Package 'titrationCurves'

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Type Package

Title Acid/Base, Complexation, Redox, and Precipitation Titration
Curves

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Description A collection of functions to plot acid/base titration
curves (pH vs. volume of titrant), complexation titration curves
(pMetal vs. volume of EDTA), redox titration curves (potential
vs.volume of titrant), and precipitation titration curves (either
pAnalyte or pTitrant vs. volume of titrant). Options include the
titration of mixtures, the ability to overlay two or more
titration curves, and the ability to show equivalence points.

License GPL-2

LazyData TRUE

RoxygenNote 5.0.1

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

Author David Harvey [aut, cre]

Repository CRAN

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R topics documented:

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derivative   *Derivative Titration Curves*

Description

Given a two-column data frame, with volumes of titrant in the first column and pH, pAnalyte, pTitrant, pMetal, or solution potential in the second column, this function calculates and plots the associated first-derivative and second derivative titration curves.

Usage

```
derivative(df, plot = TRUE, ...)
```

Arguments

df	A data frame with two columns; the first column must contain the volumes of titrant and the second column must contain values for the associated pH, pAnalyte, pTitrant, pMetal, or solution potential. A typical object to pass to this function is that created by the other functions in this package; however, the data frame can be one prepared separately, provided that it matches the structure defined above.
plot	Logical; if TRUE, plots the titration curve.
...	Additional arguments to pass to plot() function.

Value

A list that consists of two data frames, one for the first derivative titration curve and one for the second derivative titration curve.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Derivative weak acid/strong base titration curves
ab = wa_sb()
ex16 = derivative(ab)
str(ex16)
```

---

diwa_sb   *Titration Curve for Diprotic Weak Acid*

Description

This function calculates and plots the titration curve for a diprotic weak acid analyte using a mono-protic strong base as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
diwa_sb(conc.acid = 0.1, conc.base = 0.1, pka1 = 5, pka2 = 9,
  pkw = 14, vol.acid = 50, plot = TRUE, eqpt = FALSE, overlay = FALSE,
  ...)
```

Arguments

conc.acid	Molar concentration of the diprotic weak acid analyte; defaults to 0.10 M.
conc.base	Molar concentration of the strong base titrant; defaults to 0.10 M.
pka1	The pKa1 value for the diprotic weak acid analyte; defaults to a pKa1 of 5.
pka2	The pKa2 value for the diprotic weak acid analyte; defaults to a pKa2 of 9.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.acid	Initial volume, in mL, of the solution that contains the weak acid analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. `<harvey@depauw.edu>`

Examples

```
### Simple titration curve with equivalence points
ex5 = diwa_sb(eqpt = TRUE)
head(ex5)

### Overlay titration curves using different pKa1 and pKa2 values
diwa_sb(pka1 = 5, pka2 = 9, eqpt = TRUE)
diwa_sb(pka1 = 6, pka2 = 10, overlay = TRUE)
diwa_sb(pka1 = 4, pka2 = 8,  overlay = TRUE)
```

---

diwb_sa   *Titration Curve for Diprotic Weak Base*

Description

This function calculates and plots the titration curve for a diprotic weak base analyte using a mono-protic strong acid as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
diwb_sa(conc.base = 0.1, conc.acid = 0.1, pka1 = 5, pka2 = 9,
  pkw = 14, vol.base = 50, plot = TRUE, eqpt = FALSE, overlay = FALSE,
  ...)
```

Arguments

conc.base	Molar concentration of the diprotic weak base analyte; defaults to 0.10 M.
conc.acid	Molar concentration of the strong base titrant; defaults to 0.10 M.
pka1	The pKa1 value for the diprotic weak base analyte's conjugate weak acid; defaults to a pKa1 of 5, or a pKb2 of 9 for the weak base analyte.
pka2	The pKa2 value for the diprotic weak base analyte's conjugate weak acid; defaults to a pKa2 of 9, or a pKb1 of 5.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.base	The initial volume, in mL, of the solution that contains the weak base analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. `<harvey@depauw.edu>`

Examples

```
### Simple titration curve with equivalence points
ex6 = diwb_sa(eqpt = TRUE)
head(ex6)

### Overlay titration curves using different pKa1 and pKa2 values
diwb_sa(pka1 = 5, pka2 = 9, eqpt = TRUE)
diwb_sa(pka1 = 6, pka2 = 10, overlay = TRUE)
diwb_sa(pka1 = 4, pka2 = 8,  overlay = TRUE)
```

---

metal_edta   *Complexation Titration Curve*

Description

This function calculates and plots the titration curve for a metal ion analyte using EDTA as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed concentration of the metal ion, pM, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
metal_edta(conc.metal = 0.1, conc.edta = 0.1, vol.metal = 50, ph = 10,
  logkf = 8.79, alpha.metal = 1, plot = TRUE, eqpt = TRUE,
  overlay = FALSE, ...)
```

