Isoelectric Point Calculation

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By rearranging the Henderson-Hasselbalch equation:

$$\mathrm{pH} = \mathrm{pK_a} + \log\left(\frac{[\mathrm{A^-}]}{[\mathrm{HA}]}\right)$$

we can get the ratio between an acid and its conjugate base:

$$\frac{[\mathrm{HA}]}{[\mathrm{A^-}]} = 10^{(\mathrm{pK_a}-\mathrm{pH})}$$

and between an base and its conjugate acid:

$$\frac{[\mathrm{B}]}{[\mathrm{BH^+}]} = 10^{(\mathrm{pH}-\mathrm{pK_a})}$$

Thus, the proportion of deprotonated acid is calculated as follows:

$$\frac{[\mathrm{A^-}]}{[\mathrm{A}]_{\mathrm{total}}} = \frac{[\mathrm{A^-}]}{[\mathrm{HA}]+[\mathrm{A^-}]} = \frac{1}{1+\frac{[\mathrm{HA}]}{[\mathrm{A^-}]}} = \frac{1}{1+10^{(\mathrm{pK_a}-\mathrm{pH})}}$$

Similarly, for basic species:

$$\frac{[\mathrm{BH^+}]}{[\mathrm{B}]_{\mathrm{total}}} = \frac{[\mathrm{BH^+}]}{[\mathrm{B}]+[\mathrm{BH^+}]} = \frac{1}{1+\frac{[\mathrm{B}]}{[\mathrm{BH^+}]}} = \frac{1}{1+10^{(\mathrm{pH}-\mathrm{pK_a})}}$$

http://fields.scripps.edu/DTASelect/20010710-pI-Algorithm.pdf