Answer on Question #76210, Chemistry / Inorganic Chemistry

a) By writing molecular orbital configuration for each of following molecules calculate the bond order and also determine whether it is paramagnetic or diamagnetic.
(i) NO (ii) CO (iii) O2
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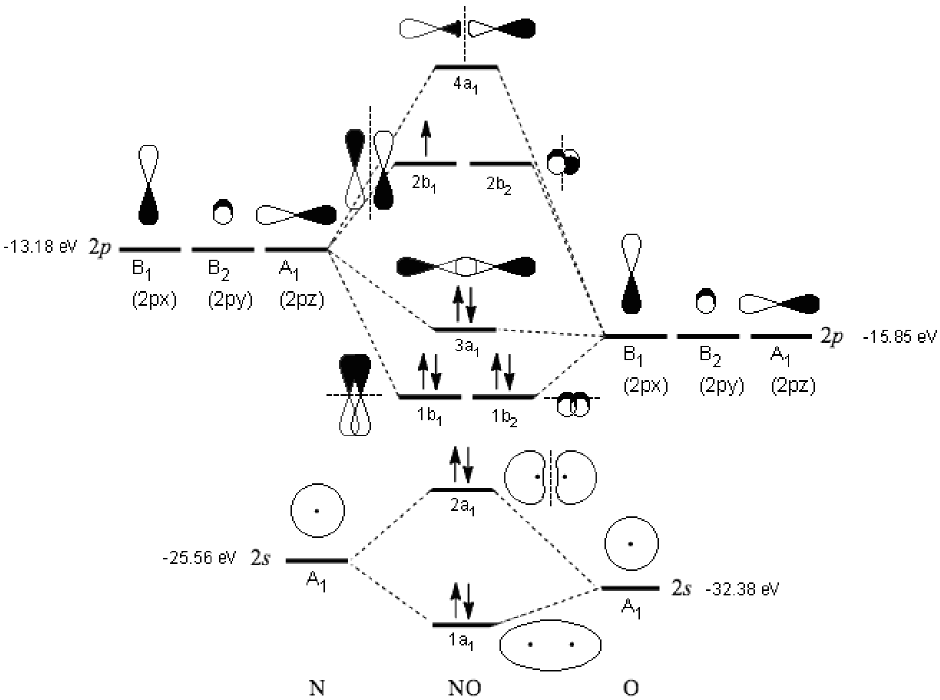
Solution

(i) The electronic configuration of N atom is : $_7N$ [He]$2s^22p^3$.

The electronic configuration of O atom is: $_8O$ [He]$2s^22p^4$.

Nitrogen has 5 electrons in the valence shell, and oxygen has 6 electrons in the valence shell. The total number of valence electrons in the NO molecule is 6+5 =11. The total of 11 electrons are to be accommodated in the molecular orbitals of NO molecule. Molecular orbitals of NO are formed of atomic orbitals of oxygen and atomic orbitals of N. Because of higher electronegativity of oxygen it's atomic orbitals would be of lower energy than the corresponding atomic orbitals of nitrogen. MO diagram of NO is:



Electronic configuration of NO molecule is: $(\sigma_{2s})^2(\sigma^*_{2s})^2$ $(\pi_{2p})^4$ $(\sigma_{2p})^2$ $(\pi^*_{2p})^1$

Bonding orbitals: $(\sigma_{2s})^2$ $(\pi_{2p})^4$ $(\sigma_{2p})^2$, number of electrons in bounding orbitals is: 2+2+4= 8

Antibounding orbitals: $(\sigma^*_{2s})^2(\pi^*_{2p})^1$, number of electrons in antibounding orbitals is: 2+1=3

Bound order = (number of electrons in bounding orbitals – number of electrons in antibounding orbitals)/2

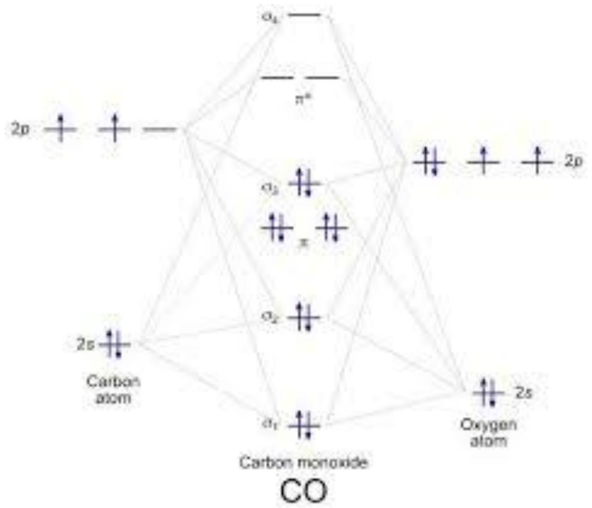
Bound order of NO = (8-3)/2 = 2.5

NO molecule is paramagnetic as it has at least one electron that is not paired.