Arguments

conc.metal	Molar concentration of the metal ion analyte; defaults to 0.10 M.
conc.edta	Molar concentration of the EDTA titrant; defaults to 0.10 M.
vol.metal	Initial volume, in mL, of the solution that contains the metal ion analyte; defaults to 50.00 mL.
ph	The pH of the solution, which is used to calculate the fraction of EDTA present in its fully deprotonated form; defaults to a pH of 10.
logkf	The log of the formation constant, Kf, for the metal-EDTA complex; defaults to 8.79, which is the value for the complex of Mg^{2+} and EDTA.

alpha.metal	The fraction of the metal ion analyte that is not complexed by an auxiliary complexing agent; defaults to 1, the value when there is no secondary complexing agent present.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pMetal in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence point
ex11 = metal_edta(eqpt = TRUE)
head(ex11)

### Overlay titration curves using different pH values
metal_edta(ph = 12, eqpt = TRUE)
metal_edta(ph = 10, overlay = TRUE)
metal_edta(ph = 8, overlay = TRUE)
```

---

ppt_analyte   *Precipitation Titration Curve: Monitoring pAnalyte*

Description

This function calculates and plots the precipitation titration curve for an analyte and a titrant that form a precipitate with a 1:1 stoichiometry. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed concentration of the analyte, expressed as pAnalyte, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
ppt_analyte(conc.analyte = 0.025, conc.titrant = 0.05, vol.analyte = 50,
  pksp = 16.08, plot = TRUE, eqpt = FALSE, overlay = FALSE, ...)
```

Arguments

`conc.analyte`	Molar concentration of the analyte; defaults to 0.025 M.
`conc.titrant`	Molar concentration of the titrant; defaults to 0.050 M.
`vol.analyte`	The initial volume, in mL, of the solution containing the analyte; defaults to 50.00 mL.
`pksp`	The pKsp value for the precipitate; defaults to 16.08, which is the pKsp for AgI.
`plot`	Logical; if TRUE, plots the titration curve.
`eqpt`	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
`overlay`	Logical; if TRUE, adds the current titration curve to the existing titration curve.
`...`	Additional arguments to pass to `plot()` function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pAnalyte in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence point
ex13 = ppt_analyte(eqpt = TRUE)
head(ex13)

### Overlay titration curves using different pKsp values
ppt_analyte(pksp = 16, eqpt = TRUE)
ppt_analyte(pksp = 14, overlay = TRUE)
ppt_analyte(pksp = 12, overlay = TRUE)
```

---

ppt_mixture   *Precipitation Titration Curve: Mixture of Analytes*

Description

This function calculates and plots the precipitation titration curve for a mixture of two analytes using a titrant that form precipitates with 1:1 stoichiometries. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed concentration of titrant, expressed as pTitrant, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
ppt_mixture(conc.analyte1 = 0.05, conc.analyte2 = 0.05, vol.analyte = 25,
  conc.titrant = 0.05, pksp1 = 16.08, pksp2 = 11.97, plot = TRUE,
  eqpt = FALSE, overlay = FALSE, ...)
```

Arguments

`conc.analyte1`	Molar concentration of the first analyte; defaults to 0.050 M.
`conc.analyte2`	Molar concentration of the second analyte; defaults to 0.050 M.
`vol.analyte`	The initial olume, in mL, of the solution containing the analyte; defaults to 25.00 mL.
`conc.titrant`	Molar concentration of the titrant; defaults to 0.050 M.
`pksp1`	The pKsp value for the first analyte's precipitate; defaults to 16.08, which is the pKsp for AgI.
`pksp2`	The pKsp value for the second analyte's precipitate; defaults to 11.97, which is the pKsp for AgSCN.
`plot`	Logical; if TRUE, plots the titration curve.
`eqpt`	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
`overlay`	Logical; if TRUE, adds the current titration curve to the existing titration curve.
`...`	Additional arguments to pass to `plot()` function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pTitrant in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence points
ex15 = ppt_mixture(eqpt = TRUE)
head(ex15)

