2.8: PREDICTING ACID-BASE REACTIONS FROM PKA VALUES

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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

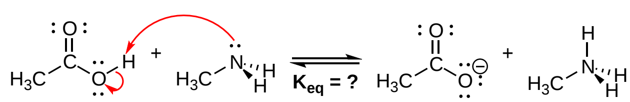
USING PK$_A$ VALUES TO PREDICT REACTION EQUILIBRIA

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 ΔpK_a is the pK_a of product acid minus pK_a of reactant acid

Consider a reaction between methylamine and acetic 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

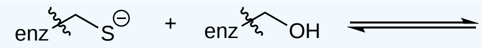
$$K_{eq} = 10^{\Delta pK_a} = 10^{10.6-4.8} = 10^{5.8} = 6.3 \times 10^5$$

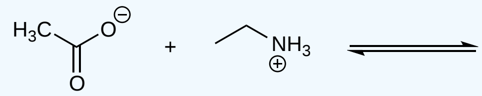
So K_{eq} is a very large number (much greater than 1) and the equilibrium lies far to the right-hand side of the equation, just as we had predicted.

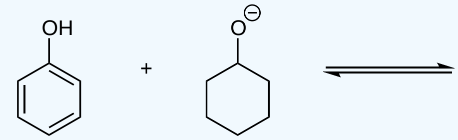
If you had just wanted to approximate an answer without bothering to look for a calculator, you could have noted that the difference in pK_a values is approximately 6, so the equilibrium constant should be somewhere in the order of 10^6, or one million. Using the pK_a table in this way, and making functional 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.

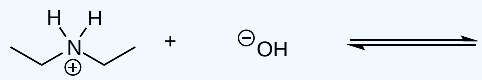
EXAMPLE 2.8.1

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

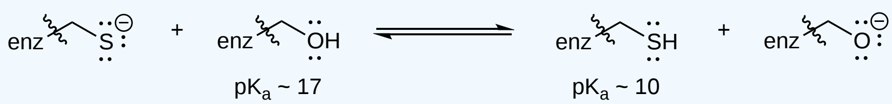
a) 

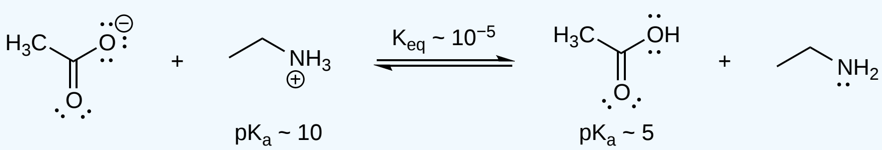
b) 

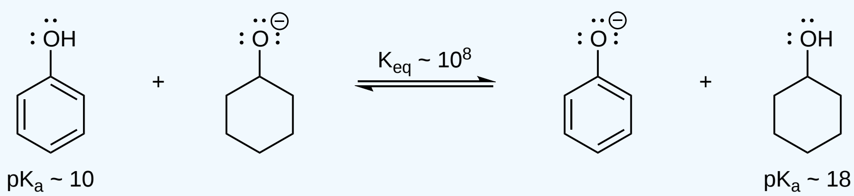
c) 

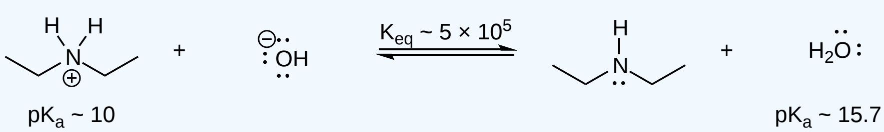
d) 

Answer

a) 

b) 

c) 

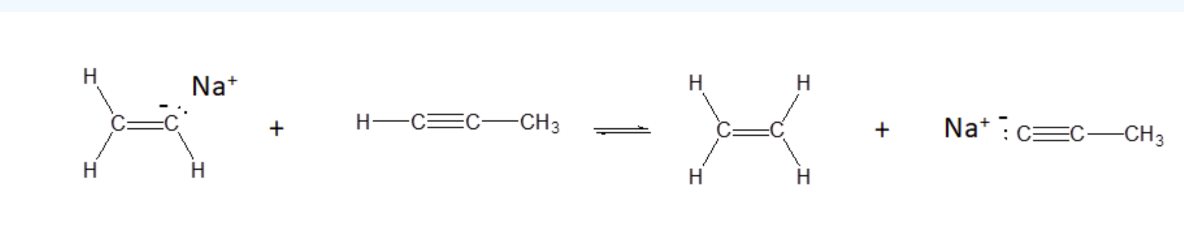
d) 

The pK_a of water is 14.0. Thus the K_{eq} for reaction d) is ~ 10^4.

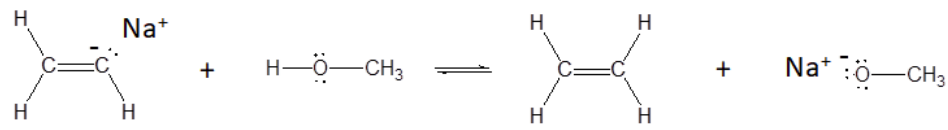
EXERCISES

? EXERCISE 2.8.1

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)

b) 

c) 

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.

$CH_3CH_2OH \quad NO_2 \longrightarrow$

$CH_3OH \quad H_2O \longrightarrow$

SOLUTIONS

S2.9.1

$$CH_3CH_2OH + NO_2 \longrightarrow \underset{\text{Conjugate base}}{CH_3CH_2O^-} + \underset{\text{Conjugate acid}}{HNO_2}$$

$$CH_3OH + H_2O \longrightarrow \underset{\text{Conjugate base}}{CH_3O^-} + \underset{\text{Conjugate acid}}{H_3O^+}$$