2.4: Predicting the Outcome of Acid–Base Reactions

## Using pKa values to predict reaction equilibria

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:

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

where $\Delta pK_a = pK_a$ of product acid minus pK_a of reactant acid

Consider a reaction between methylamine and acetic acid:

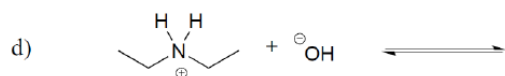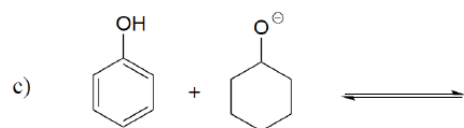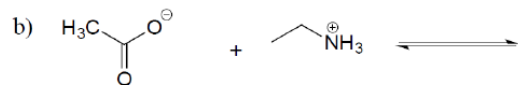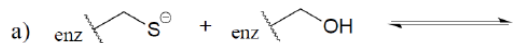pKa = 4.8
(stronger acid)

pKa = 10.6
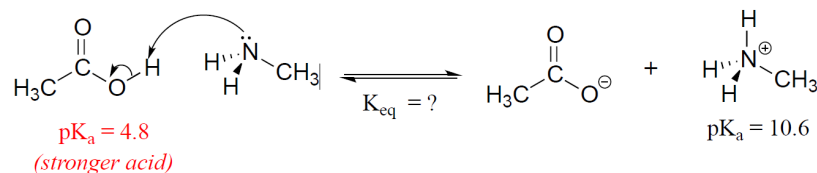
First, we need to identify the acid species on either side of the equation. On the left side, the acid is of course acetic acid, while on the right side the acid is methyl ammonium. The specific pK_a values for these acids are not on our very generalized pK_a table, but are given in the figure above. 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

$$K_{eq} = 10^{\Delta pKa} = 10^{(10.6 - 4.8)} = 10^{5.8} = 6.3 \times 10^5$$
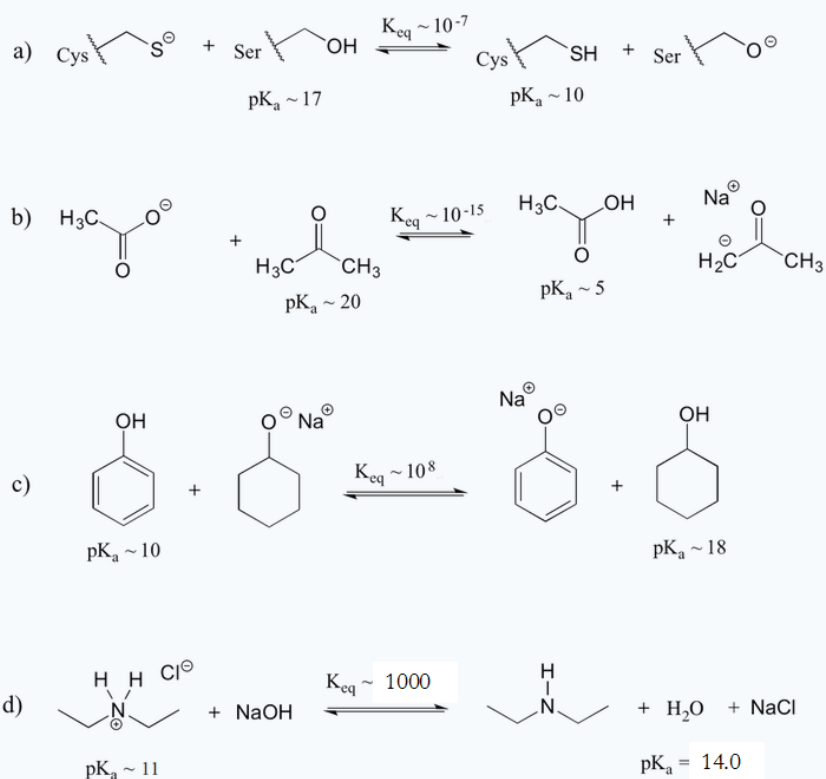
So K_{eq} is a very large number (much greater than 1) and the equilibrium lies far to the right-hand side of the equation, just as we had predicted. If you had just wanted to approximate an answer without bothering to look for a calculator, you could have noted that the difference in pK_a values is approximately 6, so the equilibrium constant should be somewhere in the order of 10^6, or one million. Using the pK_a table in this way, and making functional group-based pK_a 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.

Exercise 2.4.1

Show the products of the following acid-base reactions, and estimate the value of K_{eq}. Use the pKa table from Section 2.3 and/or from the Reference Tables.

