Functions for Generating and Plotting Titration Curves

Gathered here are functions for generating and plotting normal titration curves using R, including acid-base titrations, complexation titrations, redox titrations, and precipitation titrations.

Acid-Base Titrations

The following functions are available for the titration of acids and bases.

function	analyte(s)	titrant
sa_sb	monoprotic strong acid	strong base
sb_sa	monoprotic strong base	strong acid
wa_sb	monoprotic weak acid	strong base
wb_sa	monoprotic weak base	strong acid
diwa_sb	diprotic weak acid	strong base
diwb_sa	diprotic weak base	strong acid
triwa_sb	triprotic weak acid	strong base
triwb_sa	triprotic weak base	strong acid
wamix_sb	mixture of two monoprotic weak acids	strong base
wbmix_sa	mixture of two monoprotic weak bases	strong acid

These functions use the general approach outlined in *Principles of Quantitative Analysis* by Robert de Levie (McGraw-Hill, 1997) in which a single master equation is used to calculate the progress of a titration. For example, the function `wa_sb` calculates the volume of strong base needed to achieve a particular pH using this equation

$$\text{volume} = V_a \times \left\{ \frac{C_a \times \alpha - \Delta}{C_b + \Delta} \right\}$$

where V_a is the initial volume of the weak acid analyte, C_a is the initial concentration of the weak acid analyte, C_b is the concentration of the strong base titrant, α is the fraction of the weak acid present in its conjugate weak base form

$$\alpha = \frac{K_a}{[\mathrm{H}^+] + K_a}$$

and Δ is equal to $[\mathrm{H}^+] - [\mathrm{OH}^-]$.

The function calculates the volume of titrant over a range of pH values that extends from a pH of 1 to a pH equal to pK_w. Because some of the calculated volumes are negative—equivalent to adding a strong acid to achieve a pH less than that of the original solution—and some of the calculate values are quite large, the function removes all negative volumes and all volumes greater than twice the volume of the titration curve's last equivalence point.

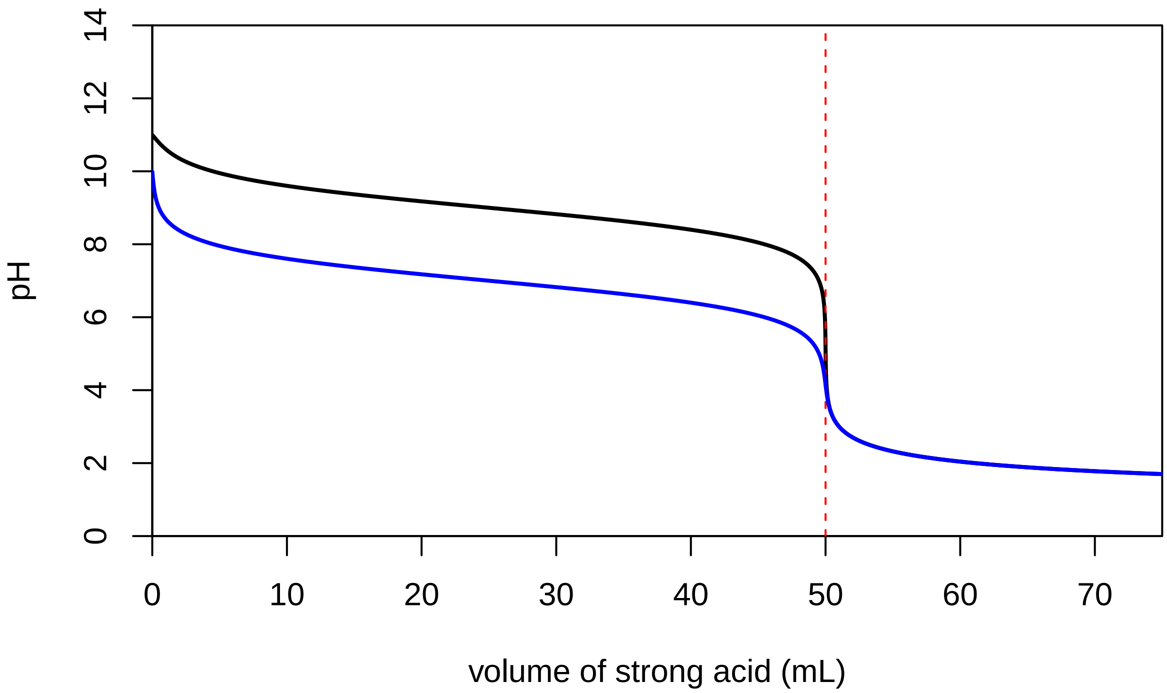
The function's arguements, all of which have default values, are intuitive; a representative example is shown here for the titration of a weak base with a strong acid

```
wb_sa = function(conc.acid = 0.1, conc.base = 0.1, pka = 9, pkw = 14,
                 vol.base = 50, eqpt = FALSE, overlay = FALSE, ...)
```

Note that the equilibrium constant(s) for a weak base are provided using the pK_a value(s) for the base's conjugate weak acid and that you can adjust the pK_a for a solvent other than water.

