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Structure Influences Acidity and Basicity

Read the instructions carefully and answer the following questions in the space provided. Then attach the PDF file on Discussion Board for peer discussion and peer review

1. In one or two sentences or with an illustration, discuss how each of the four factors below play a role in determining relative acidity strength. In other words, discuss the general trends, be concise and specific.

a. Periodic Trends
b. Resonance
c. Induction
d. Orbitals

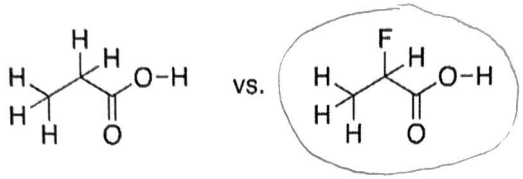
a. After deprotonation of conjugate bases, if comparable atoms are in the same row (less important), choose the more electronegative. If the atoms are in the same column (more important), choose the larger atom.

b. When we look at the conjugate bases after deprotonation, the more acidic is the structure having a resonance structure because the charge is being delocalized (more stable). Also, we can identify compounds containing a C=O bond directly to an OH bond are generally mildly acidic.

c. Induction due to electronegative atoms makes a structure more stable, which means more acidic.

d. As we increase the number of bonds a proton has, it becomes more stable; which means more acidic. This is related to hybridization of the orbitals. So, hybridization for 3 single bonds sp will tend to be more acidic, than a double bond with sp^2 hybridized, which is in turn more acidic than the single bonds found in sp^3

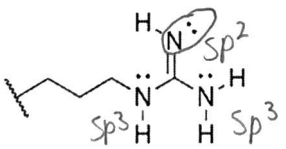
2. Analyze the two compounds below. Circle the structure which is most acidic overall. Discuss the factors that led you to this choice.



Discussion:

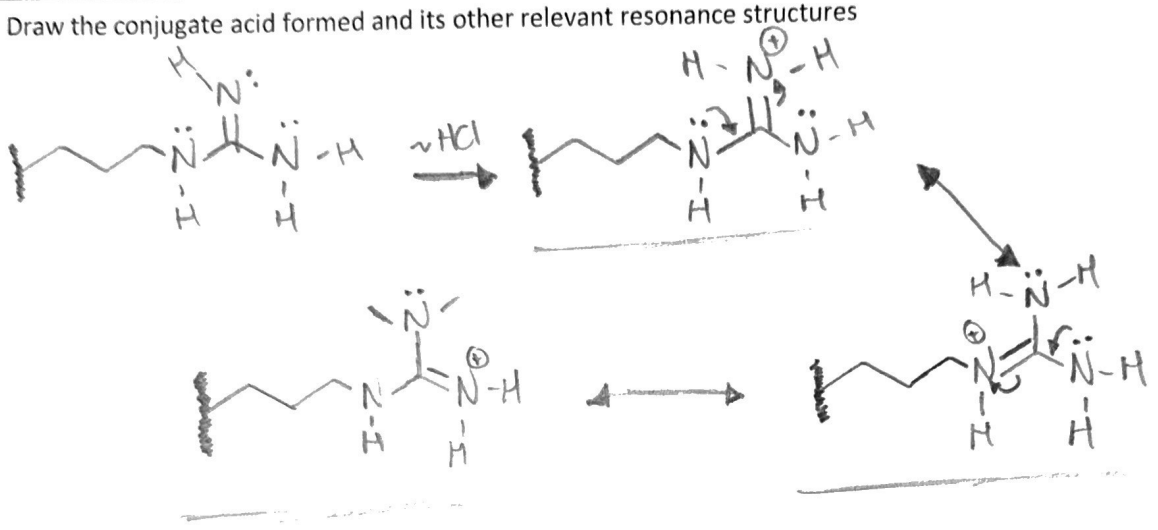
Based on chapter 3.4 of the book, we learned the four factors for differentiation of acids. It is noticeable the third factor, which is induction, differentiate the two structures. So, the compound on the right side is more acidic.

