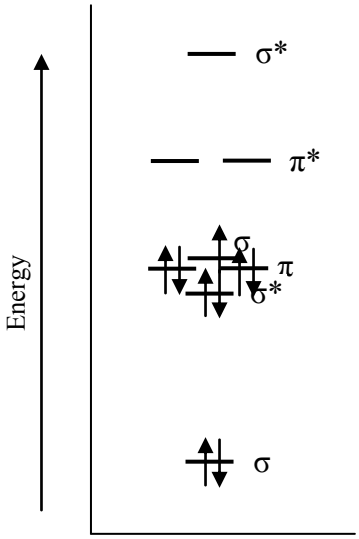
Marks 6

- Carbon and nitrogen can combine to form a cyanide ion or a neutral free radical.

The molecular orbital energy level diagram provided shows the energies of the orbitals for the valence electrons in the free radical CN. Indicate on this diagram the ground state electronic configuration of CN using the arrow notation for electron spins.



*** C has 4 valence electrons and N has 5 valence electrons, giving a total of 9 electrons to place on the diagram. These occupy orbitals from the bottom upwards, with a maximum of 2 in each. The overall configuration is shown and corresponds to $(\sigma)^2(\sigma^*)^2(\pi)^4(\sigma)^1$**

How would you expect the magnetic properties of CN to differ from that of CN^-?

CN has an unpaired electron. This makes it *paramagnetic* (it is attracted into a magnetic field).

CN^- has an extra electron. This pairs up with the electron in the highest occupied σ-orbital. As all the electrons are now paired, CN^- is *diamagnetic* (it is weakly repelled by a magnetic field).

CN is paramagnetic whereas CN^- is diamagnetic.

How would adding an electron to CN to form CN^- affect the strength of the bond between the two atoms? Explain your answer.

The extra electron in CN^- occupies a σ-orbital. This is a bonding orbital and so CN^- has more bonding electrons than CN and would be expected to have a stronger bond as a result.

Equivalently, bond order can be used to rationalize the bond strength:

bond order = ½ (number of bonding– number of antibonding electrons)

CN has 7 bonding and 2 antibonding electrons. CN^- has 8 bonding and 2 antibonding electrons. Hence,

bond order of CN = ½ (7 – 2) = 2.5
bond order of CN^- = ½ (8 – 2) = 3

CN^- has a higher bond order than CN and would therefore be expected to have a stronger bond.

ANSWER CONTINUES ON THE NEXT PAGE

Why do we only need to consider the valence electrons when discussing the bonding of CN?

The core electrons are tightly held onto by the atoms. There is little overlap between the core orbitals on the two atoms.

Even if the 1*s* core electrons on each atom are considered, they would occupy *both* the bonding σ and antibonding σ* orbitals formed from their overlap. This would not change the bond order. Their contribution to the bonding is minimal.