3. XeF₆

a. Preparation

1. By heating mixture of xenon and fluorine in molecular ratio of 1:20 at 250°C- 300°C in a sealed Ni tube under pressure of 50-60 atm.

$$Xe + 3F_2 \longrightarrow XeF_6$$

2. By reacting XeF_4 and F_2 under pressure.

$$XeF_4 + F_2 \longrightarrow XeF_6$$

b. Properties

Colourless crystalline solid with melting point 49.5°C.

1. It is reduced to Xe by the action of H₂ and NH₃ or HCl

$$XeF_6 + 3H_2 \longrightarrow Xe + 6HF$$
 $XeF_6 + 8NH_3 \longrightarrow Xe + 6NH_4F + N_2$
 $XeF_6 + 6HCl \longrightarrow Xe + 3Cl_2 + 6HF$

2. It undergoes slow hydrolysis producing XeO₃

$$XeF_6 + H_2O \longrightarrow XeO_3 + 6HF$$

3. It reacts explosively with SiO₂ giving XeO₃

$$2 \text{ XeF}_4 + \text{SiO}_2$$
 $2 \text{ XeOF}_4 + \text{SiF}_4$
 $2 \text{XeO}_4 + \text{SiO}_2$ $2 \text{ XeO}_2\text{F}_4 + \text{SiF}_4$
 $2 \text{XeO}_2\text{F}_4 + \text{SiO}_2$ 2 XeO_3 $+ \text{SiF}_4$

c. Structure and Bonding

In the formation of XeF₆ molecule, three of the 5p electrons in Xe are assumed to shift to the 5d orbitals so that there are six unpaired electrons in the excited state of Xe. One 5s, three 5p and three 5d orbitals hybridise to give seven sp³d³ hybrid orbitals. Six of the sp³d³ hybrid orbitals containing single electron overlap with the half-filled p orbitals of the six fluorine atoms forming six Xe----F bonds and seventh hybrid orbital accommodates a lone pair of electrons. The molecule has distorted octahedral structure in which all the six positions are occupied by fluorine atoms and lone pair is present at the centre of one of the triangular faces.