(ii) The electronic configuration of C atom is : $_6C$ [He]$2s^2 2p^2$.

The electronic configuration of O atom is: $_8O$ [He]$2s^2 2p^4$.

Carbon has 4 electrons in the valence shell, and oxygen has 6 electrons in the valence shell. The total number of valence electrons in the CO molecule is 4+6 =10. The total of 10 electrons are to be accommodated in the molecular orbitals of CO molecule. Molecular orbitals of CO are formed of atomic orbitals of oxygen and atomic orbitals of carbon. Because of higher electronegativity of oxygen it's atomic orbitals would be of lower energy than the corresponding atomic orbitals of carbon. MO diagram of CO is:



Electronic configuration of CO molecule is: $(\sigma_{2s})^2(\sigma^*_{2s})^2(\pi_{2p})^4 (\sigma_{2p})^2$

Bonding orbitals: $(\sigma_{2s})^2(\pi_{2p})^4 (\sigma_{2p})^2$, number of electrons in bounding orbitals is: 2+2+4= 8

Antibounding orbitals: $(\sigma^*_{2s})^2$, number of electrons in antibounding orbitals is: 2

Bound order = (number of electrons in bounding orbitals – number of electrons in antibounding orbitals)/2

Bound order of NO = (8-2)/2 = 3

CO molecule is diamagnetic as all electrons are pared in MO orbitals.

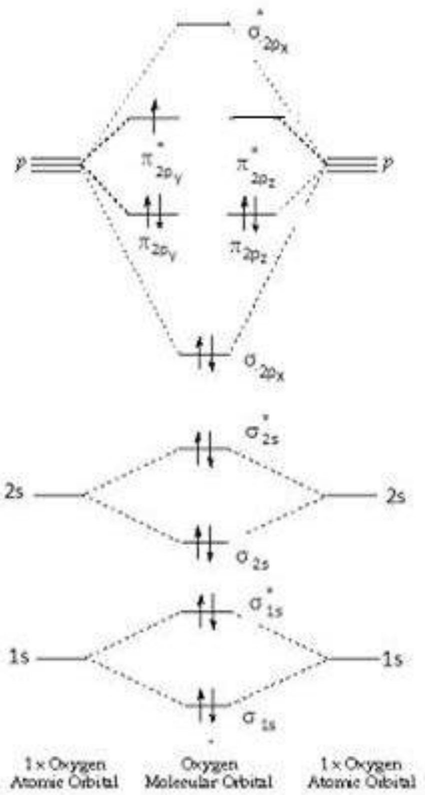
(iii) The electronic configuration of oxygen atom is:

$_8O$ [He]$2s^2 2p^4$

Oxygen has 6 electrons in it's valence shell. The total number of valence electrons in molecule of O_2 is 12, but as we consider ion O_2^+ then the total number of valence electrons is 11. The total of 11 electrons are to be accommodated in the molecular orbitals of O_2^+ ion. Molecular orbitals of O_2^+ are formed of atomic orbitals of oxygen. MO diagram of O_2^+ is:

MO diagram of O_2^+

$O^8 - 1s^2\, 2s^2\, 2p_x^2\, 2p_y^1 2p_z^1$



Electronic configuration of O_2^+ ion is: $(\sigma_{2s})^2(\sigma^*{}_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4(\pi^*{}_{2p})^1$

Bonding orbitals: $(\sigma_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4$, number of electrons in bounding orbitals is: 2+2+4= 8

Antibounding orbitals: $(\sigma^*{}_{2s})^2(\pi^*{}_{2p})^1$, number of electrons in antibounding orbitals is: 2+1=3

Bound order = (number of electrons in bounding orbitals – number of electrons in antibounding orbitals)/2

Bound order of O_2^+ = (8-3)/2 = 2.5

Ion O_2^+ is paramagnetic as it has at least one electron that is not paired.