Package 'imputeREE'

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Title Impute Missing Rare Earth Element Data Using a Lattice-Strain Derived Method

Version 0.0.1

Description Set of functions that fit a linear regression to calculate missing Rare Earth Element (REE) in zircon based on a method derived from the lattice strain theory of Blundy and Wood (1994)<doi:10.1038/372452a0>.

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R topics documented:

`add_element_data` *Add ionic radius and chondrite and mantle values, Z and Mass*

Description

This is a helper function to work with Element_norm() and Element_denorm(). Add Ionic Radius to data and chondrite values. For now, only supports 3+ in eight-fold coordination for REE, Zr and Y.Values are from Shannon(1976), McDonough and Sun (1995) and Palme and O'Neill (2014).

Usage

```
add_element_data(dat)
```

Arguments

`dat`	Long data REE format

Value

A data frame

`add_ID` *Add_ID*

Description

Add an unique ID per observation and checks that is not overwriting an existing column. If the column already exist, it will take no action. This is a wrapper of tibble::rowid_to_column() that checks that not columns is overwritten.

Usage

```
add_ID(dat, ID = "rowid")
```

Arguments

dat	a tibble or a dataframe
ID	Name of column to use for rownames. 'rowid' is used if none is specified. er parameters passed onto the `tibble::rowid_to_column()` function

Value

a data frame

---

add_IonicRadii *Add Chondrite or Mantle values for normalization.*

Description

This is a helper function to work with Element_norm() and Element_denorm(). Takes long pivoted data to match element name and add normalizing values from the Element_data dataset.

Usage

```
add_IonicRadii(dat, method = ShannonRadiiVIII_Coord_3plus)
```

Arguments

dat	a dataframe or tibble.
method	Ionic Radii from Shannon, 1976

Value

a data frame or tibble

---

add_NormValues *Add Chondrite or Mantle values for normalization.*

Description

This is a helper function to work with Element_norm() and Element_denorm(). Takes long pivoted data to match element name and add normalizing values from the Element_data dataset.

Usage

```
add_NormValues(dat, method = PalmeOneill2014CI)
```

Arguments

dat	Dataframe or tibble.
method	Values to normalize: an option from: PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI. load

Value

a data frame or tibble

---

add_parameters *Calculate relevant data from REE*

Description

Calculate the Eu and Ce anomalies, the sum or REE + Y and P as molar ratios from imputed data. It expects the result of data %>% model_ree() %>% impute_ree()

Usage

```
add_parameters(data, prefix = NULL, suffix = NULL)
```

Arguments

data	A dataframe
prefix	A prefix in your columns e.g. ICP_La
suffix	A suffix in your columns e.g. La_ppm

Value

A dataframe

Examples

```
testing_data %>%
dplyr::slice(12) %>%
model_REE(prefix = 'Zr_', suffix = '_ppm') %>%
impute_REE(prefix = 'Zr_', suffix = '_ppm')  %>%
add_parameters(prefix = 'Zr_', suffix = '_ppm')
```

calc_all *Calculate and Impute REE missing data and anomalies.*

Description

This is a wrapper for data %>% model_REE() %>% impute_REE %>% add_parameters()

Usage

```
calc_all(data, prefix = NULL, suffix = NULL, method = PalmeOneill2014CI)
```

Arguments

data	A data frame containing REE data
prefix	a string. A prefix in the columns names e.g 'Whole_rock_La', where 'Whole_rock_' is the prefix
suffix	a string. A suffix in the columns names e.g 'La_ppm', where '_ppm' is the suffix
method	an option from: 'PalmeOneill2014CI', 'Oneill2014Mantle', 'McDonough1995CI'

Value

A data frame. Includes imputed REE, model metrics, and calculated variables.

