Chem 241 Activity: Acids and Bases-Predicting Acid/Base Strength

Due Weds, Oct 17. You can work individually or in groups of 2, 3, 4 or 5.

Name(s)___________________________________________________________________________

Before you begin you will want to review sections 1.16, 1.17, 1.18, 1.20 and 1.21 in Bruice

Stability of Conjugate Base

The strength of an acid can be predicted by estimating the stability of the conjugate base formed. The stability of a base is affected by the following factors: electronegativity, hybridization and size.

Model 1

\[
\text{acid} \rightarrow \text{H}^+ + \text{A}^-
\]

Questions:
1. (a). In the forward direction of the above reaction if the conjugate base is stable, would the acid be (circle one) more likely / less likely to give up the proton?

(b). In the forward direction of the above reaction, if the conjugate base is unstable, would the acid be (circle one) more likely / less likely to give up the proton?

(c). The more stable the conjugate base, then the acid it is derived from is (circle one) stronger / weaker.

Model 2: Acidity and Electronegativity Values (see section 1.17 for understanding pKa values and section 1.3 and 1.21 for electronegativity)

<table>
<thead>
<tr>
<th>Element</th>
<th>Electronegativity</th>
<th>pKa</th>
<th>HA → H⁺ + A⁻</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>4.0</td>
<td>3.2</td>
<td>HF → H⁺ + F⁻</td>
</tr>
<tr>
<td>O</td>
<td>3.4</td>
<td>15.7</td>
<td>HOH → H⁺ + HO⁻</td>
</tr>
<tr>
<td>N</td>
<td>3.0</td>
<td>36</td>
<td>HNH₂ → H⁺ + H₂N⁻</td>
</tr>
<tr>
<td>C</td>
<td>2.5</td>
<td>40</td>
<td>HCH₃ → H⁺ + H₃C⁻</td>
</tr>
</tbody>
</table>

Compare electronegativity of elements of similar size.

Questions
2. (a). Of the four elements listed in Model 2, which element is the most electronegative? Which element is the least electronegative?

(b). An electronegative element (circle one) attracts / repels electrons.
(c). In the general reaction $\text{HA} \rightarrow \text{H}^+ + \text{A}^-$, which conjugate base (A-) would be more stable, the one derived from the more electronegative element or the least electronegative element as noted in 2a above?

(d). Of the four conjugate bases listed in Model 2, (F⁻, HO⁻, H₂N⁻, H₃C⁻) rank them from most stable to least stable.

(e). Construct a statement on how the stability of the conjugate base relates to the pKa values listed in Model 2.

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Model 3: Acidity and Size (see section 1.21)

<table>
<thead>
<tr>
<th>Element</th>
<th>pKa</th>
<th>$\text{HA} \rightarrow \text{H}^+ + \text{A}^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>3.2</td>
<td>HF $\rightarrow$ H⁺ + F⁻</td>
</tr>
<tr>
<td>Cl</td>
<td>-2.2</td>
<td>HCl $\rightarrow$ H⁺ + Cl⁻</td>
</tr>
<tr>
<td>Br</td>
<td>-9</td>
<td>HBr $\rightarrow$ H⁺ + Br⁻</td>
</tr>
<tr>
<td>I</td>
<td>-10</td>
<td>HI $\rightarrow$ H⁺ + I⁻</td>
</tr>
</tbody>
</table>

Larger

Questions:

3. From the information shown in Model 3:
   (a). Which element is the largest in size? Which element is the smallest?

   (b). How does the size of the element relate to the pKa values given?

   (c). What conclusions can you make about how size affects the stability of the base?
Model 4: Acidity and Hybridization

\[ \begin{align*}
H_3C\equiv CH_3 + BH_3 & \rightleftharpoons H_3C\equiv CH_2 + HB \quad \text{pKa}=50 \quad \text{Eq. 6} \\
H_2C\equiv CH_2 + BH_3 & \rightleftharpoons H_2C\equiv CH + HB \quad \text{pKa}=44 \quad \text{Eq. 7} \\
HC\equiv CH + BH_3 & \rightleftharpoons HC\equiv C + HB \quad \text{pKa}=25 \quad \text{Eq. 8}
\end{align*} \]

Questions:
4. (a). Using the pKa values, which compound is most acidic, that from Eq. 6, 7 or 8?

(b). Compare the conjugate base from each reaction. Focus on the atom that contains the charge and determine if there are any differences in electronegativity or size.

(c). What is the hybridization of each carbon in each of the starting materials in Eq, 6, 7, 8?

(d). Are there any differences in hybridization between the conjugate bases in Eq. 6, 7, 8?

(e). Based on hybridization, which compound has the most s-character? Which has the least s-character?

(f) Construct a statement on how the s-character (or hybridization) of the conjugate base relates to the pKa values.

Additional questions:
5. For each compound, circle the most acidic H.

6. For a and b, rank the following compounds from most acidic to least acidic (rank the protons that are bold).

(a). CH₃OCH₃, CH₃CH₂OH, HCl      (b). CH₃CH₂NH₂, (CH₃)₃N, CH₃CH₂OH

7. Which of the following compounds is the most basic (strongest base).

8. Two of the factor that determine acidity are size and Electronegativity of the conjugates base. Given the fact that the pKa of H₂S is 10 and the pKa of H₂O is 16 which of the 2 factors above do you feel is a more important determinate of acidity? (note that the electronegativity value of S is 2.5 and Oxygen is 3.5) Briefly explain.