Monoprotic Acids

$$\alpha_0 = \frac{\left[H^+\right]}{\left[H^+\right] + {}^{c}K_a} = \frac{[HA]}{C_{T,A}} \qquad \text{(A1-1)}$$

and

$$\alpha_1 = \frac{{}^{c}K_a}{\left[H^+\right] + {}^{c}K_a} = \frac{\left[A^-\right]}{C_{T,A}} \qquad \text{(A1-2)}$$

When ionic strength effects are negligible, ${}^{c}K_a = K_a$.

A1.2. IONIZATION FRACTIONS FOR MULTIPROTIC ACIDS

The exact equations for a diprotic acid, H_2A, are

$$\alpha_0 = \frac{\left[H^+\right]^2}{E} = \frac{[H_2A]}{C_{T,A}} \qquad \text{(A1-3)}$$

$$\alpha_1 = \frac{\left[H^+\right] {}^{c}K_{a,1}}{E} = \frac{\left[HA^-\right]}{C_{T,A}} \qquad \text{(A1-4)}$$

$$\alpha_2 = \frac{{}^{c}K_{a,1}\,{}^{c}K_{a,2}}{E} = \frac{\left[A^{2-}\right]}{C_{T,A}} \qquad \text{(A1-5)}$$

where $E = \left[H^+\right]^2 + \left[H^+\right] {}^{c}K_{a,1} + {}^{c}K_{a,1}\,{}^{c}K_{a,2}$. When ionic strength effects are negligible, ${}^{c}K_{a,1} = K_{a,1}$ and ${}^{c}K_{a,2} = K_{a,2}$.

For the triprotic acid, H_3A, the equations are:

$$\alpha_0 = \frac{\left[H^+\right]^3}{D} = \frac{\left[H_3A\right]}{C_{T,A}} \qquad \text{(A1-6)}$$

$$\alpha_1 = \frac{\left[H^+\right]^2 {}^{c}K_{a,1}}{D} = \frac{\left[H_2A^-\right]}{C_{T,A}} \qquad \text{(A1-7)}$$

$$\alpha_2 = \frac{\left[H^+\right]\,{}^{c}K_{a,1}\,{}^{c}K_{a;2}}{D} = \frac{\left[HA^{2-}\right]}{C_{T,A}} \qquad \text{(A1-8)}$$

$$\alpha_3 = \frac{{}^{c}K_{a,1}\,{}^{c}K_{a,2}\,{}^{c}K_{a,3}}{D} = \frac{\left[A^{3-}\right]}{C_{T,A}} \qquad \text{(A1-9)}$$

where $D = \left[H^+\right]^3 + \left[H^+\right]^2\,{}^{c}K_{a,1} + \left[H^+\right]\,{}^{c}K_{a,1}\,{}^{c}K_{a,2} + {}^{c}K_{a,1}\,{}^{c}K_{a,2}\,{}^{c}K_{a,3}$. Again if ionic strength effects are negligible, ${}^{c}K_{a,1} = K_{a,1}$, ${}^{c}K_{a,2} = K_{a,2}$, and ${}^{c}K_{a,3} = K_{a,3}$.