# Package 'imputeREE'

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Title Impute Missing Rare Earth Element Data in Zircon			
Version 0.0.5			
<b>Description</b> Set of functions to impute missing rare earth data, calculate La and Pr concentrations and Ce anomalies in zircons based on the Chondrite-Onuma and Chondrite-Lattice of Carrasco-Godoy and Campbell (2023) <doi:10.1007 s00410-023-02025-9=""> and the Logarithmic regression from Zhong et al. (2019) <doi:10.1007 s00710-019-00682-y="">.</doi:10.1007></doi:10.1007>			
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 $add\_element\_data$ 

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 3

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

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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, chondrite = PalmeOneill2014CI)
```

## **Arguments**

dat Dataframe or tibble. doc

chondrite PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI

#### Value

a data frame or tibble

Ballard\_et\_al\_Zircon

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

```
Ballard_et_al_Zircon
```

# **Format**

A data frame with 210 rows and 18 variables:

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

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```
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

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)

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(dat, prefix = NULL, suffix = NULL, chondrite = PalmeOneill2014CI)
```

#### **Arguments**

dat A data frame with REE data in ppm
prefix A prefix in your columns e.g. ICP\_La
suffix A suffix in your columns e.g. La\_ppm

chondrite an option from: PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI

# Value

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

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# **Examples**

```
Ballard_et_al_Zircon %>% 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 Er, 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  $model_REE()$ 

```
correct_heavy(
  dat,
  Y_correction_fact = 1/0.72,
  Ho_correction_fact = 1,
  Er_correction_fact = 1/0.974,
  Tm_correction_fact = 1,
  Yb_correction_fact = 1/0.907,
  Lu_correction_fact = 1/0.926
)
```

correct\_middle 7

# Arguments

#### Value

a data frame

correct\_middle

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_middle(
  dat,
  Nd_correction_fact = 1/0.989,
  Sm_correction_fact = 1/1.022,
  Gd_correction_fact = 1/1.033,
  Tb_correction_fact = 1/1.05,
  Dy_correction_fact = 1/1.032,
  Pr_correction_fact = 1/0.918
)
```

# **Arguments**

```
dat A dataframe

Nd_correction_fact

a number: correction factor for underestimated Nd 1/0.0.989

Sm_correction_fact

a number: correction factor for overestimated Sm 1/1.022
```

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Gd\_correction\_fact

a number: correction factor for overestimated Gd 1/1.033

Tb\_correction\_fact

a number: correction factor for overestimated Tb 1/1.050

Dy\_correction\_fact

a number: correction factor for overestimated Dy 1/1.032

Pr\_correction\_fact

a number: correction factor for overestimated Pr 1/0.918

#### 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 11 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

**Z\_Zhong** numbers assigned by Zhong et al. (2019) for a logarithmic regression to calculate Zircon REE. ...

element\_denorm 9

#### **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

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

Zhong, S., Seltmann, R., Qu, H., and Song, Y., 2019, Characterization of the zircon Ce anomaly for estimation of oxidation state of magmas: a revised Ce/Ce\* method: Mineralogy and Petrology, v. 113, no. 6, p. 755–763. doi:10.1007/s0071001900682y

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

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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",
  chondrite = 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

chondrite 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 = 0.95)
```

# **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 model.

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 0.95. This limit is flexible and method dependent. As guidelines, the Chondrite-Lattice mthod should consider R-squared > 0.95 for at least 3 points. The Chondrite-Onuma method should consider R-squared > 0.98 for at least 4 points.

#### Value

A dataframe

# Examples

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

modelChondrite\_lattice

Model REE contents using the Chondrite-Lattice method of Rhrefhttps://link.springer.com/article/10.1007/s00410-023-02025-9Carrasco-Godoy and Campbell (2023)

# **Description**

This function apply the Chondrite-Lattice method which is a linear regression between the misfit parameter from the lattice strain equation and the logarithm of their chondrite normalized values. At least 2 points are required to use this method. This method is based on the work of Blundy and Wood (1994) but using chondrite normalized values as noted by Carrasco-Godoy and Campbell (2023). Refer to Carrasco-Godoy and Campbell (2023) for details.

# Usage

