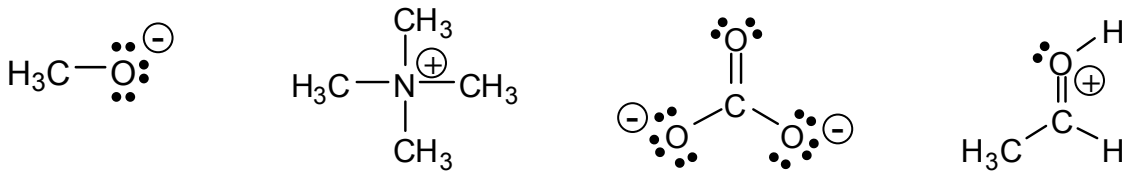
Chemistry 2301

Workshop 4 Solutions
Charge and Resonance

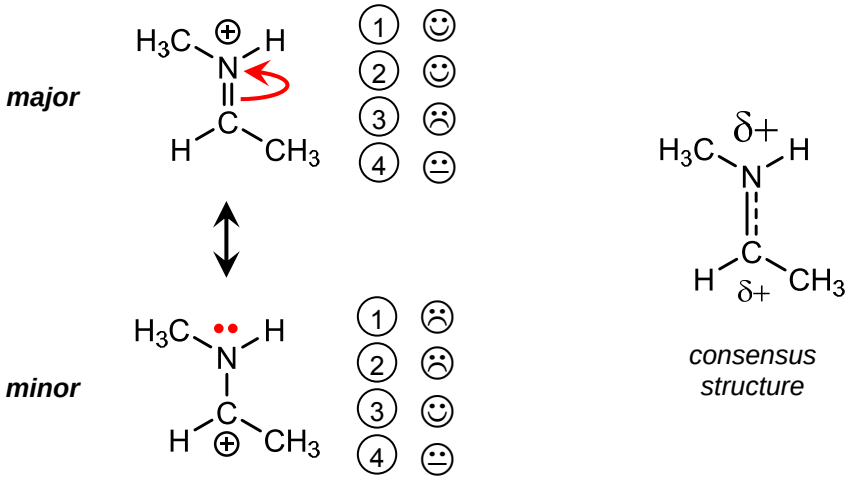
1.



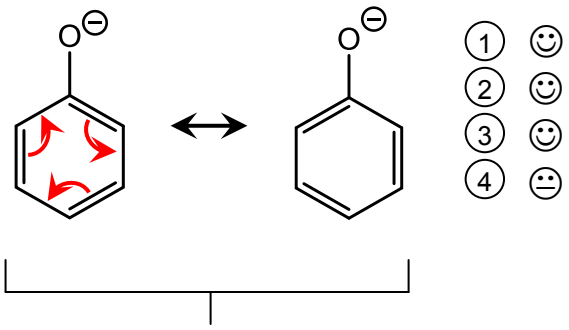
In my opinion, the best way to keep track of this is to look for a number of bonds that doesn't match the typical valency of an atom (2 for oxygen, 3 for nitrogen).

2. When we evaluate resonance structures, we use four criteria, in order of importance:

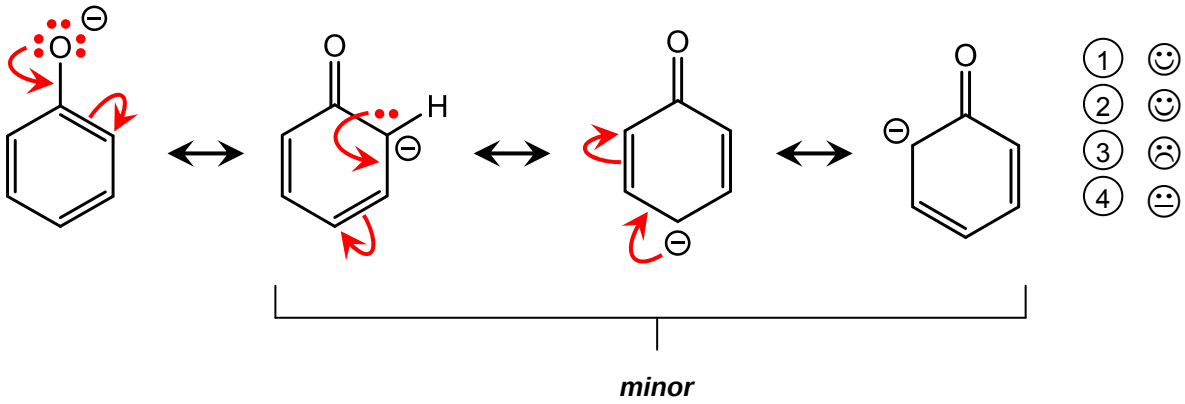
   1. Filled octets are better than unfilled octets.
   2. More bonds (in total) are better than fewer bonds.
   3. If a molecule has charges, they should be matched with atoms of similar (relative) electronegativity.
   4. Fewer formal charges is better than more formal charges.



