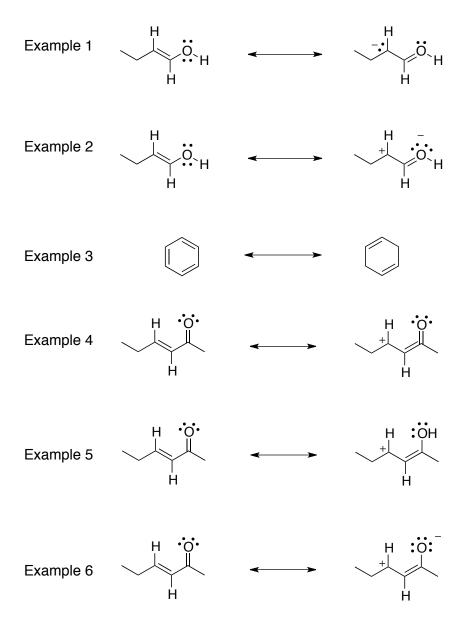
## **CHAPTER 2: RESONANCE THEORY**

**The Basics.** Use the 'Rules for writing acceptable contributing structures' for this exercise (some hydrogens have been added for clarity)

- 1. For each example, add curved arrows to the left structure to show a reallocation of elections that would result in the Lewis structure on the right.
- 2. If an example proposes a resonance structure that is not valid (use the 'Rules for writing acceptable contributing structures'), place an X through the example. Use the space to the right of the example to provide a brief explanation of what the problem is.
- 3. If an example proposes a resonance structure that IS valid, use the 'Relative Importance of Resonance Contributing Structures' to identify and circle the preferred/most relevant resonance structure. Use the space to the right of the example to provide a brief explanation for your choice.



**Now YOU try.** For each example below, draw all the *relevant* resonance structures that you can. I've tried to simplify things and give you hints as to how many relevant resonance structures can be drawn (where I've drawn the first one). When you're finished, use numbers to rank them in order of their relevance - where 1 is the best.

Make sure you draw curved arrows to show the reallocation of electrons that lead to your proposed resonance structure(s)

Chemistry! Now let's use resonance theory to describe some experimental data.

Example 1. In comparison to cyclohexanol, phenol is a much stronger acid. This means that the conjugate base of phenol is more stable (lower energy) than the conjugate base of cyclohexanol (less stable, relatively high energy). Use resonance theory/structures to explain this.

Example 2. In the first step of a hydrolysis reaction, water (the oxygen, actually) is attracted to the carbon of the right-hand molecule, as shown below. This is a relatively slow reaction.

$$H_2O + H_3C - C - OCH_3$$
 $H_3C - C - OCH_3$ 
 $H_3C - C - OCH_3$ 

In the two-step process shown below, however, the carbonyl first reacts with acid (H+), then the positively charged intermediate that it makes reacts with water. This second reaction is relatively fast when compared to the reaction that used no acid catalyst. Use resonance theory/structures to explain this.

$$OCH_3$$
 + H+

 $OCH_3$ 
 $OCH_3$ 

Example 3. When 3,4-dihydropyran is treated with acid (H+), one of three reactions is possible (each are shown below). A box is added around the H+ so you can follow where it goes on the right side of each of the reaction arrows. As shown, only the bottom reaction prevails. Use resonance theory/structures to explain this.

Example 4. When a hydroxyl functional group acts as an acid and donates a proton (H+), the oxygen of the resulting conjugate base will become negatively charged and will hold three lone-pairs of electrons. Of the four hydroxyl groups on ascorbic acid, **A** is the most acidic; describe why (be specific). Use resonance theory/structures to explain this. (this question was on last year's second exam!)

Example 5. Each of these reactions represent an  $S_N2$  alkylation reaction between imidazole (the nitrogen-containing molecule) and isobutyliodide; something we'll learn much more about later in the semester and especially in CHM 224.

Although these reactions appear quite similar, treatment of imidazole with isobutyliodide in the presence of base ONLY follows reaction pathway  $\bf A$  - not  $\bf B$ . Use resonance theory/structures to explain this.

Example 6. Acetophenone (shown below) is made of an acetyl group (COCH $_3$ ) attached to a benzene ring. Using a Nuclear Magnetic Resonance spectrometer (NMR), it can be shown that the six carbons that make up the benzene ring are not all magnetically unique; in fact there are four unique carbons they are labeled  $\bf a$ ,  $\bf b$ ,  $\bf c$  and  $\bf d$ . What can also be determined from the NMR data is that carbons  $\bf a$ ,  $\bf b$  and  $\bf d$  are electron deficient (meaning they have a partial positive charge) when compared to the carbons labeled as  $\bf c$ . One can argue carbon  $\bf a$  is electron deficient because of an inductive effect (the carbonyl oxygen is pulling electrons toward itself; through-bond communication). Use resonance theory/structures, explain why carbons  $\bf b$  and  $\bf d$  are electron deficient when compared to  $\bf c$ .