Answer
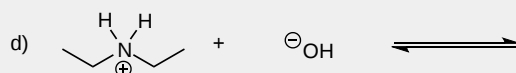
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a) Cys–S⁻ + Ser–OH $\xrightleftharpoons{K_{eq} \sim 10^{-7}}$ Cys–SH + Ser–O⁻

$pK_a \sim 17$ $pK_a \sim 10$

b) H_3C–CO–O⁻ + H_3C–CO–CH_3 $\xrightleftharpoons{K_{eq} \sim 10^{-15}}$ H_3C–CO–OH + Na⁺ ⁻H_2C–CO–CH_3

$pK_a \sim 20$ $pK_a \sim 5$

c) PhOH + cyclohexyl–O⁻ Na⁺ $\xrightleftharpoons{K_{eq} \sim 10^8}$ Na⁺ ⁻O–Ph + cyclohexyl–OH

$pK_a \sim 10$ $pK_a \sim 18$

d) $R_2NH_2^+$ Cl⁻ + NaOH $\xrightleftharpoons{K_{eq} \sim 1000}$ R_2NH + H_2O + NaCl

$pK_a \sim 11$ $pK_a = 14.0$

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Example 7.3

Exercise 7.3 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) enz~CH₂S⁻ + enz~OH ⇌
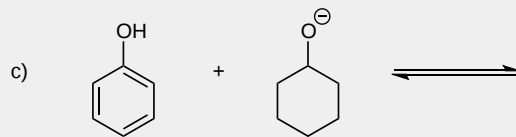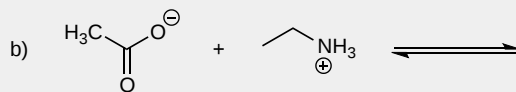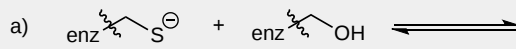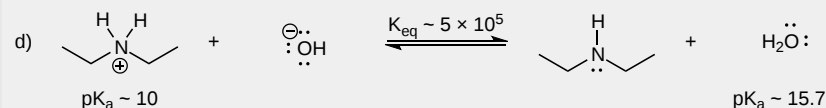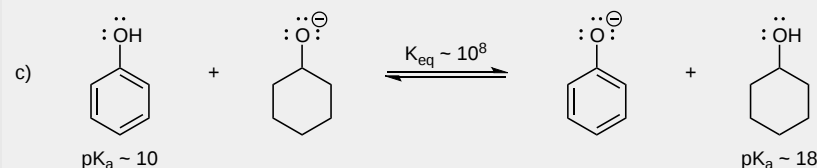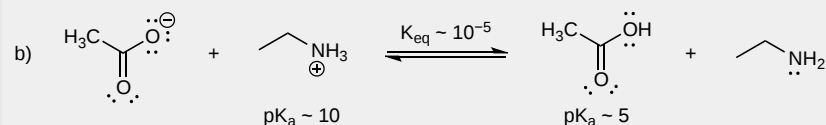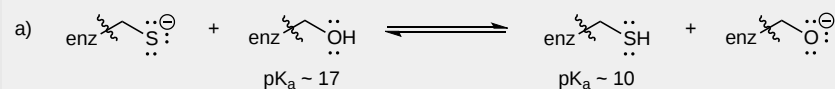
b) H_3C-C(O)-O⁻ + $CH_3CH_2NH_3^+$ ⇌

c) phenol-OH + cyclohexyl-O⁻ ⇌

d) $(CH_3CH_2)_2NH_2^+$ + ⁻OH ⇌

Solution

a) enz~CH₂S⁻ + enz~OH ⇌ enz~CH₂SH + enz~O⁻
   pKₐ ~ 17 (under OH)   pKₐ ~ 10 (under SH)

b) H_3C-C(O)-O⁻ + $CH_3CH_2NH_3^+$ ⇌ (Keq ~ 10⁻⁵) H_3C-C(OH)(O⁻) + $CH_3CH_2NH_2$
   pKₐ ~ 10   pKₐ ~ 5

c) phenol-OH + cyclohexyl-O⁻ ⇌ (Keq ~ 10⁸) phenol-O⁻ + cyclohexyl-OH
   pKₐ ~ 10   pKₐ ~ 18

d) $(CH_3CH_2)_2NH_2^+$ + ⁻OH ⇌ (Keq ~ 5 × 10⁵) $(CH_3CH_2)_2NH$ + H_2O
   pKₐ ~ 10   pKₐ ~ 15.7

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