Resonance and formal charge

Tuesday, 27 February 2024 11:12 am

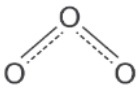
Resonance hybrids
Resonance hybrids may occur when there is more than one possible position for a double bond in a molecule
Resonance - the Lewis structure of a molecule that has more than one possible position for a double bond

Show the resonance structure as:

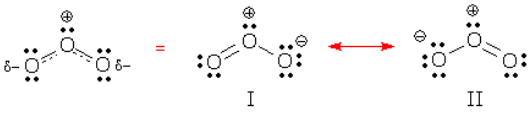
The molecule achieve this by delocalizing one of pair of electron - means no longer fixed to one bonding position: its spread over two positions (the position of atom is constant)

Delocalizing - an electron that is not associate with one specific atom and is free to move within the molecular structure

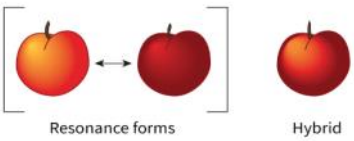
Electron delocalization is represent using a dashed line



Present of resonance hybrid



All represent resonance hybrid



Resonance hybrid structures can be used to represent molecules for which there are more than one valid Lewis formula in terms of electron

Resonance hybrid structure have intermediate properties as they lies between these number of extreme structure - bond length in resonance is same
Strength of bond (single bond 1, double bond 2, triple bond 3)
In a resonance hybrid the bond order is 1.5

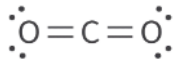
Bond order is calculate by the average value of single bond and double bond

(average strength of bond)

Resonance in other molecules and ions(eg: 3 possible structure in carbonate

As there is no 'choice' of where to place the C=O bond in the carbon dioxide molecule, this cannot experience resonance.
Carbon dioxide is the element that form as the structure is defined

Carbon dioxide:



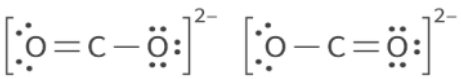
Which there are only 1 possibility where the bond are placed

HL Difficulty:

Chemical species that can form two or more plausible structures with potential alternative places for a double bond are said to demonstrate resonance ✓ .

These structures exist because the pair of electrons that would make up the double bond become delocalized ✓ . If there are two positions for the double bond to be placed the value of the overall bond order is 1.5 ✓ but if there are three positions for the double bond to be placed the value of the overall bond order is 1.33.

In the carbonite ion, there are two possible places for the C=O bond; this ion can experience resonance



Formal charge
The charge of the each atom in a molecule - larger structures and more in depth explanations of bonding systems often require more sophistic concepts and theories of bonding (eg: expanding octet)

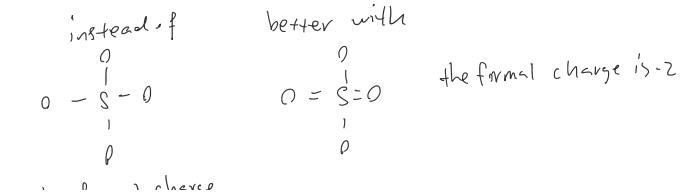
Formal charge = ve - (Bonding pair + nonbonding electron(or is the lone pair / 2))
B - bonding pair on atom
Ve = valence shell on neutral atom

Formal charge of molecule, all up all the formal charge on each atom

Formal charge in resonance - each hybrid resonance has the same molecular formular but they differ from the formal charge.
To determine the structure is more likely to be, choose the structure with formal charge is zero or the absolute value as low as possible.

Formal charge = the number of valence electron around that atom In free atom - the number of non bonding electron - 1/2number of bonding electron

eg: SO_4^{2-}



the formal charge
is -4