Delocalized π electrons

1) Describe the hybridization of the carbon atoms in the benzene molecule.

2) Describe the location of the π electrons in the benzene molecule according to the valance bond theory and the molecular orbital theory.

3) Which theory gives a more accurate description of the bonding in the benzene molecule? Explain your answer.

4)

a) Draw the 3 resonance structures for the nitrate ion (NO_3^-). Describe the hybridisation of the nitrogen atom and the bond angle around the nitrogen atom.

b) Draw the resonance hybrid structure for the nitrate ion.

c) Describe the location of the π electrons in the resonance structures and the resonance hybrid structure. Comment on the nitrogen to oxygen bonds in the resonance hybrid structure.

Answers:

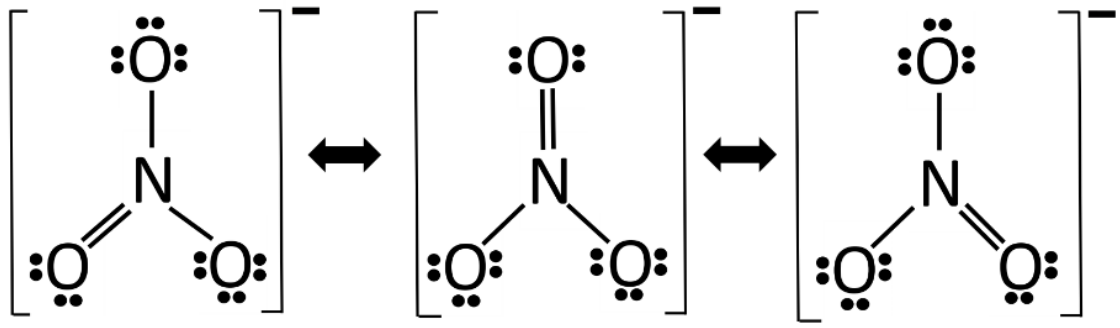
1) The carbon atoms in the benzene molecule have sp^2 hybridisation. There are three sp^2 hybrid orbitals around each carbon atom and one unhybridized p orbital. The bond angle around the carbon atoms is 120°, trigonal planar.

2) According to the valance bond theory, π electrons are localized between the carbon atoms in π bonds (produced by sideways overlap of unhybridized p orbitals).

According to the molecular orbital theory, π electrons are delocalized and spread out in π bonded regions (delocalized π electron clouds) above and below the plane of the molecule.

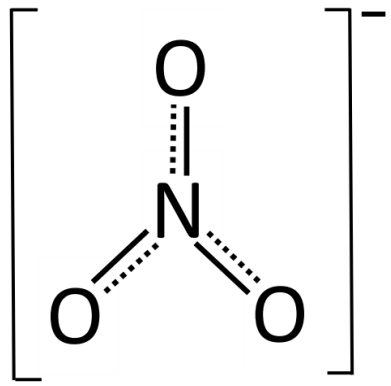
2) The molecular orbital theory gives a more accurate description of the bonding in the benzene molecule. The valence bond theory has two resonance structures with alternating single and double carbon to carbon bonds. However, the length and strength of the carbon to carbon bonds in the benzene molecule are identical (intermediate between a single and a double bond).

3) a)



The nitrogen atom has sp^2 hybridisation. The bond angle around the nitrogen atom is 120°, trigonal planar.

b)



c) In the resonance structures, the π electrons are localized between the nitrogen and oxygen atom (in the π bond that forms the double bond).
In the resonance hybrid structure, the π electrons are delocalised and spread over all four atoms. The nitrogen to oxygen bonds are all of identical length and strength (intermediate between a single and a double bond).