Chem M3LC. R. Corn

Diprotic Weak Acid Ampholyte

Constants: K1, K2, Kw, Ctot

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

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

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

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

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

Ctot = [H2A] + [HA-] + [A2-] mass balance 1

Ctot = [Na+] mass balance 2

Full equations for [H+]

Ctot = [H2A] + [HA-] + [A2-] mass balance 1

Ctot = [Na+] mass balance 2

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

[H+] = [A2-] - [H2A] + [OH-]

[H+] = Ka2[HA-]/[H+] - [H+][HA-]/Ka1 + Kw/[H+]

$[H+]^2$ = (Ka2[HA-] + Kw)/(1 + [HA-]/Ka1)

[H+] = sqrt[(Ka2[HA-] + Kw)/(1 + [HA-]/Ka1)]

Ampholyte Disproportionation:

$2HA \rightarrow H2A + A2-$

$Kd = [H2A][A2-]/[HA-]2 = ([H2A]/[HA-][H+])([H+][A2-]/[HA-]) = K2/K1 << 1$

$[H2A] = [A2-] = [HA-]sqrt(Kd)$

$[H+] = K1[H2A]/ [HA-] = K1sqrt(Kd) = sqrt(K1K2)$

$pH = (pK1 + pK2)/2$