

### **What is clathrate compound give example?**

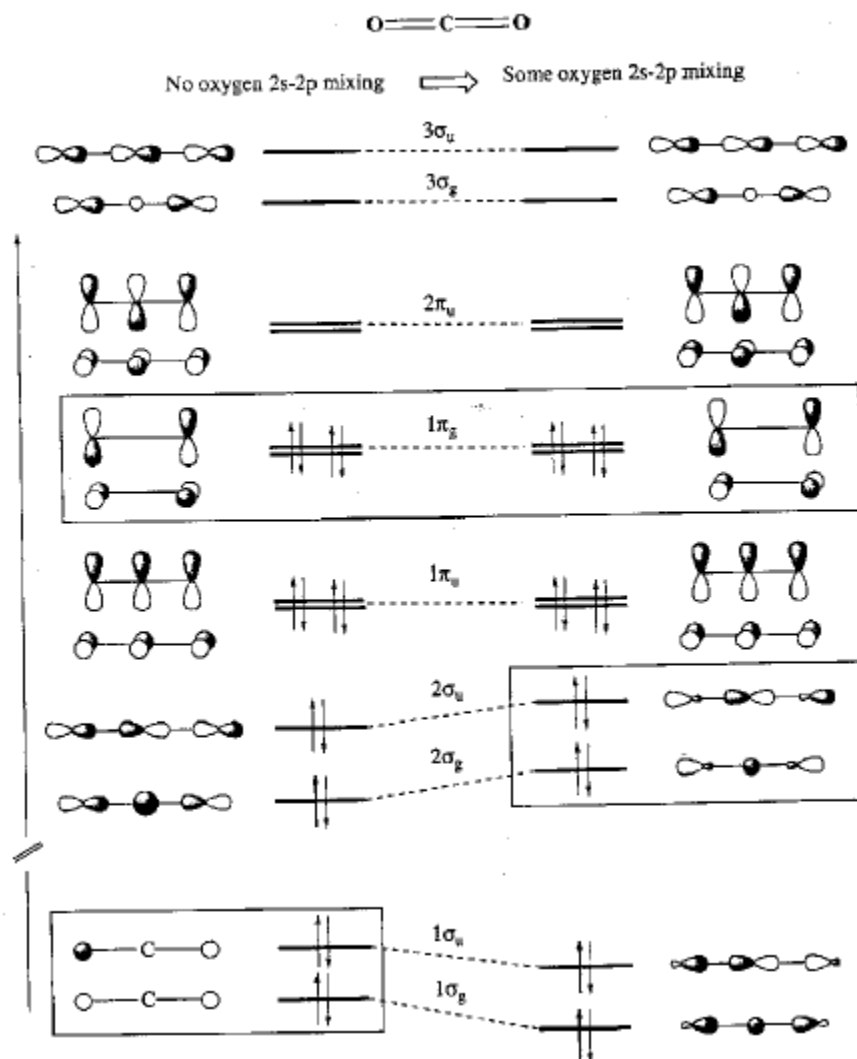
**clathrate** A **compound** in which molecules of one substance, commonly a noble gas, are completely enclosed within the crystal structure of another substance. Typical **examples** are Kr and Xe encapsulated in zeolite structures, or Ar, Kr, and Xe trapped in water ice.

**Clathrate hydrates**, or **gas clathrates**, **gas hydrates**, **clathrates**, **hydrates**, etc., are crystalline water-based solids physically resembling ice, in which small non-polar molecules (typically gases) or polar molecules with large hydrophobic moieties are trapped inside "cages" of hydrogen bonded, frozen water molecules. In other words, clathrate hydrates are clathrate compounds in which the host molecule is water and the guest molecule is typically a gas or liquid. Without the support of the trapped molecules, the lattice structure of hydrate clathrates would collapse into conventional ice crystal structure or liquid water. Most low molecular weight gases, including O<sub>2</sub>, H<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S, Ar, Kr, and Xe, as well as some higher hydrocarbons and freons, will form hydrates at suitable temperatures and pressures. Clathrate hydrates are not officially chemical compounds, as the sequestered molecules are never bonded to the lattice. The formation and decomposition of clathrate hydrates are first order phase transitions, not chemical reactions. Their detailed formation and decomposition mechanisms on a molecular level are still not well understood. Clathrate hydrates were first documented in 1810 by Humphry Davy who found that water was a primary component of what was earlier thought to be solidified chlorine