Examples

```
testing_data %>% calc_all(prefix = 'Zr_', suffix = '_ppm')
```

CleanColnames *Clean variable names that have prefixes or suffixes*

Description

This is a helper function

Usage

```
CleanColnames(dat, prefix = NULL, suffix = NULL)
```

Arguments

dat	a data frame
prefix	A character of length 1
suffix	A character of length 1

Value

A data frame

`correct_heavy` *Corrects for the model deviations of Yb, Lu and Y*

Description

Calculated value of Yb, Lu and Y slightly deviates from the linear regression. This function apply a correction to compensates those deviations. This function is wrapped inside model_REE()

Usage

```
correct_heavy(
  dat,
  Y_correction_fact = 1.29,
  Yb_correction_fact = 1/0.8785,
  Lu_correction_fact = 1/0.8943
)
```

Arguments

`dat`	A dataframe
`Y_correction_fact`	a number: correction factor for underestimated Y. 1.29 by default.
`Yb_correction_fact`	a number: correction factor for underestimated Yb 1/0.8785
`Lu_correction_fact`	a number: correction factor for underestimated Lu 1/0.8943

Value

a data frame

`Element_Data` *Element data for calculations*

Description

A dataset containing CI and Mantle values for normalization for selected elements. The data used is from IUPAC, Palme and O'Neill (2014), and McDonough and Sun (1995). Ionic Radii are from Shannon (1976).

Usage

```
Element_Data
```

Format

A data frame with 77 rows and 10 variables:

Z Atomic Number

Element_name Element Symbol

Atomic_Mass Atomic Mass from IUPAC

Unit Measure Unit of the Concentrations, ppm = parts per million, pct = percentage

PalmeOneill2014CI Chondrite values from Palme and Oneil (2014)

PalmeOneill2014CI_RSD Uncertainty from chondrite values from Palme and O'Neill (2014) as RSD (Relative standard Deviation)

PalmeOneill2014Mantle Primitive Mantle values from Palme and O'Neill (2014)

PalmeOneill2014Mantle_RSD Uncertainty from Primitive Mantle Values from Palme and O'Neill (2014) as RSD (Relative standard Deviation)

McDonough1995CI Chondrite values from McDonough and Sun (1995)

ShannonRadiiVIII_Coord_3plus Shannon (1976) Ionic Radii for elements in Eight-fold coordination and 3+ charge ...

Source

IUPAC Website (https://iupac.org/)

Palme, H., and O'Neill, H. St. C., 2014, 3.1 - Cosmochemical Estimates of Mantle Composition, in Holland, H. D. and Turekian, K. K. eds., Treatise on Geochemistry (Second Edition): Oxford, Elsevier, p. 1-39.(doi:10.1016/B9780080959757.002011)

McDonough, W. F., and Sun, S. -s., 1995, The composition of the Earth: Chemical Geology, v. 120, p. 223-253.(doi:10.1016/00092541(94)001404)

Shannon, R. D., 1976, Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides: Acta Crystallographica Section A, v. 32, p. 751-767. doi:10.1107/S0567739476001551

`element_denorm` *Denormalize chrodrite Normalize to ppm*

Description

Denormalize chrodrite Normalize to ppm

Usage

```
element_denorm(dat, method = PalmeOneill2014CI)
```

Arguments

`dat`	A dataframe
`method`	an option from: 'PalmeOneill2014CI', 'Oneill2014Mantle', 'McDonough1995CI'

Value

A dataframe

`Element_norm` *Calculate normalized values for a list of elements*

Description

Element norm normalize values according to published values for the Primitive mantle and chondrites. By defect, it uses the values from Palme and O'Neill (2014). By default, REE + Y list is provided

Usage

```
Element_norm(
  data,
  return = "rect",
  method = PalmeOneill2014CI,
  prefix = NULL,
  suffix = NULL,
  Element_list = REE_plus_Y_Elements
)
```

Arguments

`data`	a data frame
`return`	a character from: "rect" for a wide data return,"raw" for a long data return,"append" to append the results to the input data
`method`	an option from: PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI
`prefix`	A prefix in your columns e.g. ICP_La
`suffix`	A suffix in your columns e.g. La_ppm
`Element_list`	a character vector: indicating the elements that should be normalized. REE + Y by default

Value

a data frame

impute_REE *Impute Rare earth elements*

Description

Imputes missing REE after modelling. Expect the output of 'model_REE()' function. Only missing values are replaced.

Usage

```
impute_REE(data, prefix = NULL, suffix = NULL, rsquared = 0.9)
```

Arguments

data	A dataframe resulting from 'model_ree()'
prefix	A prefix in your columns e.g. ICP_La
suffix	A suffix in your columns e.g. La_ppm
rsquared	A numerical value between 0 and 1. Tolerance to mis-fitting models. set as 0.9 by default.

Details

By default, exclude models with R-squared lower than 0.9.

