Resonance Part 1

1. Introduction

Organic chemists communicate with skeletal representations. These contain all the information needed to plan complex syntheses. While these are good at showing the position of atoms they can be bad for electrons.

In many molecules, electrons are ***delocalised*** and can be drawn in multiple positions.

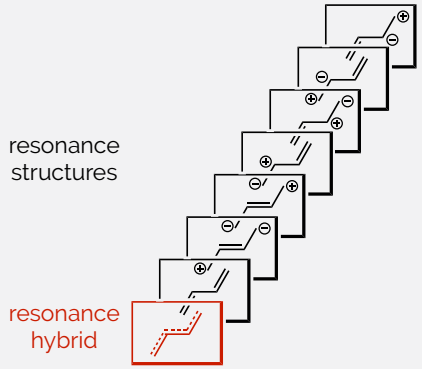
These molecules are best represented by multiple Lewis structures or ***resonance structures*** .

2. Conjugation

Delocalisation of electrons occurs when π bonds are ***conjugated*** or a lone pair is ***conjugated*** with a π bond.

Conjugation occurs when a π bond is separated from a second π bond or lone pair by a single σ bond.

3. Resonance structures & resonance hybrids



If electrons are ***delocalised*** then it will be possible to draw multiple ***allowable*** Lewis structures. Each one of these is a different representation of the ***same*** molecule. They are not different molecules. They are not switching back and forth. They are called resonance structures.

They can be thought of as overlapping to give the real molecule - this is called the ***resonance hybrid***.

4. Drawing resonance

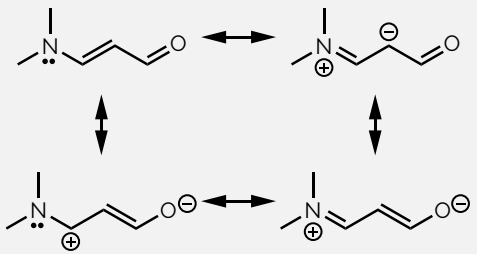
When drawing each resonance structure, they must:

i) Obey the octet rule (they cannot exceed a full valence shell but can have fewer electrons)

ii) Only differ by the position of π bonds or lone pairs of electrons

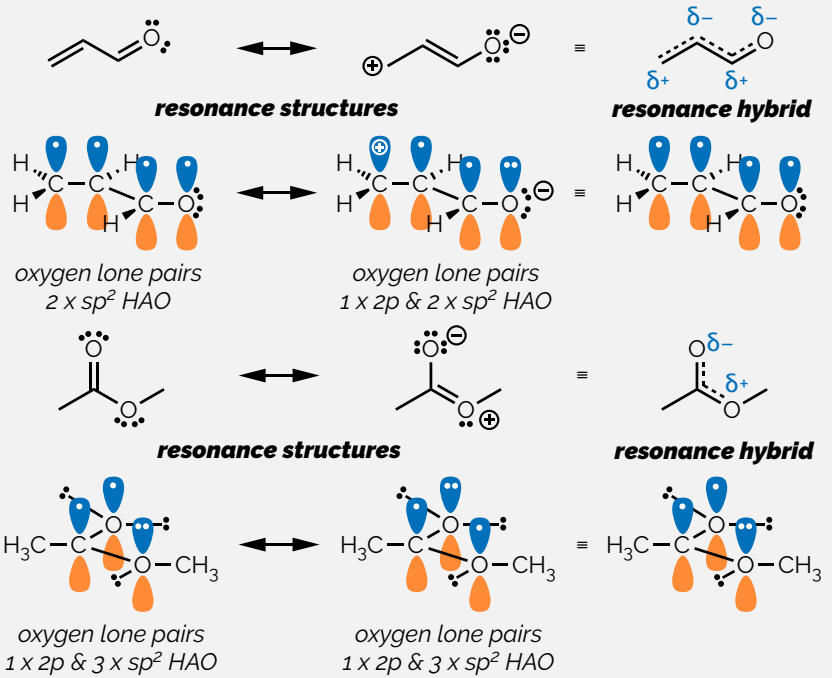
iii) All atoms and σ bonds are in the same place

iv) The overall charge must be the same for all structures



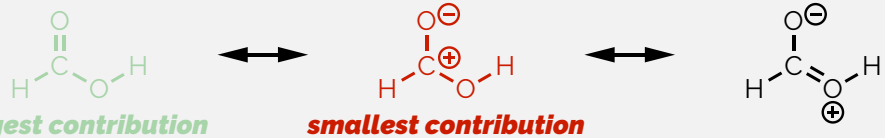
i) All structures obey octet rule (only bottom left has one atom with less than 8 valence electrons). ii & iii) Only differ by position of electrons. iv) All structures are neutral overall.

5. Valence Bond Representations



As all resonance structures represent the same molecule they must invoke the same orbitals. This is only possible if delocalised electrons are in non-hybridised *2p* atomic orbitals. This explains the exception to the hydridisation guidelines on a separate summary sheet.

6. Contribution of resonance structures



largest contribution
all atoms obey octet
no formal charges

smallest contribution
carbon has 6 valence electrons
formal charges on adjacent atoms

The overlap analogy of resonance structures giving the resonance hybrid is not correct. Some resonance structures contribute more to the resonance hybrid. Ranking resonance structures in order of importance (greatest contribution first):

all atoms have full valence shells > no formal charges > formal charges are on correct atoms > formal charges are far apart