Chem M3LC. R. Corn

Diprotic Weak Acid

Constants: K1, K2, Kw, Ctot

Five species: [H2A], [HA-], [A2-], [H+], [OH-]

$K1 = [H+][HA-]/[H2A]$ acid dissociation 1

$K2 = [H+][A2-]/[HA-]$ acid dissociation 2

$Kw = [H+][OH-]$ water dissociation

$[H+] = [HA-]+ 2[A2-] + [OH-]$ charge balance

$Ctot = [H2A] + [HA-] + [A2-]$ mass balance

Alpha Fractions

$[H2A]/Ctot = (1 + K1/[H+] + K1K2/[H+]^2)^{-1}$

$[HA-]/Ctot = ([H+]/K1 + 1 + K2/[H+])^{-1}$

$[A2-]/Ctot = ([H+]/K2 + [H+]^2/K1K2 + 1)^{-1}$

Iterative eqns for [H+]

$[H+][HA-] = K1[H2A]$

$[H+]([H+] - [OH-] – 2[A2-]) = K1[H2A]$

$[H+]^2 - 2[H+][A2-] - Kw = K1[H2A]$

$[H+]^2 = K1[H2A] + 2K2[HA-] + Kw$

Initial Guess: $[H+] = sqrt (K1*Ctot + Kw)$

Calculate [H2A], [HA-], [A2-]

$[H+] = sqrt(K1[H2A] + 2K2[HA-] + Kw)$