# Package 'simplex'

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**Title** Data Reduction Software for Secondary Ion Mass Spectrometry

**Version** 0.1

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**Description** Processes Secondary Ion Mass Spectrometery (SIMS) data within the confines of the simplex, i.e. the data space of compositions. Accommodates input files for both Cameca and SHRIMP instruments. Models the data using a combination of multinomial and logistic normal statistics. Keeps track of inter-sample error correlations caused by using a common standard for multiple samples. Includes applications for U-Pb geochronology and stable isotope geochemistry.

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**Depends** R (>= 3.0.0)

**Imports** MASS, graphics, IsoplotR

**License** GPL-3

**URL** https://github.com/pvermees/simplex

**LazyData** true

**RoxygenNote** 6.1.1

**Encoding** UTF-8

## R topics documented:

## avg_Lm *Average logratios*

### Description

Takes time resolved logratio estimates as input and produces a single spot logratio vector and covariance matrix as output.

### Usage

```
avg_Lm(Lm)
```

### Arguments

| | |
|---|---|
| Lm | A time resolved list of logratio vectors and Hessian matrices. |

### Details

Uses a weighted mean algorithm with correlated uncertainties.

### Value

A list with a single vector of logratios and its covariance matrix.

### Examples

```
data(Cameca,package='simplex')
Lm <- raw_count_ratios(samp=Cameca[[1]])
aLm <- avg_Lm(Lm)
```

## Cameca *Example datasets for testing* simplex

### Description

a Plesovice and Qinghu zircon dataset from the Cameca SIMS instrument at the Chinese Academy of Sciences Beijing.

### Usage

```
Cameca
```

### Format

An object of class simplex.

## plot_timeresolved *Plot and fit raw time-resolved SIMS data.*

### Description

Shows the raw data for a single spot in a SIMS dataset.

### Usage

```
plot_timeresolved(samp, fit = FALSE, c64 = NULL)
```

### Arguments

| | |
|---|---|
| samp | One item of a simplex dataset. |
| fit | Set to TRUE to show the maximum likelihood fit on the plot. |
| c64 | (optional) common Pb composition ($^{2}06$Pb/$^{2}04$Pb ratio). |

### Value

Produces a multi-panel scatter plot.

### Examples

```
data(Cameca,package="simplex")
plot_timeresolved(Cameca[[1]],fit=TRUE)
```

## raw_count_ratios *Time-resolved logratios*

### Description

Calculate the time-resolved logratios for a single spot.

### Usage

```
raw_count_ratios(samp)
```

### Arguments

| | |
|---|---|
| samp | One item in an object of class simplex. |

### Value

A list with a vector of logratios and its covariance matrix.

## See Also

plot_timeresolved

## Examples

```
data(package="simplex")
Lm <- raw_count_ratios(samp=Cameca[[1]])
```

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`read_directory` *Read data directory*

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## Description

Read all the input files in a data directory

## Usage

```
read_directory(dname, instrument = "Cameca", suffix = NULL)
```

## Arguments

| | |
|---|---|
| `dname` | path to the input directory |
| `instrument` | text string with the type of ICP-MS. Currently only `'Cameca'`. |
| `suffix` | (optional) file extension of the input files. |

## Value

An object of class `simplex`, i.e. a list of lists containing the following items: `ions`, `ions`, `dwelltime`, `detector`, `yield`, `background`, `cps`, `counts`, `sbm`, and `time`.

## Examples

```
datadir <- system.file(package="simplex")
dat <- read_directory(paste0(datadir,'/'),instrument='Cameca',suffix='.asc')
```

subset_samples *Subset a dataset of class* simplex

## Description

Select a subset of samples aor standards from a simplex dataset.

## Usage

```
subset_samples(dat, prefix = "Plesovice")
```

## Arguments

| | |
|---|---|
| dat | A dataset to subset |
| prefix | Text string to match |

## Value

an object with the same class as dat

## See Also

read_directory

## Examples

```
data(Cameca,package="simplex")
stand <- subset_samples(Cameca,prefix='Plesovice')
```

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