Acid-Base Titration Equations
Kelly Lancaster
August 11, 2009

The following equations were derived from ones given in the 5th edition of *Quantitative Chemical Analysis* by Harris. Each titration case was coded in Octave, an open-source version of MATLAB available for free download at http://www.gnu.org/software/octave/.

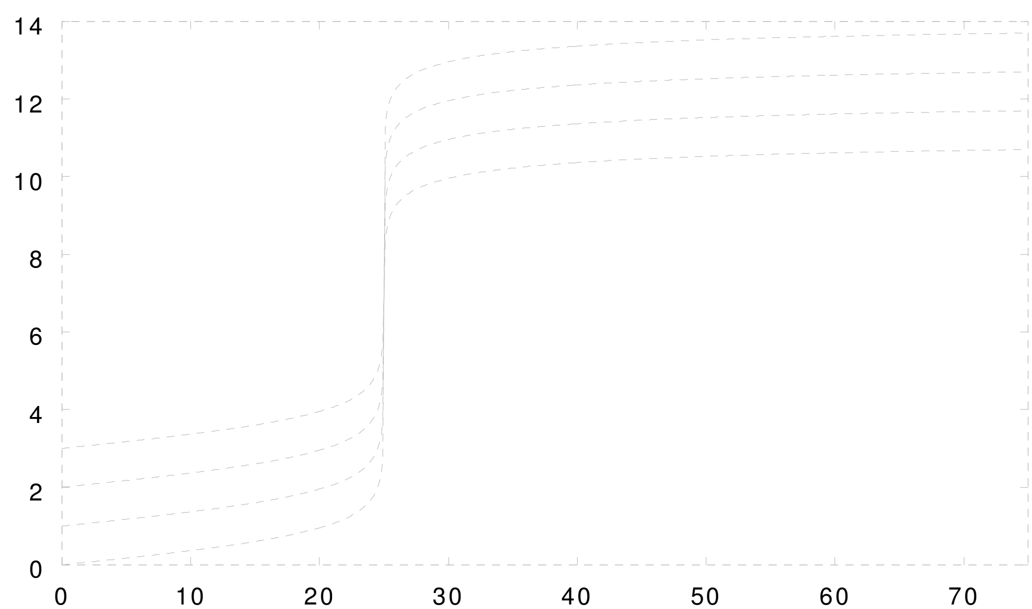
Strong acid/strong base

In this case and the one below, the equation can be solved analytically.

$$(V_a + V_b)[H^+]^2 - (C_a V_a - C_b V_b)[H^+] - K_w(V_a + V_b) = 0$$

To generate the titration curve, call: `strongacid (Ca, Cb, Va, Vb)`

Here is an example that uses the existing parameters of the simulation:
`strongacid (Ca, Cb, 25, 0:0.1:75)`
where Ca and Cb are varied from 0.001 M to 1 M.



Strong base/strong acid

$$-(V_a + V_b)[H^+]^2 + (C_a V_a - C_b V_b)[H^+] + K_w(V_a + V_b) = 0$$

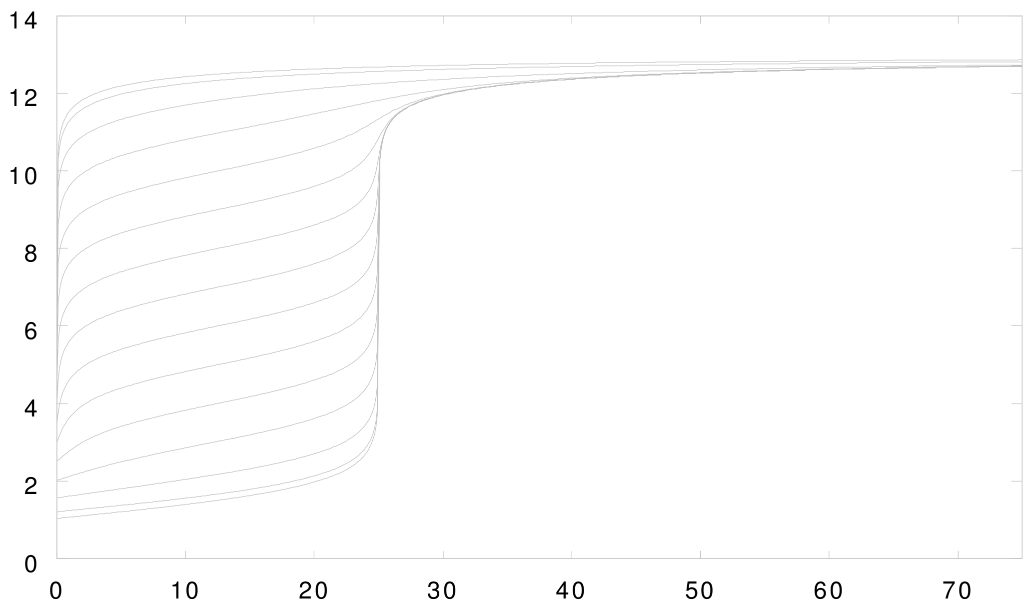
Weak acid/strong base

In this case and the ones that follow, the equation must be solved numerically.

