

Package ‘IsoplotR’

May 20, 2016

Title Statistical Toolbox for Radiometric Geochronology

Version 0.3

Description An R implementation of Ken Ludwig's popular Isoplot add-in to Microsoft Excel. Currently plots U-Pb data on Wetherill and Tera-Wasserburg concordia diagrams, taking into account error correlations. Future versions will include functionality for the Ar-Ar, Rb-Sr, Sm-Nd, Re-Os, U-Th-He, fission track and cosmogenic nuclide methods, including isochrons, age spectra, ternary diagrams, kernel density estimates, radial plots, banana diagrams and multidimensional scaling plots. A graphical user interface is provided as an RStudio Shiny app.

Author Pieter Vermeesch [aut, cre]

Maintainer Pieter Vermeesch <p.vermeesch@ucl.ac.uk>

Depends R (>= 3.0.0)

Imports methods

License GPL-2

LazyData true

RoxygenNote 5.0.1

R topics documented:

concordia.age	2
concordia.plot	3
ellipse	3
I.R	4
lambda	5
read.data	6
read.matrix	7
settings	7
UPb	8
Index	9

concordia.age	<i>Calculate U-Pb concordia ages</i>
---------------	--------------------------------------

Description

Evaluates the equivalence of multiple ($^{206}\text{Pb}/^{238}\text{U}$ - $^{207}\text{Pb}/^{235}\text{U}$ or $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{206}\text{Pb}/^{238}\text{U}$) compositions, computes the weighted mean isotopic composition and the corresponding concordia age using the method of maximum likelihood, computes the mswd of equivalence and concordance and their respective Chi-squared p-values.

Usage

```
concordia.age(x, wetherill = TRUE)
```

Arguments

x	an object of class UPb
wetherill	boolean flag to indicate whether the data should be evaluated in Wetherill (TRUE) or Tera-Wasserburg (FALSE) space

Value

a list with the following items:

x: a named vector with the weighted mean U-Pb composition

x.cov: the covariance matrix of the mean U-Pb composition

age: the concordia age (in Ma)

age.err: the standard error of the concordia age

mswd: a list with two items (equivalence and concordance) containing the MSWD (Mean of the Squared Weighted Deviates, a.k.a the reduced Chi-squared statistic outside of geochronology) of isotopic equivalence and age concordance, respectively.

p.value: a list with two items (equivalence and concordance) containing the p-value of the Chi-square test for isotopic equivalence and age concordance, respectively.

Examples

```
data(UPb)
fit <- concordia.age(UPb)
print(paste('age = ', fit$age, '+/-', fit$age.err, 'Ma, MSWD = ', fit$mswd))
```

concordia.plot	<i>Concordia diagram</i>
----------------	--------------------------

Description

Wetherill and Tera-Wasserburg concordia diagrams

Usage

```
concordia.plot(x, limits = NULL, alpha = 0.05, wetherill = TRUE,
  show.numbers = FALSE, ellipse.col = rgb(0, 1, 0, 0.5),
  concordia.col = "darksalmon", dcu = TRUE, show.age = 0)
```

Arguments

x	an object of class UPb
limits	age limits of the concordia line
alpha	confidence cutoff for the error ellipses
wetherill	boolean flag (FALSE for Tera-Wasserburg)
show.numbers	boolean flag (TRUE to show grain numbers)
ellipse.col	background colour of the error ellipses
concordia.col	colour of the concordia line
dcu	show decay constant uncertainty?
show.age	one of either 0: don't show the age 1: calculate the concordia age (2: fit a discordia line - not implemented yet)

Examples

```
data(UPb)
concordia.plot(UPb)
```

ellipse	<i>Get coordinates of error ellipse for plotting</i>
---------	--

Description

Construct an error ellipse age a given confidence level from its centre and covariance matrix

Usage

```
ellipse(x, y, covmat, alpha = 0.05)
```

Arguments

x	x-coordinate (scalar) for the centre of the ellipse
y	y-coordinate (scalar) for the centre of the ellipse
covmat	covariance matrix of the x-y coordinates
alpha	the probability cutoff for the error ellipses

Value

a [50x2] matrix of plot coordinates

Examples

```
x = 99; y = 101;
covmat <- matrix(c(1,0.9,0.9,1),nrow=2)
ell <- ellipse(x,y,covmat)
plot(c(90,110),c(90,110),type='l')
polygon(ell,col=rgb(0,1,0,0.5))
points(x,y,pch=21,bg='black')
```

I.R	<i>Isotopic ratios</i>
-----	------------------------

Description

Gets or sets natural isotopic ratios.

Usage

```
I.R(ratio, x = NULL, e = NULL)
```

Arguments

ratio	one of either 'U238U235', 'Ar40Ar36', 'Ar38Ar36', 'Rb85Rb87', 'Sr88Sr86', 'Sr87Sr86', 'Sr84Sr86', 'Re185Re187', 'Os184Os192', 'Os186Os192', 'Os187Os192', 'Os188Os192', 'Os189Os192'
x	new value for ratio
e	new value for its standard error

Value

if x == e == NULL, returns a two-item vector containing the mean value of the requested ratio and its standard error, respectively.

