Resonance

This sheet should help you understand what resonance is and when it should be considered

What is Resonance?

In some Lewis structures, **electrons can be drawn in multiple positions**, thus creating **multiple allowed Lewis structures** for a single species.

1. Consider that we can obtain **two allowable Lewis structures for acetate** in which the **negative charge** can reside on **either oxygen atom**.



Recall: Allowable Lewis structures are those in which atoms do not exceed a full valence shell and formal charges do not exceed +1 or -1

Rules for drawing resonance structures: do not break single bonds only move electrons

2. We can use curved arrows to show the electron flow required to convert between these two structures, which are referred to as resonance contributors.



Reminder: the double headed arrow indicates the two structures are related through resonance

3. Since either oxygen atom can hold the negative charge, this suggests that the negative charge is shared **(delocalized**) between the two oxygen atoms in acetate.

Thus, let's consider how to represent the average of these two structures, called the **resonance** hybrid.



resonance hybrid (less common representaion)

The electrons are delocalized and the negative charge is shared over the two oxygen atoms, represented by a partial charge δ^{-}

Resonance in Delocalized Lone Pairs

The hybridization of atoms *with lone pairs* is affected *if* the lone pair is delocalized through resonance.

Consider the **negatively charged oxygen** in resonance contributor 1 of acetate, which is adjacent to the C=O π bond and delocalized through resonance.



To correctly assign the hybridization of an atom with a delocalized lone pair, we must first consider resonance.

The delocalized lone pair mst be in a p orbital Therefore, the negatively charged oxygen is not sp^3 , but is actually sp^2 -hybridized



Conclusion:

1) Any lone pair that is involved in resonance MUST be in a p orbital and is delocalized

2) We must first consider resonance to determine the hybridization of an atom with a delocalized lone pair



Resonance in π Bonds

Resonance delocalization requires a *p* orbital at each atom involved. Since π bonds (and conjugated π bonds) are by definition formed between overlapping *p* orbitals, resonance occurs in molecules containing π bonds and conjugated π bonds.

Note: sp^3 -hybridized atoms do not have a *p* orbital and cannot participate in resonance.





Note: sp-hybridized atoms can also participate in resonance as they have *p* orbitals

Consider propylbenzene

Similar to acetate (page 1 and 2), wherein two Lewis structures were possible, there are two Lewis structures that represent the π bonding in any benzene ring. These two structures are also resonance contributors.



To illustrate the continuous overlap of p orbitals in benzene rings, we can consider the resonance hybrid (which best describes the delocalization in benzene rings).

various representations of the resonance hybrid of benzene





overlap of *p* orbitals