$$(V_a + V_b)[H^+]^3 + (C_b V_b + V_a K_a + V_b K_a)[H^+]^2 - (C_a V_a K_a - C_b V_b K_a + V_a K_w + V_b K_w)[H^+] - (V_a K_a K_w + V_b K_a K_w) = 0$$

To generate the titration curve, call: `weakacid (Ca, Cb, Va, Vb, Ka)`

Here is an example that uses the existing parameters of the simulation:
`weakacid (0.1, 0.1, 25, 0:0.1:75, Ka)`
where Ka is varied from 1e0 to 1e-14.



Weak base/strong acid

$$-(V_a + V_b)[H^+]^3 - \left(C_b V_b - C_a V_a + \frac{V_a K_w}{K_b} + \frac{V_b K_w}{K_b}\right)[H^+]^2 + \left(\frac{C_a V_a K_w}{K_b} + V_a K_w + V_b K_w\right)[H^+] + \left(\frac{V_a K_w^2}{K_b} + \frac{V_b K_w^2}{K_b}\right) = 0$$

Diprotic acid/strong base

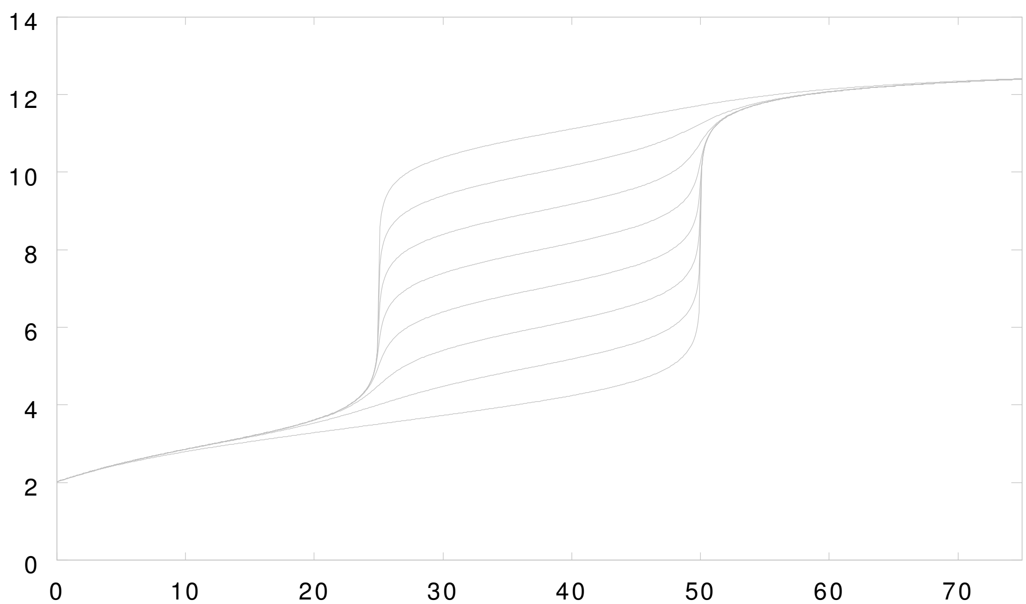
$$(V_a + V_b)[H^+]^4 + (C_bV_b + V_aK_1 + V_bK_1)[H^+]^3$$
$$+ (C_bV_bK_1 - C_aV_aK_1 + V_aK_1K_2 + V_bK_1K_2 - V_aK_w - V_bK_w)[H^+]^2$$
$$+ (C_bV_bK_1K_2 - 2C_aV_aK_1K_2 - V_aK_1K_w - V_bK_1K_w)[H^+]$$
$$- (V_aK_1K_2K_w + V_bK_1K_2K_w) = 0$$

To generate the titration curve, call: `diproticacid (Ca, Cb, Va, Vb, K1, K2)`

Here is an example that uses the existing parameters of the simulation:

```
diproticacid (0.1, 0.1, 25, 0:0.1:75, 1e-3, K2)
```

where K2 is varied from 1e-4 to 1e-11.



One can also solve the equation for a triprotic acid, but such a solution may not address any new learning goals.