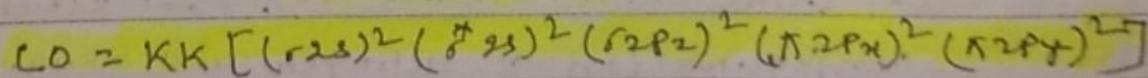


[Heteronuclear Diatomic Molecules]Dr. Sanjay Kumar Yadav
Lecture Notes Series - 24

In heteronuclear diatomic molecules the electronegativity of two atoms is different. Therefore the molecular orbital diagram will not be symmetrical like homonuclear diatomic molecules. However the principles involved in the distribution of electrons are the same as discussed before. Due to difference in the electronegativity of the atoms the electrons in bonding MO spend more time near the more electronegative atoms, the electrons in antibonding are closer to the less electronegative atom.

Let us discuss electronic configuration and molecular orbital level diagram of some heteronuclear diatomic molecules.

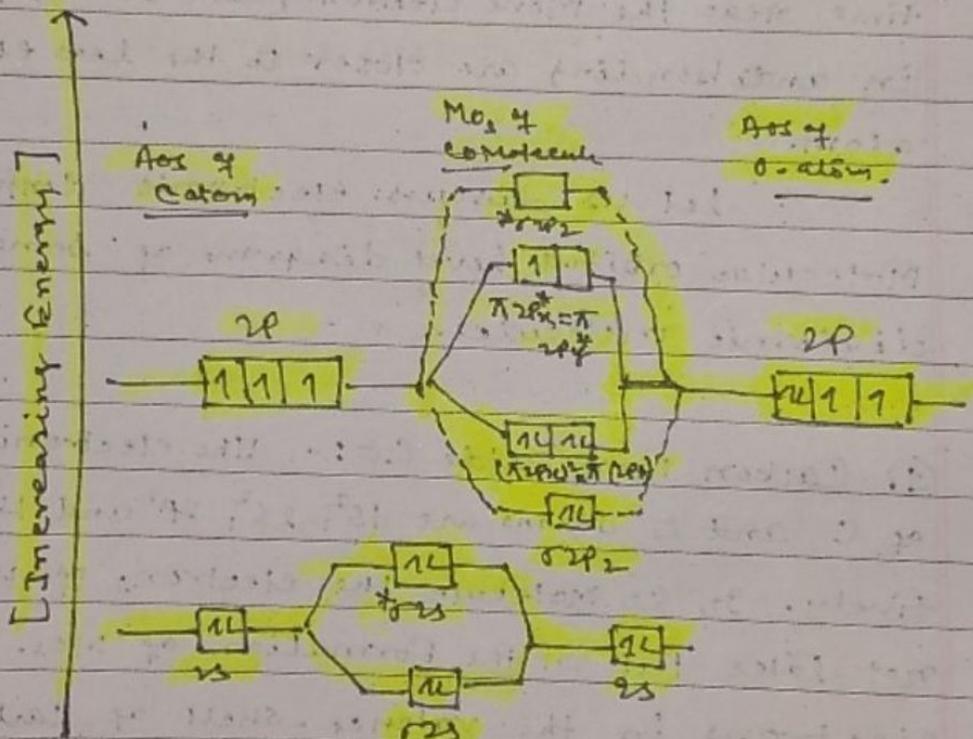
① Carbon monoxide CO:- The electronic configuration of C and O atoms are $1s^2, 2s^2, 2p^2$ and $1s^2, 2s^2, 2p^4$ respectively. In CO molecule the electrons of K-shell do not take part in the formation of MOs. There are 4 electrons in the valence shell of carbon and 6 electrons in the valence shell of oxygen. Thus CO molecule has in all ten electrons which will be accommodated in the various MOs as follows.



$$\text{Bond order} = \frac{8-2}{2} = \frac{6}{2} = 3$$

Thus CO molecule contains a triple bond. Its bond dissociation energy is 1067 KJ/mole and bond

length is equal to 1.14 \AA . The atomic orbitals of oxygen will be of lower energy than the corresponding atomic orbitals of carbon due to higher electronegativity of oxygen. The bonding mo will be closer to the atomic orbitals of more electronegative oxygen and the antibonding mo will be closer to the atomic orbitals of less electronegative carbon atom as shown in fig.



