Full Form-MOT (Molecular Orbital Theory)

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Introduction:

Let's consider homonuclear diatomic molecules. The diatomic ions are formed by two atoms of the same element. This concept can be extended for heteronuclear diatomic species as well that are formed by the combination of two atoms or ions of different elements. They can also be extended to polyatomic molecules and solids that are composed of huge numbers of atoms and ions.

Types:

(a). Bonding

(b). Antibonding

(c). Nonbonding

(a). Bonding orbital formation takes place from the constructive interference of neighbouring atomic orbitals. The orbital ψ_+ is an example of a **bonding orbital** because in this, energy gets lowered as compared to the separated atoms if this orbital is occupied by electrons.

(b). Antibonding orbital formation takes place from the destructive interference of neighbouring atomic orbitals which is indicated by nodes present between the atoms. The orbital is ψ_- an example of an **antibonding orbital** because energy becomes higher as compared to the separated atoms if this orbital is occupied by electrons.

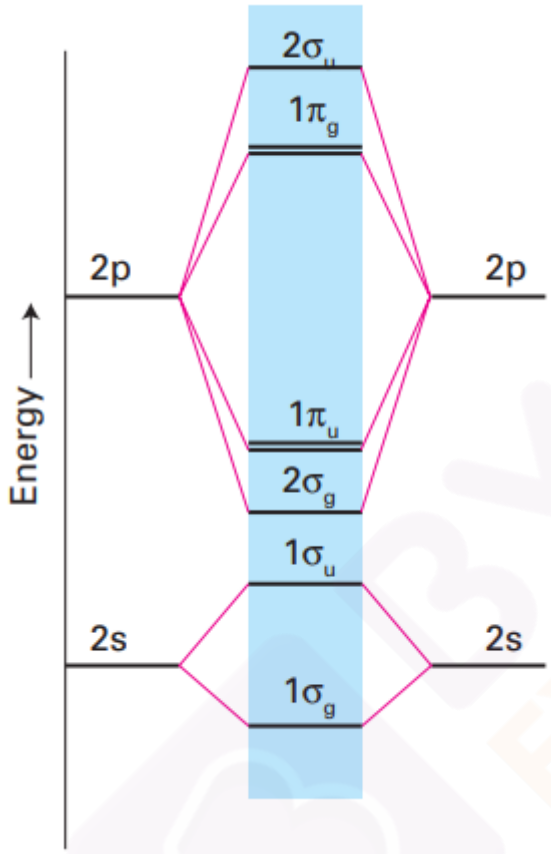
(c). Apart from the above two, it is possible to generate a molecular orbital having the same energy as the initial atomic orbitals. In this case, the electron occupying this orbital neither stabilizes nor destabilizes the molecule. This orbital consists of a single orbital on one atom because of the absence of an atomic orbital of the correct symmetry for it to overlap on a neighbouring atom.

Homonuclear diatomic molecules

1. From the basis set of four atomic orbitals on each atom, eight molecular orbitals can be constructed.

2. Out of these eight molecular orbitals, four are σ orbitals and four are π orbitals.

3. The four σ orbitals span a range of energies, as is strongly bonding and another one is strongly antibonding, while the remaining two will lie between these extremes.
4. The four π orbitals form one doubly degenerate pair of bonding orbital and one doubly degenerate pair of antibonding orbitals.



The above figure represents the molecular orbital energy level diagram for the later period 2 homonuclear diatomic molecules. This diagram is used for O_2 and F_2.

The building up principle is generally used in conjunction with the molecular orbital energy level diagram in the same way as for atoms where each orbital can accommodate a maximum of two electrons. In the case of more than one orbital available for occupation, then the orbitals are occupied separately. For example, the electron configuration of N_2 having 10 valence electrons can be written as:

N_2: $1\sigma_g^2 1\pi_u^4 2\sigma_g^2$

The **highest occupied molecular orbital** (HOMO) is the molecular orbital that, according to the building-up principle, is occupied last. The **lowest unoccupied molecular orbital** (LUMO) is the next higher molecular orbital.

Heteronuclear diatomic molecules

These molecules are polar in nature due to the difference in electronegativity of the bonded atoms. In this, bonding electrons are found on the more electronegative atom and antibonding electrons on the less electronegative atom. It can be explained by taking an example of hydrogen fluoride.

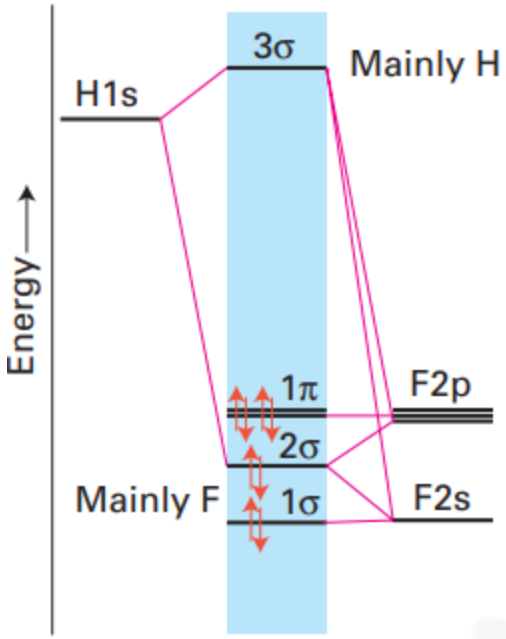
In HF, the bonding electron will be more concentrated towards the F atom while antibonding will be on the H atom. In this, five valence orbitals will be available to form molecular orbital, and these are the 1s orbital of H and the 2s and 2p orbitals of F; there are 1 + 7 = 8 valence electron to accommodate in the five molecular of HF can be constructed from the five basis orbitals. The σ orbitals of HF can be constructed when an H1s orbital overlaps with the F2s and $F2p_z$ orbitals (z being the internuclear axis). These atomic orbitals on combination gives three σ molecular orbitals that can be represented as:

$$\psi = c_1\chi_{H1s} + c_2\chi_{F2s} + c_3\chi_{F2p}$$

By following the above process, $F2p_x$ and $F2p_y$ orbitals remain unaffected due to the absence of π symmetry and there is no valence H orbital of the symmetry. The 1σ bonding orbitals will contain predominantly F2s character due to the large energy difference between it and the H1s orbital due to which it is confined mainly to the F atom and will be antibonding. As compared to 1σ, 2σ orbital is more bonding and has both H1s and F2p characters. On the other hand, 3σ orbital is antibonding, and principally H1s character: the 1s orbital has a relatively high energy (compared with the fluorine orbitals) and hence contributes predominantly to the high energy antibonding molecular orbital. Out of the eight valence electrons, two will enter the 2σ orbital that results in the formation of a bond between two atoms. Six more enter the 1σ and 1π orbitals; these two orbitals will be largely nonbonding and confined mainly to the F atom. The configuration can be written as:

$$1\sigma^2 2\sigma^2 1\pi^4 .$$

One important point to be noted is that all the electrons occupy orbitals that are predominantly on the F atom. It follows that the HF molecule is polar in nature in which F contains partial negative charge which is found experimentally.



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