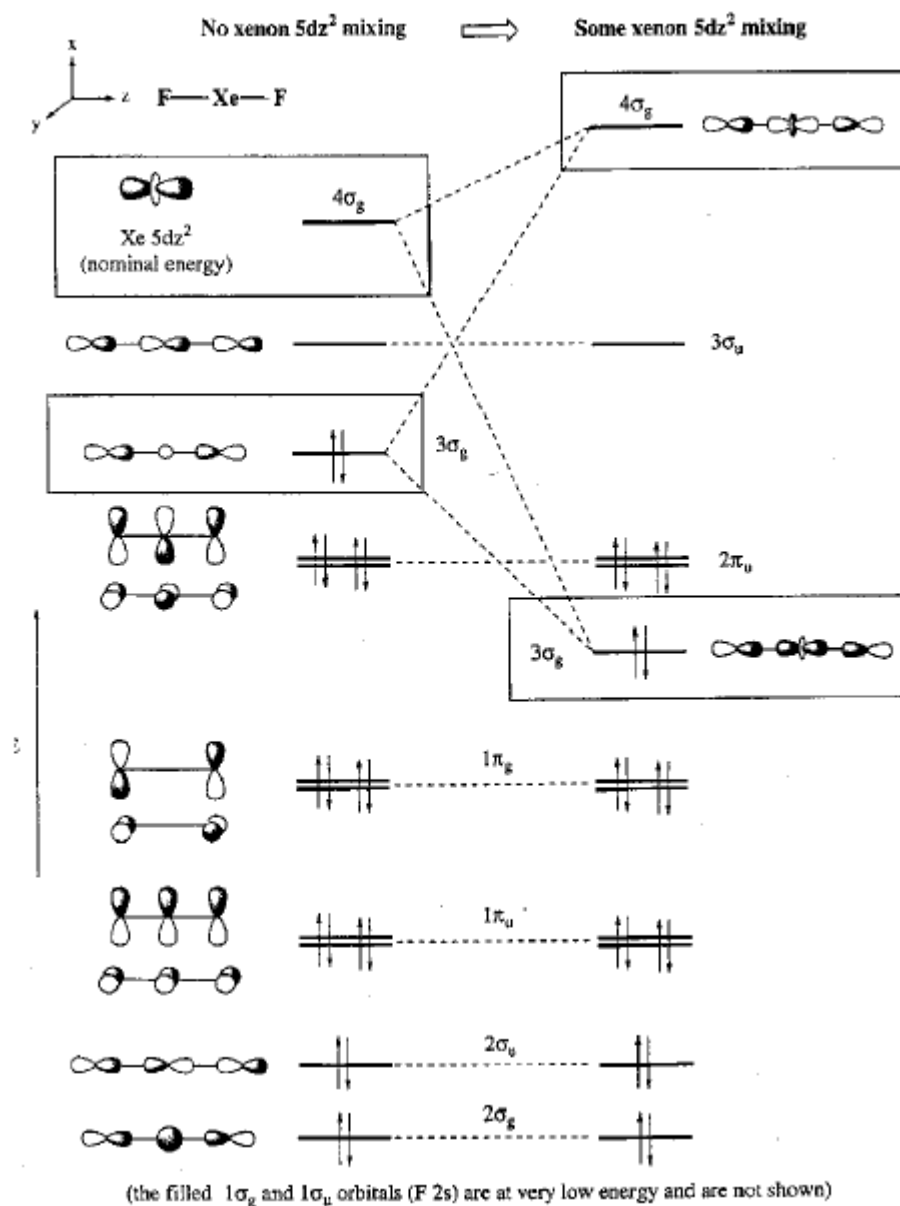
**Clathrates** (also known as cage compounds) are compounds of **noble gases** in which they are trapped within cavities of crystal lattices of certain organic and inorganic substances. The stable electronic configuration of the **noble gases** probably restricted the attempts to prepare chemical compounds of the elements.

### ***Bonding in XeF<sub>2</sub>***

This is one of the simplest examples of a post-transition metal hypervalent compound. Xe atoms have 8 valence electrons in 5s and 6p orbitals (full octet) while each of the terminal F atoms provides (in a Lewis picture) a further electron to the bonding. Hence the Xe atom has 10 electrons around it. This can be rationalised by considering resonance forms of F<sup>-</sup> and <sup>+</sup>Xe-F. This suggested delocalised bonding with an average XeF bond order of 0.5. This can just about be rationalised by valence bond theory by invoking the use of 5d<sub>z<sup>2</sup></sub> orbitals on Xe (although these are very high in energy). An MO description is best developed by first considering CO<sub>2</sub>, which has the same symmetry analysis (except that XeF<sub>2</sub> brings np valence AOs as well as the ns AOs). CO<sub>2</sub> possess 16 valence electrons, and these form a framework of σ and π bonds like so:



