Objective

After completing this section, you should be able to

- use $pK_a$ values to calculate $K_{eq}$
- use $pK_a$ values to predict the equilibrium direction of an acid-base reaction.

Key Terms

Make certain that you can define, and use in context, the key term below.

- $pK_a$

Using $pK_a$ values to predict reaction Equilibria

Edit section

By definition, the $pK_a$ value tells us the extent to which an acid will react with water as the base, but by extension, we can also calculate the equilibrium constant for a reaction between any acid-base pair. Mathematically, it can be shown that:

$$K_{eq} \text{ (for the acid base reaction in question)} = 10^\Delta pK_a$$

where $\Delta pK_a$ is the $pK_a$ of product acid minus $pK_a$ of reactant acid.

Consider a reaction between methylamine and acetic acid:

\[
\begin{align*}
\text{H}_3\text{C} & \quad \text{O} \quad \text{H} + \quad \text{H}_3\text{C} & \quad \text{N} & \quad \text{H} \\
\text{pK}_a &= 4.8 & \text{pK}_a &= 10.6
\end{align*}
\]

$pK_a = 4.8$ (stronger acid)

First, we need to identify the acid species on either side of the equation. On the left side, the acid is of course acetic acid, while on the right side the acid is methyl ammonium. The specific $pK_a$ values for these acids are not on our very generalized $pK_a$ table, but are given in the figure above. Without performing any calculations, you should be able to see that this equilibrium lies far to the right-hand side: acetic acid has a lower $pK_a$, is a stronger acid, and thus it wants to give up its proton more than methyl ammonium does. Doing the math, we see that

$$\Delta pK_a = 10.6 - 4.8 = 5.8$$

So $K_{eq}$ is a very large number (much greater than 1) and the equilibrium lies far to the right-hand side of the
equation, just as we had predicted.

If you had just wanted to approximate an answer without bothering to look for a calculator, you could have noted that the difference in pKₐ values is approximately 6, so the equilibrium constant should be somewhere in the order of $10^6$, or one million. Using the pKₐ table in this way, and making functional group-based pKₐ approximations for molecules for which we don’t have exact values, we can easily estimate the extent to which a given acid-base reaction will proceed.

**Example \(\PageIndex{1}\)**

Show the products of the following acid-base reactions, and estimate the value of $K_{eq}$. Use the pKₐ table from Section 2.8 and/or from the Reference Tables.

a) $\text{enz} - \text{S}^\ominus + \text{enz} \text{OH} \rightleftharpoons$  

b) $\text{H}_3\text{C} = \text{O}^- + \text{NH}_3 \rightleftharpoons$  

c) $\text{OH} + \text{O}^- \rightleftharpoons$  

d) $\text{H} \text{N} \ominus + \text{OH} \rightleftharpoons$

**Answer**

a) $\text{enz} - \text{S}^\ominus + \text{enz} \text{OH} \rightleftharpoons \text{enz} \text{H} + \text{enz} \text{O}^- \quad \text{pK}_a = 17 \quad K_{eq} \approx 10^{-5}$

b) $\text{H}_3\text{C} = \text{O}^- + \text{NH}_3 \rightleftharpoons \text{H}_3\text{C} \text{OH} + \text{NH}_2 \quad \text{pK}_a = 10 \quad K_{eq} \approx 10^{-5}$

c) $\text{OH} + \text{O}^- \rightleftharpoons \quad \text{pK}_a = 10 \quad K_{eq} \approx 10^{5}$

d) $\text{H} \text{N} \ominus + \text{OH} \rightleftharpoons \quad \text{pK}_a = 10 \quad K_{eq} \approx 5 \times 10^{5}$

The pKₐ of water is 14.0. Thus the $K_{eq}$ for reaction d) is $\approx 10^4$. 
Exercises

Exercise \( \PageIndex{1} \)

Use the pKa table from Section 2.8 and/or from the Reference Tables to determine if the following reactions would be expected to occur:

a)

\[
\text{Na}^+ + \text{H}^+ + \text{C} = \text{O} \rightarrow \text{Na}^- + \text{C} = \text{O}^2- + \text{H}^+
\]

b)

\[
\text{Na}^+ + \text{H}^+ + \text{C} = \text{O} \rightarrow \text{Na}^- + \text{C} = \text{O}^2- + \text{H}^+
\]

c)

\[
\text{Na}^+ + \text{H}^+ + \text{C} = \text{O} \rightarrow \text{Na}^- + \text{C} = \text{O}^2- + \text{H}^+
\]

Answer

a) Yes - alkenes have pK\(_a\) values of ~35 while alkynes have pK\(_a\) values of ~25. This means that alkynes are more acidic and more likely to donate a proton.

b) Yes - alkenes have pK\(_a\) values of ~35 while alcohols have pK\(_a\) values of ~16-18. This means that alcohols are more acidic and more likely to donate a proton.

c) No - carboxylic acids have pK\(_a\) values of ~4-5 while alcohols have pK\(_a\) values of ~16-18. This means that carboxylic acids are more acidic and more likely to donate a proton (so the reverse reaction would be expected to occur).

Questions

Q2.9.1

In the following reactions give the resulting products and label the conjugate acid and bases.

\[
\text{CH}_3\text{CH}_2\text{OH} \quad \text{NO}_2 \quad \rightarrow
\]

\[
\text{CH}_3\text{OH} \quad \text{H}_2\text{O} \quad \rightarrow
\]
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