As shown below, the function produces a plot of the titration curve, with options to overlay two or more titration curves and to add a marker for the equivalence point. The axes are fixed to display the pH from 0 to 14 and to display the volume of titrant from 0 to 1.5× the titration curve's final equivalence point; you can pass along other plot options, such as color.

```
wb_sa(eqpt = TRUE)
wb_sa(pka = 7, col = "blue", overlay = TRUE)
```



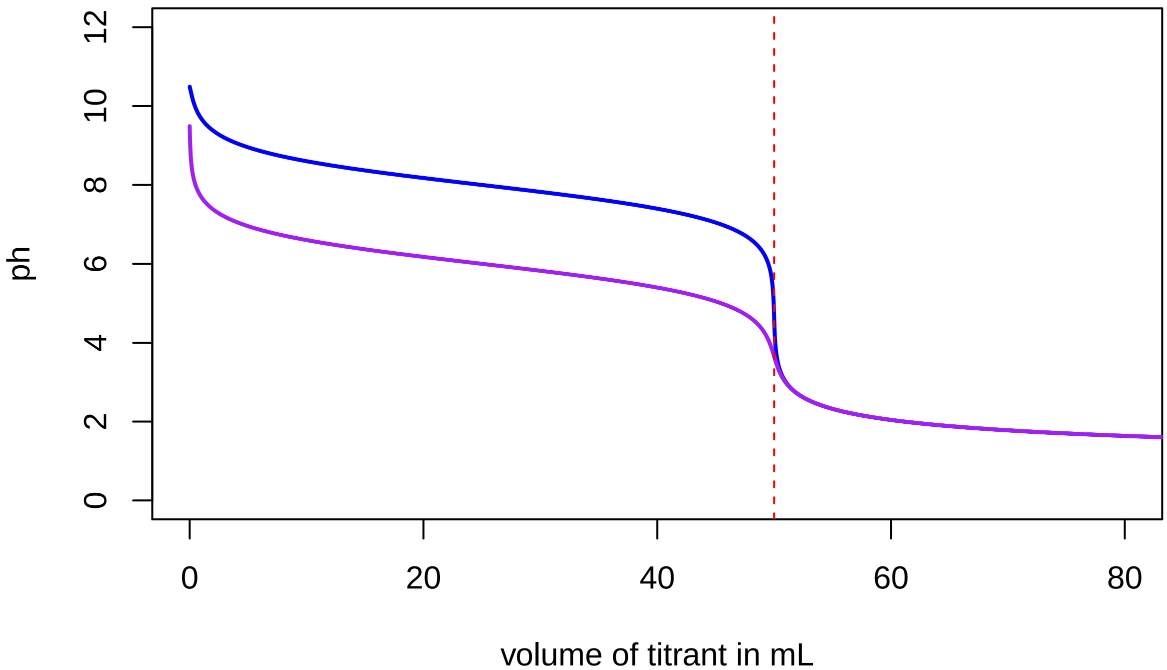
If you assign the function to an object, then the function returns to the object a dataframe with volumes in the first column and pH values in the second column. You can use this object to prepare customized plots.

```
wb1 = wb_sa(pka = 8)
wb2 = wb_sa(pka = 6)
```

```
head(wb1)
```

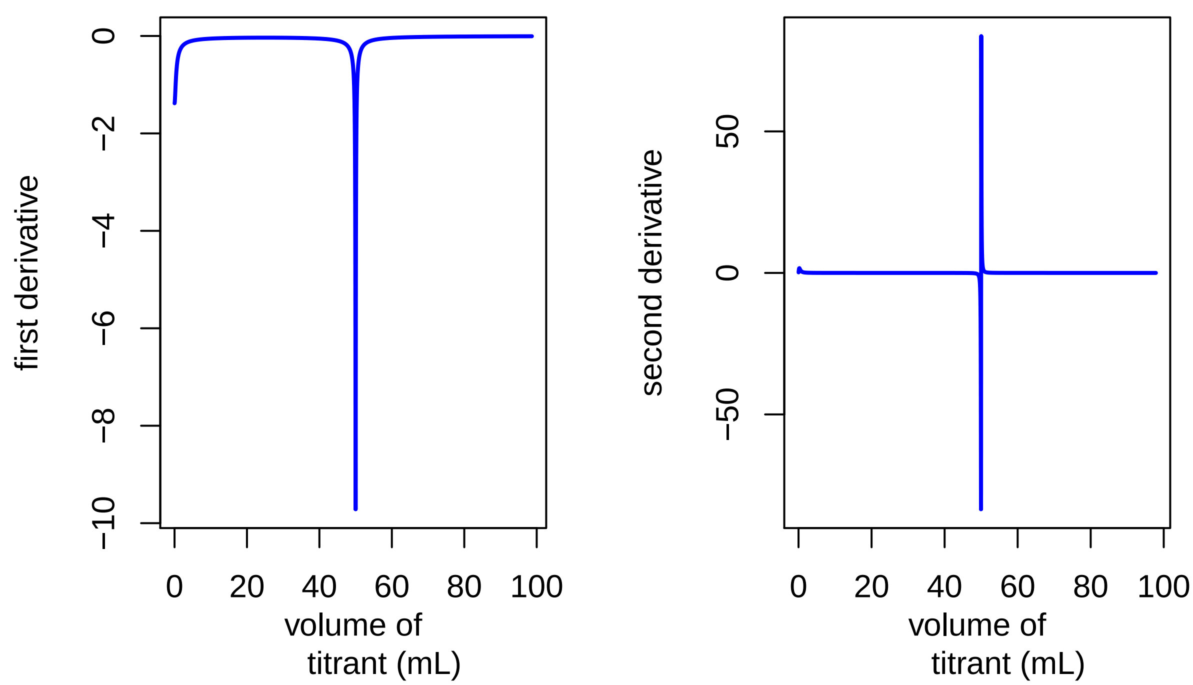
```
##        volume    ph
## 1 0.006739371 10.49
## 2 0.013979345 10.48
## 3 0.021226851 10.47
## 4 0.028485659 10.46
## 5 0.035759545 10.45
## 6 0.043052291 10.44
```

```
plot(wb1, ylim = c(0,12), xlim = c(0,80), type = "l", col = "blue",
     lwd = 2, xlab = "volume of titrant in mL")
lines(wb2, col = "purple", lwd = 2)
abline(v = 50, col = "red", lty = 2)
```



