Weak Acid/Weak Base Equilibrium Calculations

Starting with an acid (proton donor)

$A + H_2O \rightleftharpoons N + H_3O^+$

$K_a = \frac{[N]\,[H_3O^+]}{[A]}$

$R-COOH + H_2O \rightleftharpoons R-COO^- + H_3O^+$

$\frac{[N]}{[A]} = 10^{(pH - pK_a)}$

$$\text{Fraction of charged conjugate} = \frac{\frac{[N]}{[A]}}{\frac{[N]}{[A]} + 1}$$

$P + H_2O \rightleftharpoons B + H_3O^+$

$K_a = \frac{[B]\,[H_3O^+]}{[P]}$

$R-NH_3^+ + H_2O \rightleftharpoons R-NH_2 + H_3O^+$

$\frac{[P]}{[B]} = 10^{(pK_a - pH)}$

$$\text{Fraction of charged conjugate} = \frac{\frac{[P]}{[B]}}{\frac{[P]}{[B]} + 1}$$

		Lower pH			pH =pKa	Higher pH			
	2	1.5	1	0.5		0.5	1	1.5	2
$A + H_2O \rightleftharpoons N + H_3O^+$									
Percent Negative	1%	3%	9%	24%	50%	76%	91%	97%	99%
					pH =pKa				
$P + H_2O \rightleftharpoons B + H_3O^+$									
Percent Positive	99%	97%	91%	76%	50%	24%	9%	3%	1%

Starting with a base (proton acceptor)

$B + H_2O \rightleftharpoons P + OH^-$

$K_b = \frac{[P]\,[OH^-]}{[B]}$

$R-NH_2 + H_2O \rightleftharpoons R-NH_3^+ + OH^-$

$N + H_2O \rightleftharpoons A + OH^-$

$K_b = \frac{[A]\,[OH^-]}{[N]}$

$R-COO^- + H_2O \rightleftharpoons R-COOH + OH^-$

Water $H_2O + H_2O \rightleftharpoons OH^- + H_3O^+$ $\quad K_w = 10^{-14}$

Conjugate acid/base pair $\quad K_a K_b = 10^{-14}$