

Using an Excel Spreadsheet to Calculate K_A from pH and Initial Concentration

Since $K_A = \frac{[H^+]^2}{I - [H^+]}$, where $I = \text{acid's initial concentration}$,

We obtain $[H^+]^2 = K(I - [H^+])$.

Let $x = [H^+]$

$$\begin{aligned}x^2 &= K(I - x) \\x^2 + Kx - KI &= 0 \\ \text{so for } ax^2 + bx + c &= 0,\end{aligned}$$

$$a = 1$$

$$b = K$$

$$c = -KI$$

Substituting these values in to the quadratic formula $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ we obtain:

$$[H^+] = \frac{-K \pm \sqrt{K^2 + 4KI}}{2}$$

So if you enter the values for initial concentration and K_A 's for various acids into columns of a spreadsheet Excel can, in a new column, calculate the H^+ from:

$$=(-K1+SQRT(K1^2+4* I1*K1))/2$$

(We entered K and I into columns K and I to reduce confusion)

Notice that you do not have to worry about the (-) part of the \pm , since the negative value is meaningless in this context.

Then pH can be calculated in a fourth column using:

$$=-\log(L)$$

This is assuming that H^+ was calculated in column L.