

# Package ‘imputeREE’

July 19, 2022

**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](https://doi.org/10.1038/372452a0)>.

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**NeedsCompilation** no

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## R topics documented:

add_element_data . . . . .	2
add_ID . . . . .	2
add_IonicRadii . . . . .	3
add_NormValues . . . . .	3
add_parameters . . . . .	4
calc_all . . . . .	5
CleanColnames . . . . .	5
correct_heavy . . . . .	6

Element_Data . . . . .	6
element_denorm . . . . .	7
Element_norm . . . . .	8
impute_REE . . . . .	9
model_REE . . . . .	10
REE_Elements . . . . .	11
REE_plus_Y_Elements . . . . .	11
testing_data . . . . .	12

<b>Index</b>	<b>14</b>
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add_element_data	<i>Add ionic radius and chondrite and mantle values, Z and Mass</i>
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### 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
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### Value

A data frame

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add_ID	<i>Add_ID</i>
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### 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 <code>tibble::rowid_to_column()</code> function

**Value**

a data frame

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add_IonicRadii	<i>Add Chondrite or Mantle values for normalization.</i>
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**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

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add_NormValues	<i>Add Chondrite or Mantle values for normalization.</i>
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**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

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add_parameters	<i>Calculate relevant data from REE</i>
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**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')
```

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calc_all	<i>Calculate and Impute REE missing data and anomalies.</i>
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---

**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')
```

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CleanColnames	<i>Clean variable names that have prefixes or suffixes</i>
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**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

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correct_heavy	<i>Corrects for the model deviations of Yb, Lu and Y</i>
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**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

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Element_Data	<i>Element data for calculations</i>
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**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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1107/S0567739476001551)

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element\_denorm

*Denormalize chrodrite Normalize to ppm*

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**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

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Element_norm	<i>Calculate normalized values for a list of elements</i>
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**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



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impute_REE	<i>Impute Rare earth elements</i>
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### 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	<i>Model REE + Y contents using an empirical method based on the lattice strain theory</i>
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### Description

Model REE will make a linear regression between the REE (+Y) and the relationship of the ideal Ionic Radii in the lattice site ( $r_0$ ) and the ionic radii of the element that use that space ( $r_i$ ) according to the relationship :  $(r_i/3 + r_0/6)(r_i-r_0)^2$ . 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 $r_0$
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	<i>Rare earth element list</i>
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**Description**

A string vector containing the elemental symbols for REE.

**Usage**

```
REE_Elements
```

**Format**

Rare earth element list

---

REE_plus_Y_Elements	<i>Rare earth element list</i>
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---

**Description**

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

**Usage**

```
REE_plus_Y_Elements
```

**Format**

Rare earth element + Y list

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testing\_data

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

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### 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>)

# Index

## \* datasets

- Element\_Data, [6](#)
- REE\_Elements, [11](#)
- REE\_plus\_Y\_Elements, [11](#)
- testing\_data, [12](#)

- add\_element\_data, [2](#)
- add\_ID, [2](#)
- add\_IonicRadii, [3](#)
- add\_NormValues, [3](#)
- add\_parameters, [4](#)

- calc\_all, [5](#)
- CleanColnames, [5](#)
- correct\_heavy, [6](#)

- Element\_Data, [6](#)
- element\_denorm, [7](#)
- Element\_norm, [8](#)

- impute\_REE, [9](#)

- model\_REE, [10](#)

- REE\_Elements, [11](#)
- REE\_plus\_Y\_Elements, [11](#)

- testing\_data, [12](#)