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Engineering ChemistryTutorial 2 - Atomic and Molecular Structure

1) Distinguish between sigma and pi molecular orbital.

Ans

Sigma molecular orbit	Pi Molecular orbit
1) The sigma molecular orbital is obtained when the atomic orbitals overlap collinearly to a large extent.	1) The pi molecular orbit is obtained when atomic orbitals overlap along the side to a lesser extent.
2) For a sigma overlap, the lobes of atomic orbitals point along the internuclear axis.	2) For pi overlap, the lobes of the atomic orbitals are perpendicular to the axis.
3) Sigma molecular orbital is denoted by $\sigma$ .	3) Pi molecular orbital is denoted by $\pi$ .
4) For sigma molecular orbital $\psi$ is along the internuclear axis and the electron density $\psi^2$ is distributed uniformly along the axis.	4) For pi molecular orbital, $\psi$ is zero along the internuclear axis and the electron density $\psi^2$ on the axis is zero.



2) What are the characteristics of aromatic compounds?

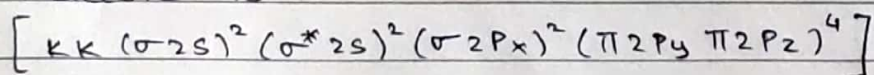
Ans. Characteristics of aromatic compounds are:

- i) They are highly unsaturated as shown by the lesser number of hydrogen atoms in their molecular formula.
- 2) They are cyclic compounds with five, six or seven membered rings.
- 3) Their molecules are flat or nearly flat as shown by physical methods such as x-ray and electron diffraction methods.
- 4) They undergo readily certain electrophilic substitution reactions such as nitration, halogenation, sulphonation, Friedel-Craft alkylations and acylations etc.

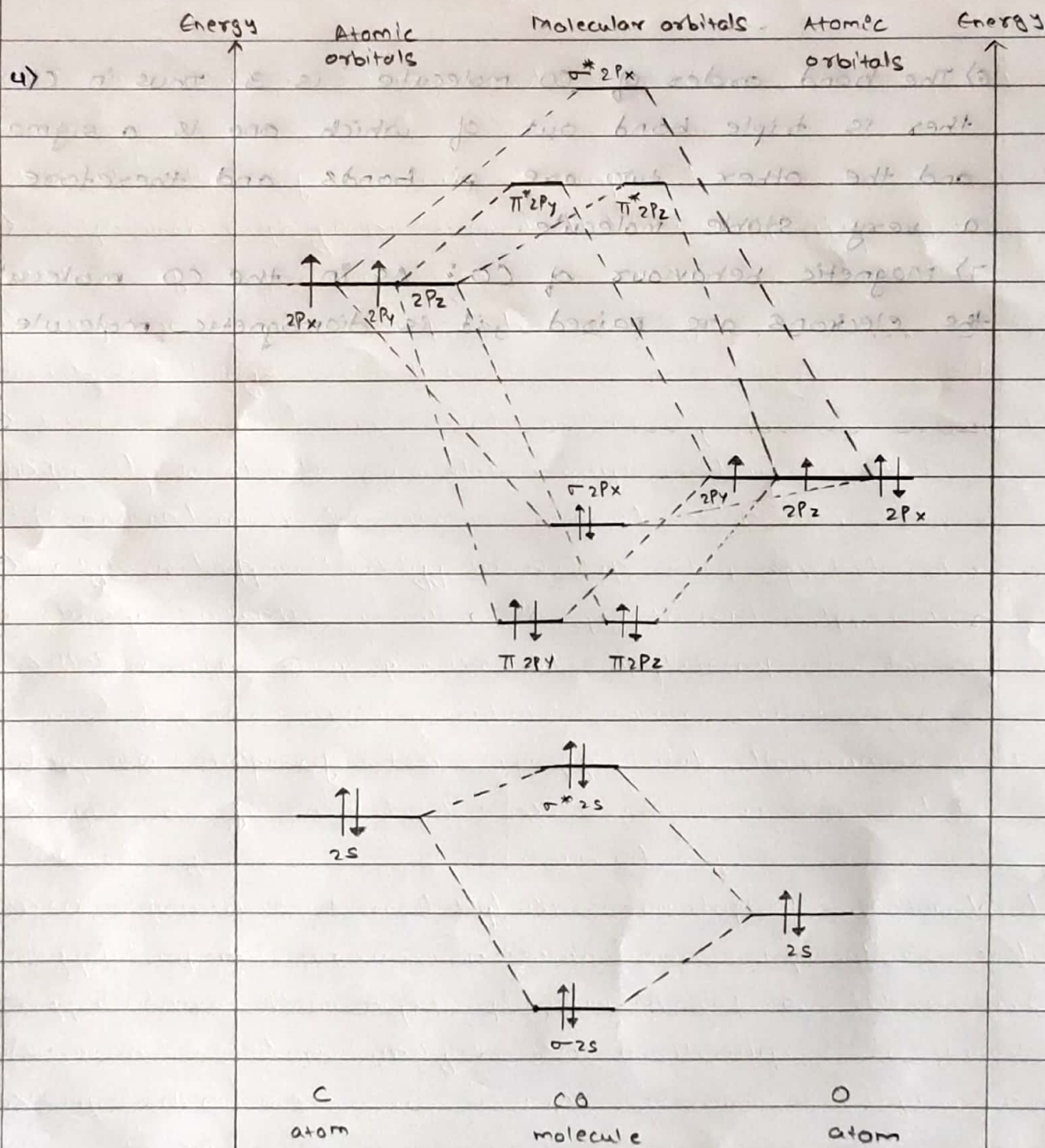
3) With the help of MO energy level diagram explain formation of CO.

Ans. i) CO molecule is formed by the overlap of carbon and oxygen atom. The carbon atom has 6 electrons and oxygen atom has eight electrons. Therefore there are fourteen electrons in the CO molecule.

2) Hence, the molecular orbital electronic configuration of CO molecule is:



3) The inner shell is non-bonding. The bonding and antibonding 2s orbitals cancel each other. A  $\sigma$  bond is formed by the filled  $\sigma 2p_x^2$  orbital. Two pi bonds are formed by the filled  $\pi 2p_y^2$  and  $\pi 2p_z^2$  orbitals.



MO Energy level diagram for CO

5) Bond order (CO) =  $\frac{1}{2} [\text{Number of electrons in bonding molecular (Nb)} - \text{Number of electrons in antibonding molecular orbitals (Na)}]$

$$= \frac{1}{2} [Nb - Na] = \frac{1}{2} (8 - 2)$$

$$= 3$$



6) The bond order of CO molecule is 3. Thus in CO molecule, there is triple bond out of which one is a sigma bond and the other two are pi bonds and therefore CO is a very stable molecule.

7) Magnetic behaviour of CO: As in the CO molecule all the electrons are paired, it is diamagnetic molecule.