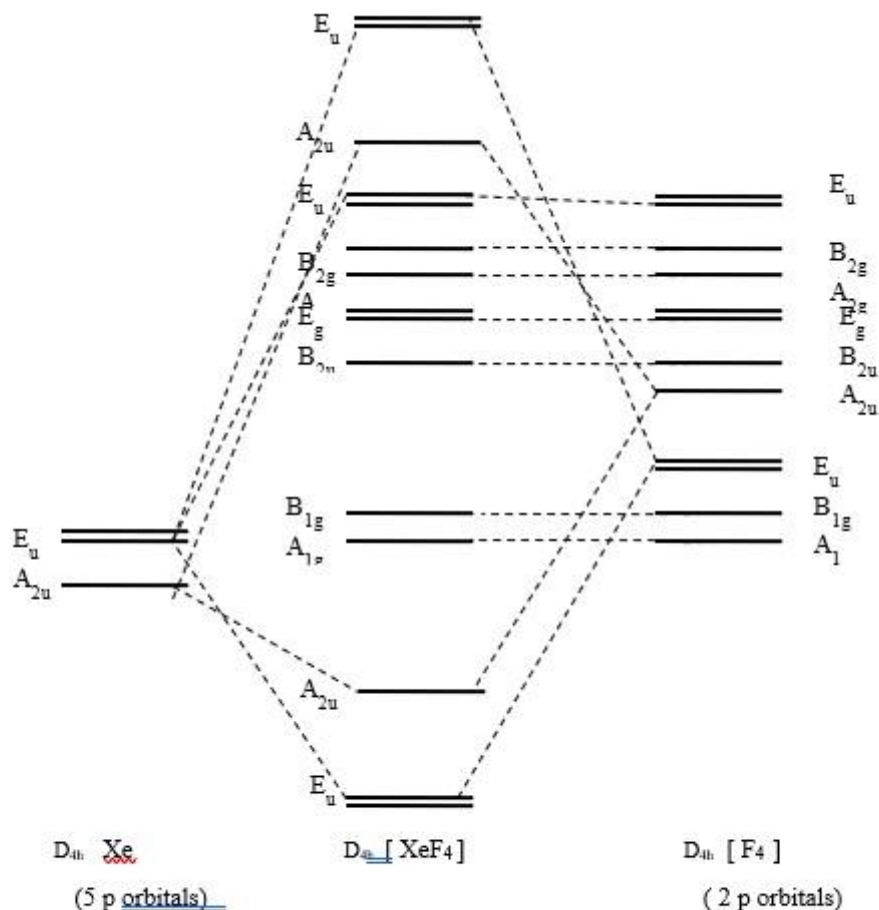
It is seen that whether or not s-p mixing is taken into account affects the results. In both descriptions however there are 8 filled MOs: 2  $\sigma$ -bonding, 2  $\pi$ -bonding, 2  $\sigma$ -non-bonding and 2  $\pi$ -non-bonding. An approximate XeF<sub>2</sub> MO description is shown below. The left hand side shows it without and 5d<sub>z<sup>2</sup></sub> contribution, while it is included on the right, where mixing with the 3 $\sigma_g$  MO stabilises the two electrons in that orbital. Antibonding character subsequently builds up in the new 4 $\sigma_g$  MO.



The 2s AOs of fluorine lie very low in energy and so they do not participate significantly in Xe-F bonding (i.e. no mixing, unlike in  $\text{CO}_2$ ). They may be reproduced without need for permission.  $\text{XeF}_2$  has 22 valence electrons (8 from Xe, and 7 from each F) to be accommodated in this MO scheme. Without the  $5dz^2$  contribution this requires the MOs to be filled up to and including the  $3\sigma_g$  level. Thus gives 11 filled MOs. This leaves only 1 antibonding MO unoccupied, compared to 4 in  $\text{CO}_2$ . In  $\text{XeF}_2$  therefore the Xe-F bonding can be considered to be based on a net  $3c4e$  interaction derived from the  $\sigma_u$  manifold. The symmetry-allowed mixing in of the  $5dz^2$  AO would have a stabilising effect by adding some

bonding character. It is not clear, however, to what extent this orbital mixing actually occurs, if at all. The  $5d_{z^2}$  AO is expected to lie fairly high in energy relative to the 5s and 5p AOs, although the electron withdrawing effects of the F atom will generate a partial positive charge on Xe that would to some extent stabilise this orbital. The key conclusion is that the bonding in  $\text{XeF}_2$  can be described without d-orbital participation (i.e. delocalised 3c-4e bonding). Any stabilisation by  $5d_{z^2}$  will not be to the same extent suggested by a formal  $sp^3d$  hybridisation model.

MO diagram of  $\text{XeF}_4$



Schematic mo diagram for [XeF<sub>4</sub>] using only the Xe 5p and F 2p as valence orbitals.