Finally, the function `derivative` accepts an object created by one of the titration functions and returns a plot of the titration curve's first and second derivatives along with a data frame that contains the values used to prepare the two titration curves.

```
wb1.d = derivative(wb1)
```

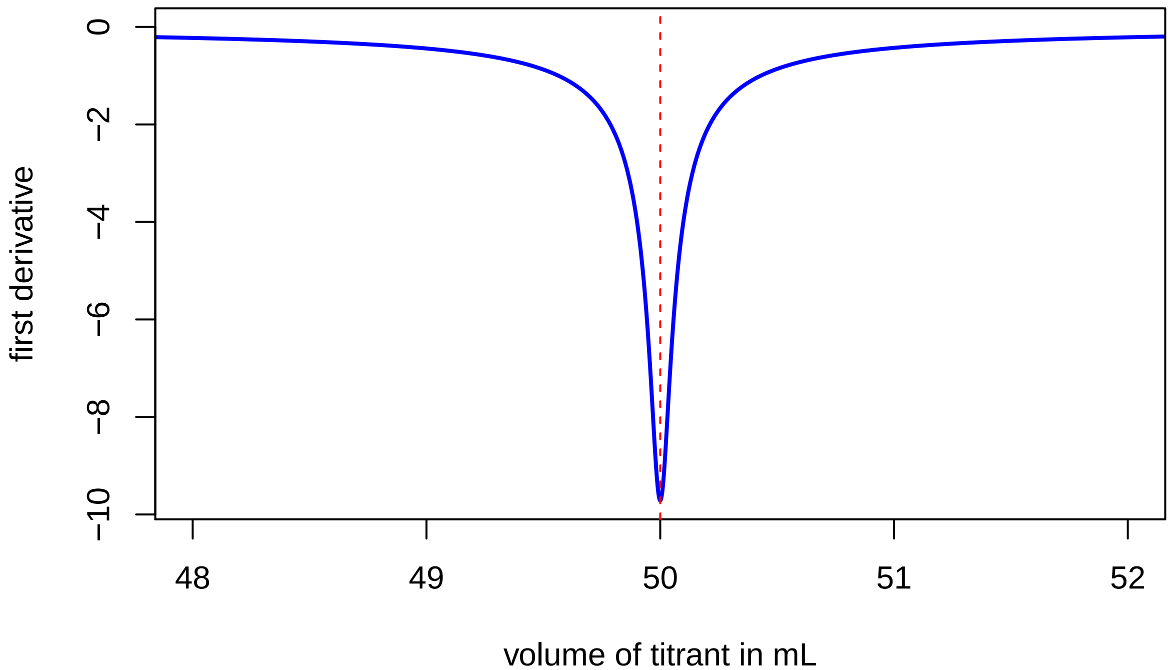



```
str(wb1.d)
```

```
## List of 2
##  $ first_deriv :'data.frame':    901 obs. of  2 variables:
```

```
##    ..$ x1: num [1:901] 0.0104 0.0176 0.0249 0.0321 0.0394 ...
##    ..$ y1: num [1:901] -1.38 -1.38 -1.38 -1.37 -1.37 ...
##   $ second_deriv:'data.frame':    900 obs. of  2 variables:
##    ..$ x2: num [1:900] 0.014 0.0212 0.0285 0.0358 0.0431 ...
##    ..$ y2: num [1:900] 0.198 0.296 0.393 0.488 0.581 ...
```

```r
plot(wb1.d$first_deriv, xlim = c(48,52), col = "blue", type = "l", lwd = 2,
     xlab = "volume of titrant in mL", ylab = "first derivative")
abline(v = 50, col = "red", lty = 2)
```



Complexation Titrations

coming soon…

Redox Titrations

coming soon…

Precipitation Titrations

coming soon…