Sample Calculations

1. Polyprotic Acids, Buffers and Alpha Fractions

H₂Z is a diprotic acid with a pK₁ = 5.92 and pK₂ = 8.77.

a) What is the pH of a solution where the alpha fractions for HZ⁻ and Z²⁻ are both equal to 0.5? [Note: you only need to report this pH with an accuracy of 0.01 pH units]

b) If the total acid concentration is 0.100M, what is the concentration of the acid species H₂Z at this pH?

2. Barium Oxalate Calculation

Barium Oxalate is only sparingly soluble in water with a K_sp = 2.3 x 10⁻⁸. The [Ba²⁺] can be changed in a system by varying the pH. Given an Oxalic Acid C_tot of 0.1M, find the [Ba²⁺] at a pH of (a) 1.0 and (b) 5.0.

Oxalic acid is a diprotic acid with a pK₁ = 1.25 and pK₂ = 4.14.

3. Mg-EDTA Complexation

Consider a Na₂MgY solution with a formal concentration of 1.50 x 10⁻³M. The solution is also buffered to a pH of 9.75, where the alpha fraction for Y⁴⁻ is 0.236.

a) Calculate the pMg = -log[Mg²⁺] for this solution.

b) Calculate the pMg = -log[Mg²⁺] for a solution with Na₂MgY = 1.50 x 10⁻³M and EDTA = 0.01M.

For the MgY²⁻ complex, log K_f = 8.69.
4. Complexation Equilibria

Acetic acid (HOAc) is a monoprotic acid with a \( pK_a = 4.75 \). \( \text{Cu}^{2+} \) ions will bind with up to two acetate ions (OAc\(^-\)). Consider a solution that (i) has a total copper concentration of \( 3.50 \times 10^{-7} \) M, (ii) has a total acetic acid concentration of 0.3750 M, and (iii) is buffered to a pH of 6.00.

a) Write down (i) the total number and (ii) the chemical formulae of ALL of the copper species that exist in this solution.
b) Calculate the acetate concentration ([OAc\(^-\)]) in this solution.
c) Calculate the \( \text{Cu}^{2+} \) ion concentration in this solution.

5. Potentiometry

Consider the electrochemical cell:

\[
\text{Pt} \mid \text{Ti}^{3+}(4.55 \times 10^{-4} \text{ M}), \text{Ti}^+(3.12 \times 10^{-6} \text{ M}) \parallel \text{Pb}^{2+}(8.93 \times 10^{-5} \text{ M}) \mid \text{Pb}
\]

a) Write down the two half cell reactions the overall reaction for this electrochemical cell.
b) Calculate the potential that you would expect to measure across this electrochemical cell.

The following electrochemical cells are required in the calculations:

\[
\begin{align*}
\text{Ti}^{3+} + 2e^- & = \text{Ti}^+ & \text{E}^\circ \text{ vs. NHE} = +1.250 \text{ V} \\
\text{Pb}^{2+} + 2e^- & = \text{Pb}(s) & \text{E}^\circ \text{ vs. NHE} = -0.126 \text{ V}
\end{align*}
\]
Answers
1. pH=8.77, [H2Z]=7e-05M

2. pH = 1.0; alpha = 2.6e-4;
   pH = 7.0; alpha = 1.0;
   \([\text{Ba}^2+] = \frac{K_{sp}}{(\alpha * 0.1)}\)

3. a) \([\text{Mg}^2+] = \sqrt{1.5-03/(\alpha \cdot K_f)}\)
   b) \([\text{Mg}^2+] = \frac{1.5-03}{(\alpha \cdot 0.01 \cdot K_f)}\)

4. Cu²⁺, Cu(Oac)²⁺, Cu(Oac)²⁺; 3.1e-07M; alpha = 0.10

5. -1.56V