Molecular Orbital Treatment For Heteronuclear Diatomic Molecules

(1) <u>Nitric oxide molecule, NO:</u> The nitrogen atom has 2 + 5 = 7 electrons and the oxygen atom has 2 + 6 = 8 electrons, making 15 electrons in the molecule. The order of energy levels of the various MO's are the same as for homonuclear diatomic molecules heavier than C_2.

The arrangement is :

$$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_x^2, \begin{Bmatrix} \pi 2p_y^2 \\ \pi 2p_z^2 \end{Bmatrix}, \begin{Bmatrix} \pi^* 2p_y^1 \\ \pi^* 2p_z^0 \end{Bmatrix}$$

B.O. = ½ (8 – 3)

= 2.5 Hence molecule exists.

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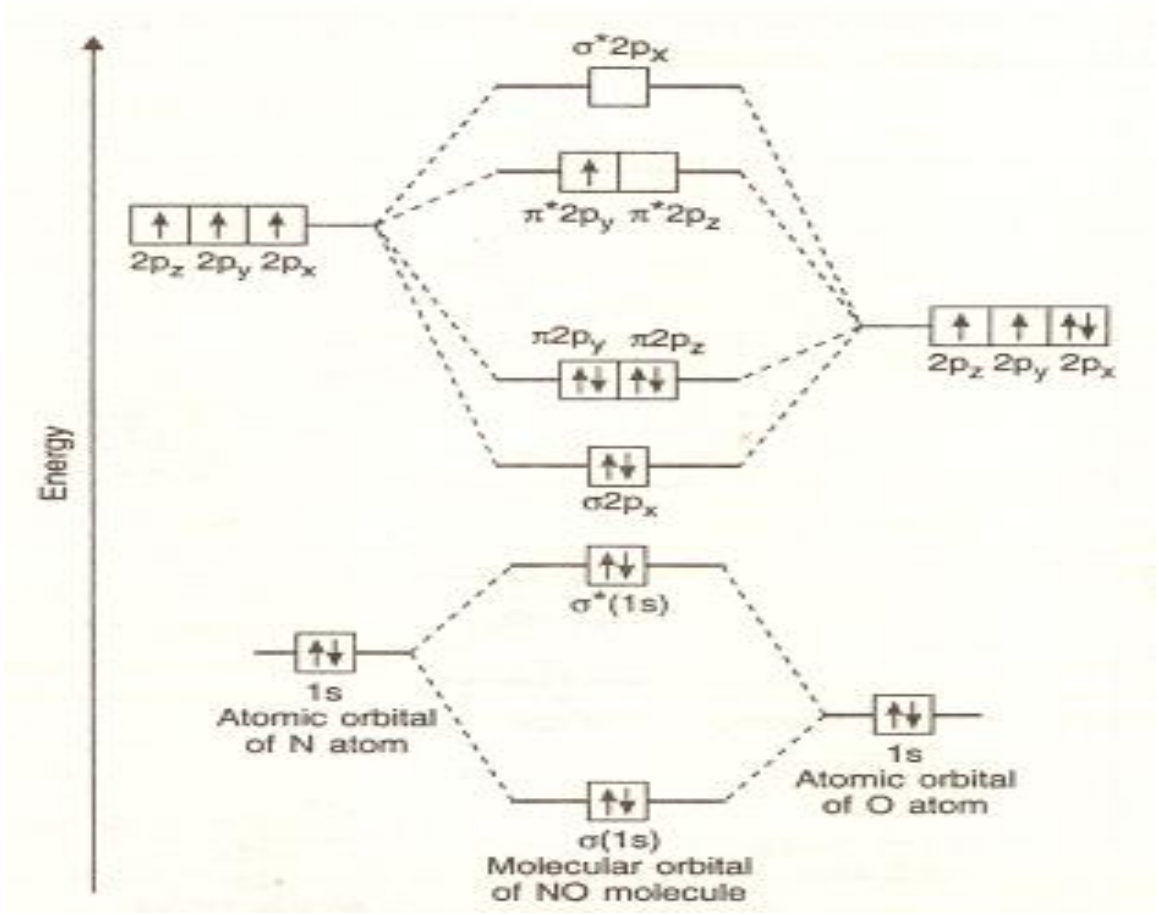
The molecule is **paramagnetic,** since it contain an unpaired electron in π*2py or π*2pz orbital.



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(2) <u>NO+ and NO- Ions:</u> The electronic configuration, bond order and magnetic character of these ions are :

Species	Electronic configuration	Bond order	Magnetic behaviour
NO^+	$kk\ \sigma(2s^2), \sigma^*2s^2\sigma(2p_x)^2, \begin{cases}\pi 2p_y^2 \\ \pi 2p_z^2\end{cases}$	$\frac{8-2}{2}=3$	Diamagnetic
NO^-	$kk\ \sigma(2s^2)\sigma^*2s^2, \sigma(2p_x)^2 \begin{cases}\pi(2p_y)^2 \begin{cases}\pi^*(2p_y)^1 \\ \pi(2p_z)^{2'} \begin{cases}\pi^*(2p_2)^1\end{cases}\end{cases}\end{cases}$	$\frac{(8-4)}{2}=2$	Paramagnetic

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(3) <u>Carbon monoxide molecule, CO:</u> The carbon atom has 2 + 4 = 6 electrons and the O atom has 2 + 6 = 8 electrons, so the CO molecule contains 14 electrons. The order is the same as for light atoms like C.

$$\sigma 1s^2, \sigma^* 2s^2, \sigma 2s^2, \sigma^* 2s^2, \begin{cases} \pi 2p_y^2 \\ \pi 2p_z^2 \end{cases}, \sigma 2p_x^2$$

B.O. = ½ (8 – 2) = 3.0

Hence Molecule exists with a triple bond.

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