Package 'NORRRM'

March 11, 2015

Type Package

Title Geochemical Toolkit for R

Version 1.0.0

Date 2015-01-29

Author Renee Gonzalez Guzman

Maintainer Renee Gonzalez Guzman <rguzman@cicese.edu.mx>

Imports ggplot2,SDMTools

Description

CIPW Norm (acronym from the surnames of the authors: Cross, Iddings, Pirrson and Washington) is the most commonly used calculation algorithm to estimate the standard mineral assemblages for igneous rocks from its geochemical composition. NORRRM (acronym from noRm, R language and
Renee) is the highly consistent program to calculate the CIPW Norm.

Depends R (>= 3.1.1)

License GPL (>= 3)

NeedsCompilation no

Repository CRAN

Date/Publication 2015-03-11 21:49:49

R topics documented:

NORRRM-package *Geochemical Toolkit for R*

Description

According to the IUGS (International Union of Geological Science), Subcommission on the Systematics of Igneous Rocks, the primary classification of igneous rocks must be based according to their modal mineral composition, expressed in volume percent. Nevertheless, where these data are not available or can not be determined owing to fine-grained mineral assemblage, glassy content or changes in the original mineralogy, then other criteria based on chemical bulk composition may be used.

Computed from the chemical composition, the normative mineralogy is an alternative approach for mineralogical classification and useful for set up the naming of igneous rocks (as parts of the TAS classification, `TASplot`). The CIPW Norm is the most commonly used calculation algorithm to estimate the standard mineral assemblages for igneous rocks `CIPW`, generated over more than a hundred years ago and thereafter modified by some authors to the passage of the years (e.g., Verma et al., 2002). It is based upon assumptions about the order of mineral formation and known phase relationships of rocks and minerals, using simplified mineral formulas.

In the option `CIPW.trace`, the trace elements that can be used are Ba, Cl, Co, Cr Cs, F, Li, Ni, Rb, S, Sr, V and Zr. Additionally, the oxides concentrations of Cr2O3, NiO and SO3 (expressed as wt. percent) are handled like trace elements as well. However Cr2O3 are preferable to Cr and NiO to Ni. Sulfur concentration when available is reported as either SO3 or S, in which case their separate identity should be maintained.

Details

Package:	NORRRM
Type:	Package
Version:	1.0.0
Date:	2015-02-28
License:	GPL-3

Author(s)

Renee Gonzalez Guzman <rguzman@cicese.edu.mx>

References

Bug reports: <rguzman@cicese.edu.mx>

AdjRock *AdjRock*

Description

The oxide data, from SiO2 to P2O5 (or CO21) are first recalculated to 100 percent on an anhydrous basis, and then Fe oxidation ratio adjustment is done according to the recommendations of Middlemost (1989), or Le Maitre (1976), or else the measured Fe2O3/FeO ratios are maintained. Finally, the oxide data is recalculated to 100 percent on an anhydrous basis from Fe2O3/FeO ratios calculated.

Usage

```
AdjRock(filename, Volcanic= TRUE, AdjTAS= TRUE, Cancrinite= FALSE,
Calcite= FALSE, digits=3)
```

Arguments

`filename`	a whole rock major and trace element chemical data. It is important to note that Fe2O3 or FeO could be Fe2O3T or FeOT if any of this values are NA or 0. On the other hands, the head format of CO2 column must be 'CO2.'
`Volcanic`	rock type, if is TRUE is shown the volcanic rock type after `TASplot` (Le Bas et al (1986)) in output, and combined with AdjTAS = FALSE, iron oxidation ratio is calculated following the equation of Le Maitre (1976) for Volcanic rocks, if is FALSE, then Plutonic adjusts are done.
`AdjTAS`	if is TRUE, iron oxidation ratio is calculated depending on rock type at `TASplot`.
`Cancrinite`	if is TRUE, CO2 will be used in whole rock adjust.
`Calcite`	if is TRUE, CO2 will be used in whole rock adjust.
`digits`	rounds the values to 'digits' after the decimal point. Default = 3, in order to keep their sum of rock oxides as close to 100 as possible.

Value

Returns a dataset of adjust oxide data on anhydrous basis.

Author(s)

Renee Gonzalez Guzman <rguzman@cicese.edu.mx>

References

Le Maitre, R.W. 1976. Some problems of the projection of chemical data into mineralogical classifications. Contribution Mineralogical Petrology. v. 56, pp. 181–189.

Middlemost, E.A.K. 1989. Iron oxidation ratios, norms and the classification of volcanic rocks. Chemical Geology. v. 77, pp. 19–26.

Examples

```
#create a dataframe with major elements indicating the appropriate parameters of rocks
data(TestTAS)#example of dataframe
AdjRock(TestTAS)
##

data(Andes)#example of dataframe
AdjRock(Andes)
##
```

Andes *Data collection of igneous rocks from Central Andes*

Description

Compilation of more than 1500 major and trace element analysis of igneous rocks from Central Andes.

Usage

```
data(Andes)
```

Format

The format is a data frame with 1511 rows and 40 columns.

Details

This data set documents compositional variations of magmas since Jurassic time to Neogene period in the Andean orogeny.

Source

The database is also available in GEOROC (Geochemistry of Rocks of the Oceans and Continents). For full details see http://georoc.mpch-mainz.gwdg.de/georoc/ .

References

Mamani, M., Worner, G., and Sempere, T. 2010. Geochemical variations in igneous rocks of the Central Andean orocline (13 S to 18 S): Tracing crustal thickening and magma generation through time and space. Bulletin of Geological Society of America. v. 122, pp. 162–182.

See Also

TestTAS

Examples

```
data(Andes)
##
```

AtomWeight *The standard atomic weights*

Description

Data frame with symbols, atom names and standard atomic weights.