3. Analyze the structure below. Circle the nitrogen atom which is considered to be overall most basic. Provide a brief discussion to explain why this nitrogen is considered to be most basic (hint: think about the orbital each nitrogen lone-pair occupies). Draw relevant resonance structures of the conjugate acid expected to form when this structure is treated with 1 equivalent of HCl. Underline the resonance structure(s) that have filled octets everywhere.

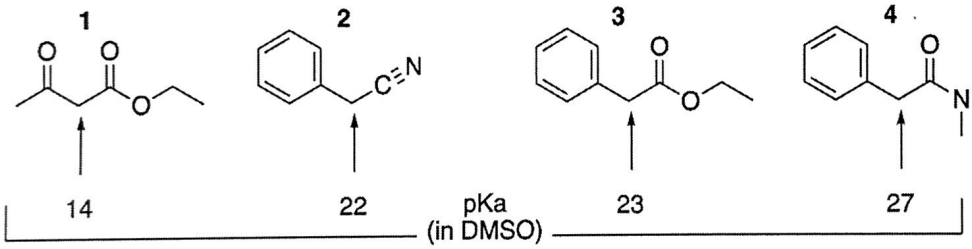


Discussion: The hybridization state of the circled nitrogen has an sp^2 compared to the other nitrogens which are sp^3 making it more basic.

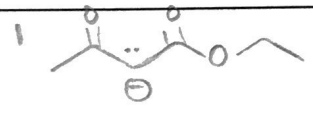
Draw the conjugate acid formed and its other relevant resonance structures

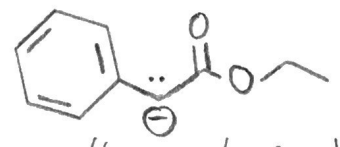


4. The pKa of the most acidic CH_2 group in each of the following compounds was measured in DMSO as solvent (reference: J. Org. Chem. 1981, 46, 4327–4331.)



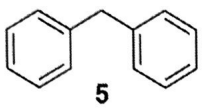
Given the pKa data above, propose an explanation why compound 1 is more acidic than compound 3.



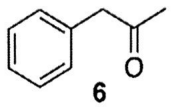


Same hybridization state on both carbons. However, the first compound has more C=O bonds. A hint from resonance structures meaning two oxygens are participating in resonance getting the negative charge on the more electronegative. In the second compound only one oxygen is involved in resonance.

Given the pKa data above, propose which of the following two compounds below (**5** or **6**) is more acidic by comparing the stability of the corresponding conjugate bases. Include (ie. draw) all relevant resonance contributors in your discussion. Do any resonance structures have greater contribution than others to the overall stability? Underline the resonance structure that is considered to be most stable overall.



5



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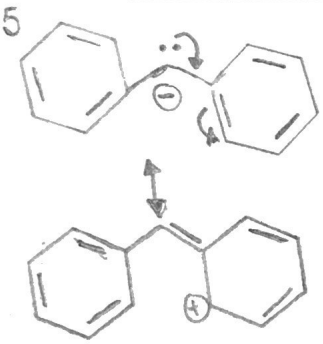
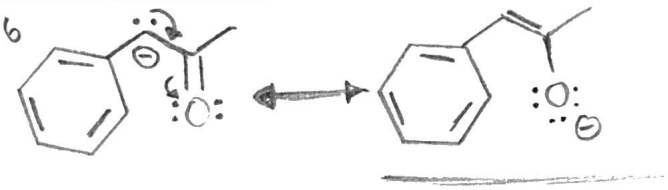
5



Even though compound number 5 is also involved in resonance, the resonance structures are C=C bonds which makes the compound less acidic than number 6.

6



It is clear compound number 6 is more acidic since its conjugate base has a C=O bond involved in resonance. Going back to chapter 2.11 when we look for a relevant contribution we follow "A structure with a negative charge on the more electronegative element will be more significant" which means the underline resonance is more stable.