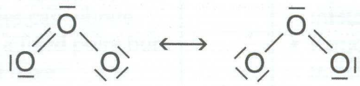
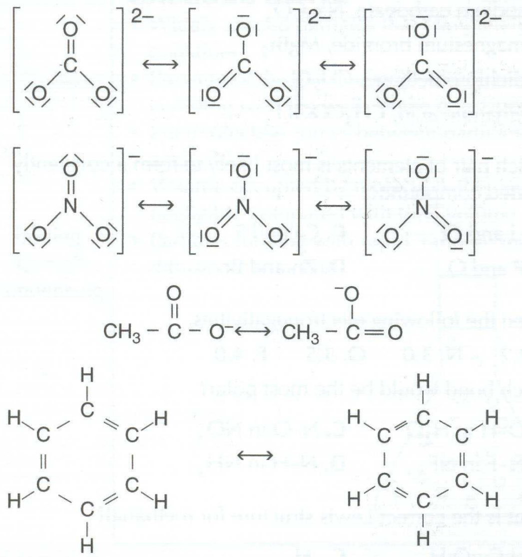
Delocalization of electrons

RESONANCE STRUCTURES

When writing the Lewis structures for some molecules it is possible to write more than one correct structure. For example, ozone can be written:

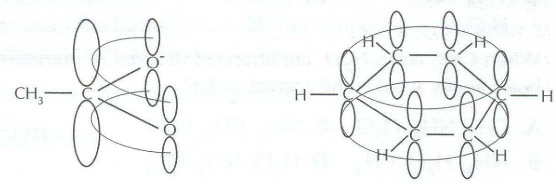


These two structures are known as resonance hybrids. They are extreme forms of the true structure, which lies somewhere between the two. Evidence that this is true comes from bond lengths, as the bond lengths between the oxygen atoms in ozone are both the same and are intermediate between an O=O double bond and an O–O single bond. Resonance structures are usually shown with a double headed arrow between them. Other common compounds which can be written using resonance structures are shown here.

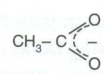


DELOCALIZATION OF ELECTRONS

Resonance structures can also be explained by the delocalization of electrons. For example, in the ethanoate ion the carbon atom and the two oxygen atoms each have a p orbital containing one electron after the σ bonds have been formed. Instead of forming just one double bond between the carbon atom and one of the oxygen atoms the electrons can delocalize over all three atoms. This is energetically more favourable than forming just one double bond. Delocalization can occur whenever alternate double and single bonds occur between carbon atoms. The delocalization energy in benzene is about 150 kJ mol^{-1}, which explains why the benzene ring is so resistant to addition reactions.



ethanoate ion shown as



benzene ring shown as

STRUCTURES OF THE ALLOTROPES OF CARBON

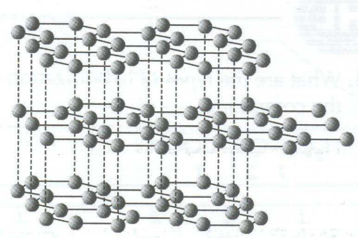
Allotropes occur when an element can exist in different crystalline forms. In diamond all the carbon atoms are sp^3 hybridized to form a macromolecule in which all the bonds are equally strong. There is no plane of weakness in the molecule, so diamond is exceptionally hard and because all the electrons are localized it does not conduct electricity.

In graphite the carbon atoms are sp^2 hybridized. This results in three very strong σ bonds between the atoms to give layers of hexagonal rings. The remaining electrons in the p orbitals are then delocalized to form very weak bonds between the layers. The layers can slide over each other so graphite is an excellent lubricant and because the electrons are delocalized it is a good conductor of electricity.

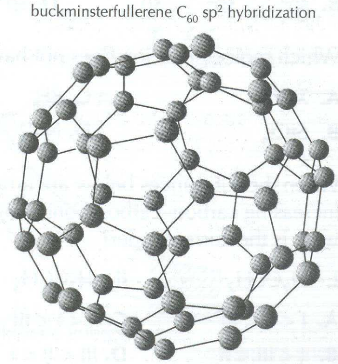
A third allotrope of carbon is buckminsterfullerene. This consists of sixty carbon atoms arranged in hexagons and pentagons to give a geodesic spherical structure similar to a football. Following the initial discovery of buckminsterfullerene a whole family of spherical carbon molecules have been isolated. They are given the collective name 'bucky balls'. In all of them the carbon atoms are sp^2 hybridized. They also contain delocalized electrons, which gives them the ability to partially conduct electricity.

Allotrope	Conductivity / S m^{-1}
graphite	7×10^{4}
buckminsterfullerene	1.7×10^{-6}
diamond	1×10^{-11}

graphite sp^2 hybridization



buckminsterfullerene C_{60} sp^2 hybridization



diamond sp^3 hybridization