### Overlay mixture titration curves using different pKsp values
ppt_mixture(pksp1 = 16, pksp2 = 12, eqpt = TRUE)
ppt_mixture(pksp1 = 14, pksp2 = 10, overlay = TRUE)
```

---

ppt_titrant   *Precipitation Titration Curve: Monitoring pTitrant*

Description

This function calculates and plots the precipitation titration curve for an analyte and a titrant that form a precipitate with a 1:1 stoichiometry. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed concentration of titrant, expressed as pTitrant, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
ppt_titrant(conc.analyte = 0.025, conc.titrant = 0.05, vol.analyte = 50,
  pksp = 16.08, plot = TRUE, eqpt = FALSE, overlay = FALSE, ...)
```

Arguments

conc.analyte	Molar concentration of the analyte; defaults to 0.025 M.
conc.titrant	Molar concentration of the titrant; defaults to 0.050 M.
vol.analyte	Initital volume, in mL, of the solution containing the analyte; defaults to 50.00 mL.
pksp	The pKsp value for the precipitate; defaults to 16.08, which is the pKsp for AgI.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pTitrant in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence point
ex14 = ppt_titrant(eqpt = TRUE)
head(ex14)

### Overlay titration curves using different pKsp values
ppt_titrant(pksp = 16, eqpt = TRUE)
ppt_titrant(pksp = 14, overlay = TRUE)
ppt_titrant(pksp = 12, overlay = TRUE)
```

---

redox_titration   *Redox Titration Curve*

Description

This function calculates and plots the titration curve for a reducing agent analyte using an oxidizing agent as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed potential, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
redox_titration(conc.analyte = 0.01, vol.analyte = 25, pot.analyte = 0.77,
  elec.analyte = 1, conc.titrant = 0.01, pot.titrant = 1.7,
  elec.titrant = 1, plot = TRUE, eqpt = FALSE, overlay = FALSE, ...)
```

Arguments

conc.analyte	Molar concentration of the analyte; defaults to 0.010 M.
vol.analyte	Initial volume, in mL, of the solution containing the analyte; defaults to 25.00 mL.
pot.analyte	Standard state or formal potential for the analyte's half-reaction in V; defaults to 0.77 V.
elec.analyte	The number, n, of electrons lost by the analyte in its oxidation half-reaction; defaults to 1.
conc.titrant	Molar concentration of the titrant; defaults to 0.010 M.
pot.titrant	Standard state or formal potential for the titrant's half-reaction in V; defaults to 1.7 V.
elec.titrant	The number, n, of electrons gained by the analyte in its reduction half-reaction; defaults to 1.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's potential in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence point
ex12 = redox_titration(eqpt = TRUE)
head(ex12)

### Overlay titration curves using different potentials for tirant
redox_titration(pot.titrant = 1.7, eqpt = TRUE)
redox_titration(pot.titrant = 1.5, overlay = TRUE)
redox_titration(pot.titrant = 1.3, overlay = TRUE)
```

---

sa_sb   *Titration Curve for a Strong Acid*

Description

This function calculates and plots the titration curve for a monoprotic strong acid analyte using a monoprotic strong base as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
sa_sb(conc.acid = 0.1, conc.base = 0.1, pkw = 14, vol.acid = 50,
  plot = TRUE, eqpt = FALSE, overlay = FALSE, ...)
```

Arguments

conc.acid	Molar concentration of the strong acid analyte; defaults to 0.10 M.
conc.base	Molar concentration of the strong base titrant; defaults to 0.10 M.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.acid	Initial volume, in mL, of the solution that contains the strong acid analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. `<harvey@depauw.edu>`

Examples

```
### Simple titration curve with equivalence point
ex1 = sa_sb(eqpt = TRUE)
head(ex1)

### Overlay titration curves
sa_sb(conc.base = 0.10)
sa_sb(conc.base = 0.15, overlay = TRUE)
sa_sb(conc.base = 0.20, overlay = TRUE)
```

---

sb_sa   *Titration Curve for a Strong Base*

Description

This function calculates and plots the titration curve for a monoprotic strong base analyte using a monoprotic strong acid as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
sb_sa(conc.base = 0.1, conc.acid = 0.1, pkw = 14, vol.base = 50,
  plot = TRUE, overlay = FALSE, eqpt = FALSE, ...)
```

Arguments

conc.base	Molar concentration of the strong base analyte; defaults to 0.10 M.
conc.acid	Molar concentration of the strong acid titrant; defaults to 0.10 M.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.base	Initial volume, in mL, of the solution that contains the strong base analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
...	Additional arguments to pass to `plot()` function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence point
ex2 = sb_sa(eqpt = TRUE)
head(ex2)

### Overlay titration curves
sb_sa(conc.acid = 0.10)
sb_sa(conc.acid = 0.15, overlay = TRUE)
sb_sa(conc.acid = 0.20, overlay = TRUE)
```

