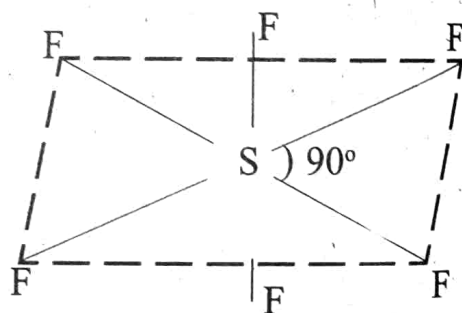
three p - orbitals and one d - orbital to form five hybridised orbitals of equal energy and identical shape. These five hybrid orbitals will overlap with the half filled 3p orbitals of five chlorine atoms. Thus, the shape of  $\text{PCl}_5$  is trigonal bipyramidal.



**sp<sup>3</sup>d<sup>2</sup> hybridisation:** Sulphur in  $\text{SF}_6$  exhibits sp<sup>3</sup>d<sup>2</sup> hybridisation. The electronic configuration of sulphur is,



This hybridisation involves the mixing of one s - orbital, three p - orbitals, and two d - orbitals to form six hybridised orbitals, directed towards the six corners of an octahedron.



**dsp<sup>2</sup> and d<sup>2</sup>sp<sup>3</sup> hybridisation:** In the case of dsp<sup>2</sup> hybridisation there is the intermixing of one s-orbital, two p -orbitals and one d -orbital of the inner shell to form four hybridised orbitals having equal energy and identical shape. These hybridised orbitals are directed to the corners of a square. e.g.  $[\text{Ni}(\text{CN})_4]^{2-}$  d<sup>2</sup>sp<sup>3</sup> hybridisation involves the intermixing of two d-orbitals in the inner shell, one s-orbital and three p-orbitals to give six hybridised orbitals of equal energy and identical shape, directed towards the corners of a regular octahedron. These vacant hybridised orbitals will overlap with the filled orbitals of  $\text{NH}_3$  in  $[\text{Co}(\text{NH}_3)_6]^{3+}$ .



## 4.7. Molecular Orbital Theory

MO theory was put forward by Hund and Mulliken. The main postulates are as follows.

- (i) In molecules, the electrons are present in a special type of orbitals called molecular orbitals.
- (ii) Molecular orbitals are formed by the combination of atomic orbitals of nearly same energy and proper symmetry.
- (iii) Molecular orbitals are associated with the nuclei of all the atoms in the molecule.
- (iv) The number of molecular orbitals formed is equal to the number of combining atomic orbitals.
- (v) The molecular orbitals are also filled in accordance with Pauli's exclusion principle, Hund's rule and Aufbau principle.



*Hund and Mulliken proposed the molecular orbital theory.*