Chem 151. R. Corn

Diprotic Weak Acid

Constants: Ka1, Ka2, Kw, C0

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

$Ka1 = [H+][HA-]/[H2A]$ acid dissociation 1

$Ka2 = [H+][A2-]/[HA-]$ acid dissociation 2

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

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

$C0 = [H2A] + [HA-] + [A2-]$ mass balance

Alpha Fractions

$[H2A]/C0 = (1 + Ka1/[H+] + Ka1Ka2/[H+]^2)^{-1}$

$[HA-]/C0 = ([H+]/Ka1 + 1 + Ka2/[H+])^{-1}$

$[A2-]/C0 = ([H+]/Ka2 + [H+]^2/Ka1Ka2 + 1)^{-1}$

Iterative eqns for [H+]

$[H+][HA-] = Ka1[H2A]$

$[H+]([H+] - [OH-] – 2[A2-]) = Ka1[H2A]$

$[H+]^2 -2[H+][A2-] - Kw = Ka1[H2A]$

$[H+]^2 = Ka1[H2A] + 2Ka2[HA-] + Kw$

Initial Guess: [H+] = sqrt (Ka1*C0 + Kw)

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

$[H+] = sqrt(Ka1[H2A] + 2Ka2[HA-] + Kw)$