```
modelChondrite_lattice(
 dat,
 exclude = c("La", "Pr", "Ce", "Eu", "Y"),
 Calibrate = T,
 prefix = NULL,
 suffix = NULL,
 r0 = 0.87,
 chondrite = PalmeOneill2014CI,
 Pr_correction_fact = 1/0.918,
 Y_correction_fact = 1/0.72,
 Dy_correction_fact = 1/1.032,
 Ho_correction_fact = 1,
 Er_correction_fact = 1/0.974,
 Tm_correction_fact = 1,
 Yb_correction_fact = 1/0.8785,
 Lu_correction_fact = 1/0.8943,
 Nd_correction_fact = 1/0.989,
 Sm_correction_fact = 1/1.022,
 Gd_correction_fact = 1/1.033,
 Tb_correction_fact = 1/1.05
)
```

# **Arguments**

dat	A data frame with REE data in ppm			
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			
Calibrate	Logical (T or F). If True, the model is calibrated using the correction factors. By default it is the reciprocal of the median REE from the work of Carrasco-Godoy and Campbell is used.			
prefix	A prefix in your columns e.g. ICP_La			
suffix	A suffix in your columns e.g. La_ppm			
r0	A number: ionic radii of the lattice site r0. By default is 0.87 A, the median value obtained by Carrasco-Godoy and Campbell.			
chondrite	an option from: PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI			
Pr_correction_fact				
	a number: correction factor for overestimated Pr 1/0.918			
Y_correction_fact				
	a number: correction factor for underestimated Y. 1/0.72 by default.			
Dy_correction_fact				
	a number: correction factor for overestimated Dy 1/1.032			
Ho_correction_fact				
	a number: correction factor for Ho. 1 by default.			
Er_correction_fact				
	a number: correction factor for underestimated Er. 1/0.97 by default.			

#### Value

a dataframe

#### See Also

```
Other model REE: modelChondrite_Onuma(), modelZhong(), model_REE()
```

# **Examples**

```
Ballard_et_al_Zircon %>% modelChondrite_lattice(prefix = 'Zr', suffix = 'ppm')
```

```
modelChondrite_Onuma Model REE contents using the Chondrite-Onuma method of Rhrefhttps://link.springer.com/article/10.1007/s00410-023-02025-9Carrasco-Godoy and Campbell (2023)
```

#### **Description**

This function apply the Chondrite-Onuma method which is a quadratic regression between the ionic radius of the REE and the logarithm of their chondrite normalized values. At least 3 non-linear points are required to use this method. This method is based on the work of Onuma et al. (1968) but using chondrite normalized values as noted by Carrasco-Godoy and Campbell (2023). Refer to Carrasco-Godoy and Campbell (2023) for details.

```
modelChondrite_Onuma(
  dat,
  exclude = c("La", "Pr", "Ce", "Eu", "Y"),
  Calibrate = T,
  chondrite = PalmeOneill2014CI,
```

```
prefix = NULL,
    suffix = NULL,
    Pr_correction_fact = 1/1,
    Nd_correction_fact = 1/1.026486418,
    Sm_correction_fact = 1/0.971111041,
    Gd_correction_fact = 1/0.95928241,
    Tb_correction_fact = 1/1.000985745,
    Dy_correction_fact = 1/1.030049321,
    Ho_correction_fact = 1/1.018711009,
    Er_correction_fact = 1/0.996610693,
    Tm_correction_fact = 1/0.992656111,
    Lu_correction_fact = 1/0.952608321,
    Y_correction_fact = 1/0.665380561
)
```

#### **Arguments**

dat A data frame with REE data in ppm 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 Calibrate Logical (T or F). If True, the model is calibrated using the correction factors. By default it is the reciprocal of the median REE from the work of Carrasco-Godoy and Campbell is used. an option from: PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI chondrite prefix A prefix in your columns e.g. ICP\_La suffix A suffix in your columns e.g. La\_ppm Pr\_correction\_fact a number: correction factor for overestimated Pr 1/0.918 Nd\_correction\_fact a number: correction factor for underestimated Nd 1/0.0.989 Sm\_correction\_fact a number: correction factor for overestimated Sm 1/1.022 Gd\_correction\_fact a number: correction factor for overestimated Gd 1/1.033 Tb\_correction\_fact a number: correction factor for overestimated Tb 1/1.050 Dy\_correction\_fact a number: correction factor for overestimated Dy 1/1.032 Ho\_correction\_fact a number: correction factor for Ho. 1 by default. Er\_correction\_fact a number: correction factor for underestimated Er. 1/0.97 by default. Tm\_correction\_fact a number: correction factor for Tm. 1 by default.

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```
Yb_correction_fact
a number: correction factor for underestimated Yb. 1/0.8785 by default.

Lu_correction_fact
a number: correction factor for underestimated Lu. 1/0.8943 by default.

Y_correction_fact
a number: correction factor for underestimated Y. 1/0.72 by default.
```

#### Value

a dataframe

#### See Also

```
Other model REE: modelChondrite_lattice(), modelZhong(), model_REE()
```

# **Examples**

```
Ballard_et_al_Zircon %>% modelChondrite_Onuma(prefix = 'Zr', suffix = 'ppm')
```

modelZhong Model REE contents using the method of Rhrefhttps://link.springer.com/article/10.1007/s00710-019-00682-yZhong et al. (2019)

# **Description**

This function apply the logarithmic regression using the method of Zhong et al. (2019). This method considers the relationship between the logarithm of the REE atomic number vs their chondrite normalized values. For more information refer to the Zhong et al. (2019) and Carrasco-Godoy and Campbell (2023) for a discussion of its limitations to calculate La or Ce\*.

```
modelZhong(
  dat,
  exclude = c("La", "Pr", "Ce", "Eu", "Y"),
  Calibrate = F,
  chondrite = PalmeOneill2014CI,
  prefix = NULL,
  suffix = NULL
)
```