---

triwa_sb *Titration Curve for Triprotic Weak Acid*

Description

This function calculates and plots the titration curve for a triprotic weak acid analyte using a mono-protic strong base as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
triwa_sb(conc.acid = 0.1, conc.base = 0.1, pka1 = 4, pka2 = 7,
  pka3 = 10, pkw = 14, vol.acid = 50, plot = TRUE, eqpt = FALSE,
  overlay = FALSE, ...)
```

Arguments

conc.acid	Molar concentration of the triprotic weak acid analyte; defaults to 0.10 M.
conc.base	Molar concentration of the strong base titrant; defaults to 0.10 M.
pka1	The pKa1 value for the triprotic weak acid analyte; defaults to a pKa1 of 4.
pka2	The pKa2 value for the triprotic weak acid analyte; defaults to a pKa2 of 7.
pka3	The pKa3 value for the triprotic weak acid analyte; defaults to a pKa3 of 10.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.acid	The initial volume, in mL, of the solution that contains the weak acid analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence points
ex7 = triwa_sb(eqpt = TRUE)
head(ex7)

### Overlay titration curves using different pKa1 and pKa2 values
triwa_sb(pka1 = 4, pka2 = 7, pka3 = 10, eqpt = TRUE)
triwa_sb(pka1 = 3, pka2 = 7, pka3 = 11, overlay = TRUE)
triwa_sb(pka1 = 5, pka2 = 7, pka3 = 9, overlay = TRUE)
```

---

triwb_sa   *Titration Curve for a Triprotic Weak Base*

Description

This function calculates and plots the titration curve for a triprotic weak base analyte using a monoprotic strong acid as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
triwb_sa(conc.base = 0.1, conc.acid = 0.1, pka1 = 4, pka2 = 7,
  pka3 = 10, pkw = 14, vol.base = 50, plot = TRUE, eqpt = FALSE,
  overlay = FALSE, ...)
```

Arguments

conc.base	Molar concentration of the triprotic weak base analyte; defaults to 0.10 M.
conc.acid	Molar concentration of the strong acid titrant; defaults to 0.10 M.
pka1	The pKa1 value for the triprotic weak base analyte's conjugat weak acid; defaults to a pKa1 of 4, or a pKb3 of 10.
pka2	The pKa2 value for the triprotic weak base analyte's conjugat weak acid; defaults to a pKa2 of 7, or a pKb2 of 7
pka3	The pKa3 value for the triprotic weak base analyte's conjugat weak acid; defaults to a pKa3 of 10, or a pKb1 of 4.

pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.base	The iniital volume, in mL, of the solution that contains the weak acid analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to `plot()` function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence points
ex8 = triwb_sa(eqpt = TRUE)
head(ex8)

### Overlay titration curves using different pKa1 and pKa2 values
triwb_sa(pka1 = 4, pka2 = 7, pka3 = 10, eqpt = TRUE)
triwb_sa(pka1 = 3, pka2 = 7, pka3 = 11, overlay = TRUE)
triwb_sa(pka1 = 5, pka2 = 7, pka3 = 9, overlay = TRUE)
```

---

wamix_sb   *Titration Curve for Weak Acid Mixture*

Description

This function calculates and plots the titration curve for a mixture of two monoprotic weak acid analyte using a monoprotic strong base as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
wamix_sb(conc.acid1 = 0.1, conc.acid2 = 0.1, conc.base = 0.1, pka1 = 5,
  pka2 = 8, pkw = 14, vol.acid = 50, plot = TRUE, eqpt = FALSE,
  overlay = FALSE, ...)
```

Arguments

conc.acid1	Molar concentration of the first monoprotic weak acid analyte; defaults to 0.10 M.
conc.acid2	Molar concentration of the second monoprotic weak acid analyte; defaults to 0.10 M.
conc.base	Molar concentration of the strong base titrant; defaults to 0.10 M.
pka1	The pKa value for the first monoprotic weak acid analyte; defaults to a pKa of 5.
pka2	The pKa value for the second monoprotic weak acid analyte; defaults to a pKa of 8.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.acid	Initial volume, in mL, of the solution that contains the weak acid analytes; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence points
ex9 = wamix_sb(eqpt = TRUE)
head(ex9)

### Overlay titration curves using different pKa values
wamix_sb(pka1 = 5, pka2 = 8, eqpt = TRUE)
wamix_sb(pka1 = 4, pka2 = 7, overlay = TRUE)
wamix_sb(pka1 = 6, pka2 = 9, overlay = TRUE)
```