Value

A dataframe

Examples

```
testing_data %>%
dplyr::slice(1:100) %>%
model_REE(prefix = 'Zr', suffix = 'ppm') %>%
impute_REE(prefix = 'Zr', suffix = 'ppm')
```

`model_REE` *Model REE + Y contents using an empirical method based on the lattice strain theory*

Description

Model REE will make a linear regression between the REE (+Y) and the relationship of the ideal Ionic Radii in the lattice site (r0) and the ionic radii of the element that use that space (ri) according to the relationship : (ri/3 + r0/6)(ri-r0)^2‘ For details in the lattice strain theory, see Blundy and Wood 1994.

Usage

```
model_REE(
  dat,
  r0 = 0.84,
  exclude = c("La", "Ce", "Eu", "Y"),
  prefix = NULL,
  suffix = NULL,
  method = PalmeOneill2014CI,
  Y_correction_fact = 1.29,
  Yb_correction_fact = 1/0.8785,
  Lu_correction_fact = 1/0.8943,
  correct_heavy = TRUE
)
```

Arguments

`dat`	A data frame
`r0`	A number: ionic radii of the lattice site r0
`exclude`	a string: vector including elements that should be omitted from modelling. La, Ce and Eu are the default. Ce and Eu should be always included
`prefix`	A prefix in your columns e.g. ICP_La
`suffix`	A suffix in your columns e.g. La_ppm
`method`	an option from: PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI
`Y_correction_fact`	a number: correction factor for underestimated Y. 1.29 by default.
`Yb_correction_fact`	a number: correction factor for underestimated Yb 1/0.8785
`Lu_correction_fact`	a number: correction factor for underestimated Lu 1/0.8943
`correct_heavy`	a logical. If `TRUE` will apply a correction factor for Yb, Lu and Y.

Value

a dataframe

Examples

```
testing_data %>%  model_REE(prefix = 'Zr', suffix = 'ppm')
```

`REE_Elements` *Rare earth element list*

Description

A string vector containing the elemental symbols for REE.

Usage

```
REE_Elements
```

Format

Rare earth element list

`REE_plus_Y_Elements` *Rare earth element list*

Description

A string vector containing the elemental symbols for REE and Y.

Usage

```
REE_plus_Y_Elements
```

Format

Rare earth element + Y list

testing_data *Zircon Rare earth Element Data from Ballard et al. 2001 and 2002.*

Description

Trace element data from selected zircons from the data of Ballard et al. 2001 and 2002.

Usage

```
testing_data
```

Format

A data frame with 210 rows and 18 variables:

Reference Reference of the data

Deposit Deposit associated with the data

Zr_Y_ppm Y concentrations in ppm

Zr_P_ppm P concentrations in ppm

Zr_La_ppm La concentrations in ppm

Zr_Ce_ppm Ce concentrations in ppm

Zr_Pr_ppm Pr concentrations in ppm

Zr_Nd_ppm Nd concentrations in ppm

Zr_Sm_ppm Sm concentrations in ppm

Zr_Eu_ppm Eu concentrations in ppm

Zr_Gd_ppm Gd concentrations in ppm

Zr_Tb_ppm Tb concentrations in ppm

Zr_Dy_ppm Dy concentrations in ppm

Zr_Ho_ppm Ho concentrations in ppm

Zr_Er_ppm Er concentrations in ppm

Zr_Tm_ppm Tm concentrations in ppm

Zr_Yb_ppm Yb concentrations in ppm

Zr_Lu_ppm Lu concentrations in ppm

Source

IUPAC Website (https://iupac.org/)

Ballard, J. R., Palin, J. M., Williams, I. S., Campbell, I. H., and Faunes, A., 2001, Two ages of porphyry intrusion resolved for the super-giant Chuquicamata copper deposit of northern Chile by ELA-ICP-MS and SHRIMP: Geology, v. 29, p. 383–386. (https://pubs.geoscienceworld.org/gsa/geology/article-abstract/29/5/383/192017/Two-ages-of-porphyry-intrusion-resolved-for-the?redirectedFrom=fulltext)

Ballard, J. R., Palin, M. J., and Campbell, I. H., 2002, Relative oxidation states of magmas inferred from Ce(IV)/Ce(III) in zircon: application to porphyry copper deposits of northern Chile: Contributions to Mineralogy and Petrology, v. 144, p. 347–364. (https://link.springer.com/article/10.1007/s00410-002-0402-5)

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