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# Arguments

dat A data frame with REE data in ppm

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

Calibrate Logical (T or F). If True, the model is calibrated using the correction factors. By

default it is the reciprocal of the median REE from the work of Carrasco-Godoy

and Campbell is used.

chondrite 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

#### Value

a dataframe

#### See Also

```
Other model REE: modelChondrite_Onuma(), modelChondrite_lattice(), model_REE()
```

# **Examples**

```
Ballard_et_al_Zircon %>% modelZhong(prefix = 'Zr', suffix = 'ppm')
```

model\_REE

*Model REE* + *Y contents using different methods.* 

#### **Description**

This function models REE + Y using different methods. The Chondrite-Lattice method use a linear regression between the REE (+Y) chondrite-normalized and the missfit term from the lattice strain equation (ri/3 + r0/6)(ri-r0)^2. The Chondrite-Onuma method use the quadratic relationship between the ionic radii and chondrite normalized REE values. The method of Zhong et al. (2019) use a logaritmic relationship between the atomic number of the REE and the chondrite normalized REE. For details in the lattice strain theory, see Blundy and Wood 1994. For more details in the imputation methods see Carrasco-Godoy and Campbell (2023), and Zhong et al. (2019)

```
model_REE(
  dat,
  method = 1,
  long_format = F,
  exclude = c("La", "Pr", "Ce", "Eu", "Y"),
  r0 = 0.84,
  chondrite = PalmeOneill2014CI,
  estimate_r0 = FALSE,
```

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```
r0_{step} = 0.01,
  r0_{min} = 0.01,
  r0_{max} = 0.15,
 prefix = NULL,
  suffix = NULL,
 Calibrate = T,
 Pr_correction_fact = 1/0.918,
 Y_correction_fact = 1/0.72,
 Dy_correction_fact = 1/1.032,
 Ho_correction_fact = 1,
 Er_correction_fact = 1/0.974,
 Tm_correction_fact = 1,
 Yb_correction_fact = 1/0.8785,
 Lu_correction_fact = 1/0.8943,
 Nd_correction_fact = 1/0.989,
  Sm_correction_fact = 1/1.022,
 Gd_correction_fact = 1/1.033,
 Tb\_correction\_fact = 1/1.05
)
```

# Arguments

Y\_correction\_fact

	dat	A data frame with REE data in ppm		
	method	a number. a choice of 1 for Chondrite Lattice or 2 for Zhong et al. $(2019)$ or 3 for Chondrite-Onuma method.		
	long_format	If T, rectangular long data is returned.		
	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		
	r0	A number: ionic radii of the lattice site r0. By default is 0.87 A, the median value obtained by Carrasco-Godoy and Campbell.		
	chondrite	an option from: PalmeOneill2014CI, Oneill2014Mantle, McDonough1995CI		
	estimate_r0	If T, r0 is estimated using a method similar to the one from Loader et al. 2022.		
	r0_step	If r0 is estimated, this define the step for iteration. smaller step heavily increases the computing time.		
	r0_min	Minimun value from which the iteration starts. Calculated from r0.		
	r0_max	Maximun value at which iteration ends. Calculated from r0.		
	prefix	A prefix in your columns e.g. ICP_La		
	suffix	A suffix in your columns e.g. La_ppm		
	Calibrate	Logical (T or F). If True, the model is calibrated using the correction factors. By default it is the reciprocal of the median REE from the work of Carrasco-Godoy and Campbell is used.		
Pr_correction_fact				

a number: correction factor for overestimated Pr 1/0.918

a number: correction factor for underestimated Y. 1/0.72 by default.

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Dy\_correction\_fact

a number: correction factor for overestimated Dy 1/1.032

Ho\_correction\_fact

a number: correction factor for Ho. 1 by default.

Er\_correction\_fact

a number: correction factor for underestimated Er. 1/0.97 by default.

Tm\_correction\_fact

a number: correction factor for Tm. 1 by default.

Yb\_correction\_fact

a number: correction factor for underestimated Yb. 1/0.8785 by default.

Lu\_correction\_fact

a number: correction factor for underestimated Lu. 1/0.8943 by default.

Nd\_correction\_fact

a number: correction factor for underestimated Nd 1/0.0.989

Sm\_correction\_fact

a number: correction factor for overestimated Sm 1/1.022

Gd\_correction\_fact

a number: correction factor for overestimated Gd 1/1.033

Tb\_correction\_fact

a number: correction factor for overestimated Tb 1/1.050

#### Value

a dataframe

#### See Also

Other model REE: modelChondrite\_Onuma(), modelChondrite\_lattice(), modelZhong()

# **Examples**

```
Ballard_et_al_Zircon %>% 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

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