---

wa_sb *Titration Curve for a Weak Acid*

Description

This function calculates and plots the titration curve for a monoprotic weak acid analyte using a monoprotic strong base as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
wa_sb(conc.acid = 0.1, conc.base = 0.1, pka = 5, pkw = 14,
  vol.acid = 50, plot = TRUE, eqpt = FALSE, overlay = FALSE, ...)
```

Arguments

conc.acid	Molar concentration of the weak acid analyte; defaults to 0.10 M.
conc.base	Molar concentration of the strong base titrant; defaults to 0.10 M.
pka	The pKa value for the weak acid analyte; defaults to a pKa of 5.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.acid	Initial volume, in mL, of the solution that contains the weak acid analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence point
ex3 = wa_sb(eqpt = TRUE)
head(ex3)

### Overlay titration curves using different pKa values
wa_sb(pka = 5, eqpt = TRUE)
wa_sb(pka = 7, overlay = TRUE)
wa_sb(pka = 9, overlay = TRUE)

### Overlay titration curve for strong acid and weak acid
sa_sb(eqpt = TRUE)
wa_sb(overlay = TRUE)
```

---

wbmix_sa   *Titration Curve for Weak Base Mixture*

Description

This function calculates and plots the titration curve for a mixture of two monoprotic weak base using a monoprotic strong acid as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

```
wbmix_sa(conc.base1 = 0.1, conc.base2 = 0.1, conc.acid = 0.1, pka1 = 6,
  pka2 = 9, pkw = 14, vol.base = 50, plot = TRUE, eqpt = FALSE,
  overlay = FALSE, ...)
```

Arguments

conc.base1	Molar concentration of the first monoprotic weak base analyte; defaults to 0.10 M.
conc.base2	Molar concentration of the second monoprotic weak base analyte; defaults to 0.10 M.
conc.acid	Molar concentration of the strong acid titrant; defaults to 0.10 M.
pka1	The pKa value for the first monoprotic weak base analyte's conjugate weak acid; defaults to a pKa of 6, or a pKb of 8.
pka2	The pKa value for the second monoprotic weak base analyte's conjugate weak acid; defaults to a pKa of 9, or a pKb of 5.
pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.base	Initial volume, in mL, of the solution that contains the weak base; defaults to 50.00 mL.

plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to `plot()` function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence points
ex10 = wbmix_sa(eqpt = TRUE)
head(ex10)

### Overlay titration curves using different pKa values
wbmix_sa(pka1 = 5, pka2 = 8, eqpt = TRUE)
wbmix_sa(pka1 = 4, pka2 = 7, overlay = TRUE)
wbmix_sa(pka1 = 6, pka2 = 9, overlay = TRUE)
```

---

wb_sa   *Titration Curve for a Weak Base*

Description

This function calculates and plots the titration curve for a monoprotic weak base analyte using a monoprotic strong acid as the titrant. The calculation uses a single master equation that finds the volume of titrant needed to achieve a fixed pH, as outlined in R. de Levie's *Principles of Quantitative Chemical Analysis* (McGraw-Hill, 1997).

Usage

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

Arguments

conc.acid	Molar concentration of the strong acid titrant; defaults to 0.10 M.
conc.base	Molar concentration of the weak base analyte; defaults to 0.10 M.
pka	The pKa value for the weak base analyte's conjugate weak acid; defaults to a pKa of 9, or a pKb of 5 for the weak base analyte.

pkw	The pKw (or pKs) value for the solvent; defaults to water as a solvent with a pKw of 14.
vol.base	Initial volume, in mL, of the solution that contains the weak base analyte; defaults to 50.00 mL.
plot	Logical; if TRUE, plots the titration curve.
eqpt	Logical; if TRUE, draws a vertical line at the titration curve's equivalence point.
overlay	Logical; if TRUE, adds the current titration curve to the existing titration curve.
...	Additional arguments to pass to plot() function.

Value

A two-column data frame that contains the volume of titrant in the first column and the solution's pH in the second column. Also produces a plot of the titration curve with options to display the equivalence point and to overlay titration curves.

Author(s)

David T. Harvey, DePauw University. <harvey@depauw.edu>

Examples

```
### Simple titration curve with equivalence point
ex4 = wb_sa(eqpt = TRUE)
head(ex4)

### Overlay titration curves using different pKa values
wb_sa(pka = 9, eqpt = TRUE)
wb_sa(pka = 7, overlay = TRUE)
wb_sa(pka = 5, overlay = TRUE)

### Overlay titration curve for strong base and weak base
sb_sa(eqpt = TRUE)
wb_sa(overlay = TRUE)
```

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