References

Ar: Lee, Jee-Yon, et al. "A redetermination of the isotopic abundances of atmospheric Ar." *Geochimica et Cosmochimica Acta* 70.17 (2006): 4507-4512.

Rb: Catanzaro, E. J., et al. "Absolute isotopic abundance ratio and atomic weight of terrestrial rubidium." *J. Res. Natl. Bur. Stand. A* 73 (1969): 511-516.

Sr: Moore, L. J., et al. "Absolute isotopic abundance ratios and atomic weight of a reference sample of strontium." *J. Res. Natl. Bur. Stand.* 87.1 (1982): 1-8.

Re: Gramlich, John W., et al. "Absolute isotopic abundance ratio and atomic weight of a reference sample of rhenium." *J. Res. Natl. Bur. Stand. A* 77 (1973): 691-698.

Os: Voelkening, Joachim, Thomas Walczyk, and Klaus G. Heumann. "Osmium isotope ratio determinations by negative thermal ionization mass spectrometry." *Int. J. Mass Spect. Ion Proc.* 105.2 (1991): 147-159.

U: Hiess, Joe, et al. "²³⁸U/²³⁵U systematics in terrestrial uranium-bearing minerals." *Science* 335.6076 (2012): 1610-1614.

Examples

```
# returns the 238U/235U ratio of Hiess et al. (2012):
print(I.R('U238U235'))
# use the 238U/235U ratio of Steiger and Jaeger (1977):
I.R('U238U235', 138.88, 0)
print(I.R('U238U235'))
```

lambda

Decay constants

Description

Gets or sets the decay constants of radioactive istopes

Usage

```
lambda(nuclide, x = NULL, e = NULL)
```

Arguments

nuclide	the nuclide name
x	new value for the decay constant
e	new value for the decay constant uncertainty

Value

if x == e == NULL, returns a two-item vector containing the decay constant [in Ma⁻¹] and its standard error, respectively.

Examples

```
print(lambda('U238'))
# use the decay constant of Kovarik and Adams (1932)
lambda('U238',0.0001537,0.0000068)
print(lambda('U238'))
```

read.data

Read geochronology data

Description

Cast a .csv file into one of IsoplotR's data classes

Usage

```
read.data(fname, method = "U-Pb", format = 1, ...)
```

Arguments

fname	file name (.csv format)
method	one of 'U-Pb', 'Ar-Ar', 'Rb-Sr', 'Sm-Nd', 'Re-Os', 'U-Th-He', 'fission tracks', 'cosmogenic nuclides' or 'other'
format	formatting option, depends on the value of method. If method = 'U-Pb', then format is one of either: 1: 7/6, s[7/6], 6/8, s[6/8], 7/5, s[7/5]
...	optional arguments to the read.csv function

Value

an object of class 'UPb', 'ArAr', 'RbSr', 'SmNd', 'ReOs', 'UThHe', 'fission', 'cosmogenics', or 'other'

Examples

```
# load one of the built-in .csv files:
fname <- system.file("UPb.csv", package="IsoplotR")
UPb <- read.data(fname, 'U-Pb')
concordia.plot(UPb)
```

read.matrix	<i>Read geochronology data</i>
-------------	--------------------------------

Description

Cast a matrix into one of IsoplotR's data classes

Usage

```
read.matrix(x, method = "U-Pb", format = 1)
```

Arguments

x	a matrix
method	see read.data for details
format	see read.data for details

Value

see read.data for details

Examples

```
# load one of the built-in .csv files:
fname <- system.file("UPb.csv", package="IsoplotR")
dat <- read.csv(fname, header=TRUE)
UPb <- read.matrix(dat, method='U-Pb', format=1)
concordia.plot(UPb)
```

settings	<i>Load settings to and from json</i>
----------	---------------------------------------

Description

Get and set preferred values for decay constants and isotopic abundances from and to a .json file format

Usage

```
settings(fname = NULL)
```

Arguments

fname	the path of a .json file
-------	--------------------------

Value

if `fname==NULL`, returns a .json string

Examples

```
json <- system.file("defaults.json", package="IsoplotR")
settings(json)
print(settings())
```

UPb

An example U-Pb dataset

Description

An example U-Pb dataset provided with Ludwig's Isoplot add-in

Details

UPb is an object of class UPb, i.e. a list with two items

x: a matrix formatted according to format

format: an integer defining the format of x. Options are:

1: 7/6, s[7/6], 6/8, s[6/8], 7/5, s[7/5]

Author(s)

Ken Ludwig and Pieter Vermeesch

Examples

```
data(UPb)
concordia.plot(UPb)
```


Index

`concordia.age`, [2](#)
`concordia.plot`, [3](#)

`ellipse`, [3](#)

`I.R.`, [4](#)

`lambda`, [5](#)

`read.data`, [6](#)
`read.matrix`, [7](#)

`settings`, [7](#)

`UPb`, [8](#)