

Chem 151. R. Corn

Diprotic Weak Acid Salt

Constants: K_b , K_w , C_0

Constants: K_{a1} , K_{a2} , K_w , C_0

Six species: $[H_2A]$, $[HA^-]$, $[A^{2-}]$, $[H^+]$, $[OH^-]$, $[Na^+]$

$$K_{a1} = \frac{[H^+][HA^-]}{[H_2A]} \quad \text{acid dissociation 1}$$

$$K_{a2} = \frac{[H^+][A^{2-}]}{[HA^-]} \quad \text{acid dissociation 2}$$

$$K_w = [H^+][OH^-] \quad \text{water dissociation}$$

$$[Na^+] + [H^+] = [HA^-] + 2[A^{2-}] + [OH^-] \quad \text{charge balance}$$

$$C_0 = [H_2A] + [HA^-] + [A^{2-}] \quad \text{mass balance 1}$$

$$2C_0 = [Na^+] \quad \text{mass balance 2}$$

Alpha Fractions

$$\frac{[H_2A]}{C_0} = (1 + \frac{K_{a1}}{[H^+]} + \frac{K_{a1}K_{a2}}{[H^+]^2})^{-1}$$

$$\frac{[HA^-]}{C_0} = (\frac{[H^+]}{K_{a1}} + 1 + \frac{K_{a2}}{[H^+]})^{-1}$$

$$\frac{[A^{2-}]}{C_0} = (\frac{[H^+]}{K_{a1}} + \frac{[H^+]^2}{K_{a1}K_{a2}} + 1)^{-1}$$

Iterative Equations for $[OH^-]$

$$[OH^-][HA^-] = K_b[A^{2-}]$$

$$2C_0 + [H^+] = [HA^-] + 2(C_0 - [HA^-] - [H_2A]) + [OH^-]$$

$$[HA^-] = [OH^-] - 2[H_2A] - [H^+]$$

$$[OH^-]([OH^-] - 2[H_2A] - [H^+]) = K_b[A^{2-}]$$

$$[OH^-]^2 - 2[OH^-][H_2A] - K_w = K_b[A^{2-}]$$

$$[OH^-]^2 = K_b[A^{2-}] + 2[OH^-][H_2A] + K_w$$

$$[\text{OH}^-]^2 = K_{b2}[\text{A}^{2-}] + 2K_{b1}[\text{HA}^-] + K_w$$

Iterative Equations:

$$[\text{A}^{2-}] = C_0$$

$$[\text{OH}^-] = \sqrt{K_{b2}C_0 + K_w}$$

$$[\text{OH}^-] = \sqrt{K_{b2}[\text{A}^{2-}] + 2K_{b1}[\text{HA}^-] + K_w}$$