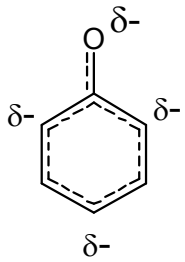
How do you get from one resonance structure to another? I've tried to illustrate how with the red arrow above; just pick up a pair of electrons from a π bond or a lone pair, and move it to another atom or bond nearby. Here, I moved electrons from a π bond towards an electron-deficient (positively charged) nitrogen atom.



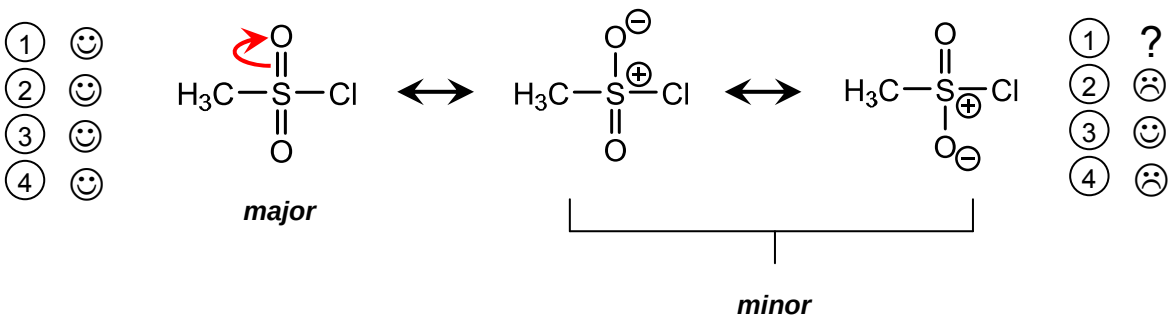
Once again, I've used curved arrows to illustrate how I can move electrons around to create resonance structures from other resonance structures. Below, you'll notice that I started one arrow from a negative charge. This is because a negative charge typically means, "I have extra lone-pair electrons." (You can't similarly move a positive charge—you can't move a lack of electrons.)



Kind of interesting—our consensus structure has partial negative charges at some carbons, but not others.

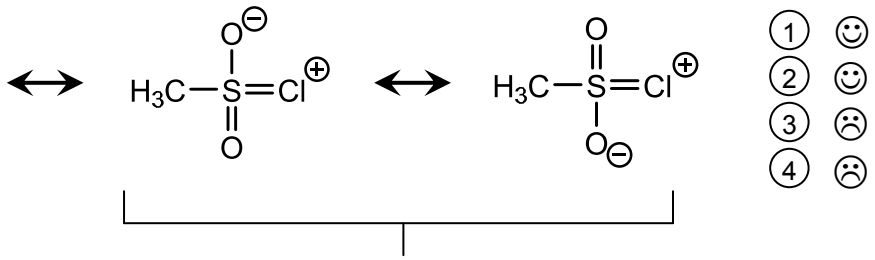


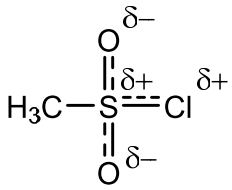
consensus structure



In the case of the 2nd and 3rd resonance structures on the previous page, I don't know how to address whether sulfur (S) has a filled octet or not. S starts with an outer shell of 12 electrons, and both resonance structures on the left have less than that. But S can accommodate 10 electrons in its outermost shell too. I've left the question open.

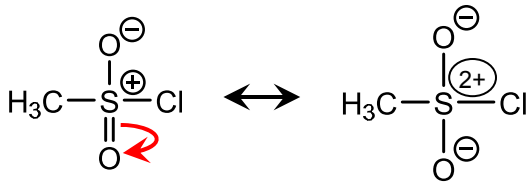
Some students ask me: "Aren't the two resonance structures on the right the same?" They look the same. But the two resonance structures would lead us to conclude that *both* oxygen atoms are partially charged, which makes good sense. If we only drew one, we might conclude that just one oxygen was partially charged, and the other was neutral, which makes no sense. (Another way of thinking about it: imagine that our oxygen atoms have names, John and Susan. Why would John be charged and Susan not?)





consensus structure

One structure that I think doesn't contribute, but which you might have come up with, puts a double-positive charge on sulfur:



The small atoms in organic molecules will do just about anything to avoid having multiple charges on the same atom. (That makes them different from the large metal ions that you dealt with in general chemistry, which can more easily accommodate charges like 2+ or 3+.)