Pharmacy 331 Thompson: Spring 2004
Problem Set #2

pH, pKa and Henderson-Hasselbalch Calculations (corrections 2/5/04)

1. Calculate the concentration of benzoic acid and benzoate in a solution whose pH = 5.2. The pKa of benzoic acid is 4.20 and the solution was prepared to be 0.005 M benzoic acid. (Connors, p. 164)

pH = pKa + log[A-/HA]
5.20 = 4.20 + log[A-/HA]
1.0 = log[A-/HA]

10 = [A-]/[HA] → says the concentration of benzoate is ten times that of benzoic acid or the fractional amount is: [A-]/([HA] + [A-]) or 1/11 [HA] and 10/11 [A-].
The fractional amount of [HA] is: 0.005 M x 1/11 = .0004545 M (4.5 x 10^{-4} M)
The fractional amount of [A-] is: 0.005 M x 10/11 = .004545 M (4.5 x 10^{-3} M)

2. From class… Calculate the pH of a buffer solution prepared by dissolving 242.2 mg of tris(hydroxymethyl)aminomethane in 10.0 mL of 0.170 M HCl and diluting it to 100 mL with water. The mw of tris = 121.1 and has a pKa = 8.08. Connors p. 170

Tris: 242.2 mg/121.1 g/mol = 2.00 mmol (or 0.002 M).
HCl: 10 mL x 0.170 M/L = 1.7 mmol or 0.0017 M)

If 1.7 mmol HCl is added to 2.0 mmol of tris then 1.7 mmol of tris-HCl forms but leaves 0.3 mmol ~~HCl~~ tris unreacted (tris HCl is ~~as~~ the conjugate acid). And….

Note: My narrative error from discussion section is denoted in blue (vs. red strikeout) above – thanks to those of you who caught it. The numbers are correct.

pH = pKa + log[A-/HA] or pH = pKa + log[tris/trisHCl] (tris is equivalent to the ionized A- and trisHCl is equivalent to the acid HA.

pH = 8.08 + log [0.3/1.7) = 7.32

3. Ephedrine (pKa = 9.6) reacts with hydrochloric acid to afford the ephedrine hydrochloride salt. If you react 1 M ephedrine with 1 M HCl what is the pH? (Cairnes p. 22)

The key is to remember is that when you add 1.0 M ephredrine to 1.0 M HCl the result is a 0.5 M solution. For example, adding 10 mL of 1 M ephedrine to 10 mL of 1.0 M HCl gives you 20 mL from the same molarity – but a net dilution of two-fold or 0.5 M. So….

pH = ½pKa – ½ log C
= ½ (9.6) – ½ log (0.5 M)
= 4.8 – (-0.15)
= 4.95

4. What is the pH of 0.05 M sodium acetate given that acetic acid pKa = 4.66. Although sodium acetate is a weak base, we can use the weak acid equation to calculate and then substract from 14.

Sodium acetate is a weak base so we substitute for pKa using the equation:
pKw = pKa + pKb or
pKw – pKb = pKa

if pH = ½pKa – ½ log C
then pH = ½ (pKw – pKb) – ½ log C
= ½ (14 - 4.66) – ½ log (0.05 M)
= 4.67 – (-0.65)
= 5.32
and
14 - 5.32 = 8.68

5. An antilog calculation!! Calculate the concentration of acetic acid needed to be added to a 0.1 M solution of sodium acetate to give a buffer of pH 5 (pKa of acetic acid= 4.66). (Cairns, p. 24)

pH = pKa + log[A-/HA]
5.0 = 4.66 + log (0.1/HA)
0.34 = log 0.1 – log[HA]
1.34 = -log[HA]
0.045 M [acetic acid]

6. Calculating the fractional amount of a compound in the ionized and unionized forms. Pentobarbitone (pKa 8.0) is a weak acid. Calculate the percentage of a dose of this drug in the plasma (pH 7.4).

First, since the pH is lower than the pKA, the higher proportion of the drug will be unionized!!!
pH = pKa + log[A-/HA]
7.4 = 8.0 + log[A-/HA]
-0.6 = log[A-/HA]
0.25 = ¼ = [A-]/[HA] or there are four HA's for every one A-. 4 + 1 = 5 total.
So the fractional amounts are 4/5 x 100% pHA] and 1/5 x 100% [A-]
80% pentobarbitone and 20% pentobarbitone anion (conjugate base).