Molecular orbital energy level diagram

of NO molecule.

Inorganic Chemistry
 B.Sc Part II, Group-B
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[2] Nitric Oxide Molecule NO . The electronic configuration of nitrogen and oxygen atoms are $1s^2, 2s^2, 2p^3$ and $1s^2, 2s^2, 2p^4$ respectively. There are five electrons in the valence shell of nitrogen and 6 electrons in the valence shell of oxygen. Thus 11 electrons are to be adjusted in different mo

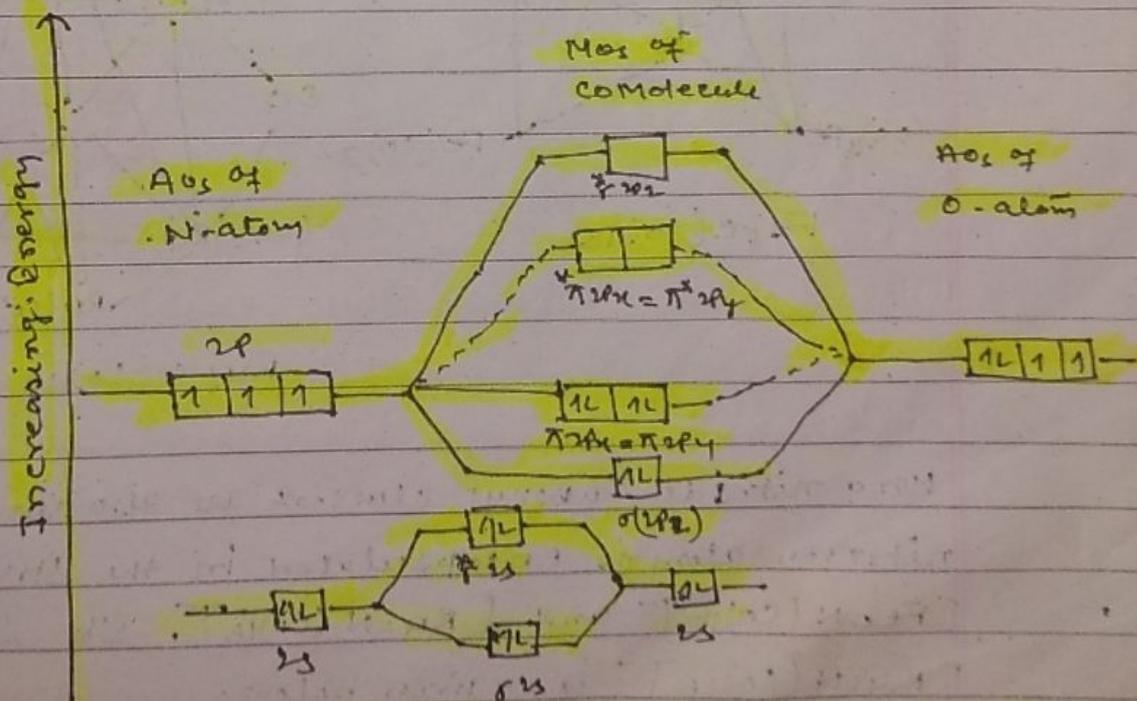
These electrons are distributed as given below.

$$NO = KK [(\sigma_{2s})^2 (\sigma_{2s}^*)^2 (\sigma_{2p_z})^2 (\pi_{2p_x})^2] \\ = (\pi_{2p_y})^2 (\pi_{2p_x}^*)^1]$$

$$\text{Bond order} = \frac{8-3}{2} = \frac{5}{2} = 2.5$$

This shows that in NO molecule nitrogen and oxygen are linked together by one σ bond and two π bonds less the antibonding effect of one unpaired electron in the $\pi_{2p_x}^*$ MO. Due to the presence of the antibonding electron NO molecule is paramagnetic and less stable (bond energy $667.8 \text{ kJ mol}^{-1}$) than N_2 molecule (bond energy $945.6 \text{ kJ mol}^{-1}$).

As in the case of CO molecule, the bonding MOs will be closer to the AOs of more electronegative oxygen and the antibonding MOs will be closer to the AOs of less electronegative N-atom as shown fig.



[Molecular orbital energy level diagram of NO molecule]