Usage

```
data(AtomWeight)
```

Format

The format is a data frame with 92 rows and 3 columns, including the row names.

Details

This table is based on the 2011 table after the IUPAC (International Union of Pure and Applied Chemistry), Commission on Isotopic Abundances and Atomic Weights. It is important to note that row names are the symbol of the elements.

Source

http://www.chem.qmul.ac.uk/iupac/AtWt/

References

Wieser, M.E., and others. 2013. Pure and Applied Chemistry. International Union of Pure and Applied Chemistry (IUPAC). v. 78, no. 11, pp. 2051–2066.

See Also

MinWeight,OxiWeight

Examples

```
data(AtomWeight)
AtomWeight['H','AWeight']
##
```

CIPW *CIPW*

Description

Computed from the chemical composition, the normative mineralogy is an alternative approach for mineralogical classification and useful for set up the naming of igneous rocks (as parts of the TAS classification, TASplot). The CIPW Norm (acronym from the surnames of the authors: Cross, Iddings, Pirrson and Washington, Cross et al., 1902) is the most commonly used calculation algorithm to estimate the standard mineral assemblages for igneous rocks, generated over more than a hundred years ago and thereafter modified by some authors to the passage of the years (e.g., Verma et al., 2002). It is based upon assumptions about the order of mineral formation and known phase relationships of rocks and minerals, using simplified mineral formulas.

Usage

```
CIPW(filename, Volcanic= TRUE, AdjTAS= TRUE, Cancrinite= FALSE,
Calcite= FALSE, digits=3)
```

Arguments

filename	a whole rock major and trace element chemical data. It is important to note that Fe2O3 or FeO could be Fe2O3T or FeOT if any of this values are NA or 0. On the other hands, the head format of CO2 column must be 'CO2.'.
Volcanic	rock type, if is TRUE is shown the volcanic rock type after TASplot (Le Bas et al (1986)) in output, and combined with AdjTAS = FALSE, iron oxidation ratio is calculated following the equation of Le Maitre (1976) for Volcanic rocks, if is FALSE, then Plutonic adjusts are done.
AdjTAS	if is TRUE, iron oxidation ratio is calculated depending on rock type at TASplot.
Cancrinite	if is TRUE, CO2 will be used in whole rock adjust. If the concentration of CO2 is more than 0, and the modal cancrinite is present then Sodium carbonate is calculated.
Calcite	if is TRUE, CO2 will be used in whole rock adjust. If the concentration of CO2 is more than 0, and the modal calcite is present then Calcite is calculated.
digits	rounds the values to 'digits' after the decimal point. Default = 3, in order to keep their sum of rock oxides as close to 100 as possible.

Value

Calculate the CIPW Norm and others geochemical parameters.

Author(s)

Renee Gonzalez-Guzman <rguzman@cicese.edu.mx>

References

Cross, W., Iddings, J.P., Pirsson, L. V., Washington, Henry S. 1902, A quantitative chemico-mineralogical classification and nomenclature of igneous rocks: The Journal of Geology, v. 10, no. 6, pp. 555–690.

Verma, S.P., Torres-Alvarado, I.S., and Velasco-Tapia, F., 2003, A revised CIPW norm: Schweizerische Mineralogische und Petrographische Mitteilungen, v. 83, no. 2, pp. 197–216.

See Also

CIPW.trace

Examples

```
#create a dataframe with major elements indicating the appropriate parameters of rocks
data(TestTAS)#example of dataframe
CIPW(TestTAS)
##
```

`CIPW.trace` *CIPW Norm (major and trace elements)*

Description

Computed from the chemical composition, the normative mineralogy is an alternative approach for mineralogical classification and useful for set up the naming of igneous rocks (as parts of the TAS classification, TASplot). The CIPW Norm (acronym from the surnames of the authors: Cross, Iddings, Pirrson and Washington, Cross et al., 1902) is the most commonly used calculation algorithm to estimate the standard mineral assemblages for igneous rocks, generated over more than a hundred years ago and thereafter modified by some authors to the passage of the years (e.g., Verma et al., 2002). It is based upon assumptions about the order of mineral formation and known phase relationships of rocks and minerals, using simplified mineral formulas.

In this option, the trace elements that can be used are Ba, Cl, Co, Cr Cs, F, Li, Ni, Rb, S, Sr, V and Zr. Additionally, the oxides concentrations of Cr2O3, NiO and SO3 (expressed as wt. percent) are handled like trace elements as well. However Cr2O3 are preferable to Cr and NiO to Ni. Sulfur concentration when available is reported as either SO3 or S, in which case their separate identity should be maintained.

Usage

```
CIPW.trace(filename, Volcanic= TRUE, AdjTAS= TRUE, Cancrinite= FALSE,
Calcite= FALSE, digits=3)
```

Arguments

filename	a whole rock major and trace element chemical data. It is important to note that Fe2O3 or FeO could be Fe2O3T or FeOT if any of this values are NA or 0. On the other hands, the format of CO2 and F column must be 'CO2.' and 'F.', respectively.
Volcanic	rock type, if is TRUE is shown the volcanic rock type after TASplot in output, and combined with AdjTAS = FALSE, iron oxidation ratio is calculated following the equation of Le Maitre (1976) for Volcanic rocks, if is FALSE, then Plutonic adjusts are done.
AdjTAS	if is TRUE, iron oxidation ratio is calculated depending on rock type at TASplot.
Cancrinite	if is TRUE, CO2 will be used in whole rock adjust. If the concentration of CO2 is more than 0, and the modal cancrinite is present then Sodium carbonate is calculated.
Calcite	if is TRUE, CO2 will be used in whole rock adjust. If the concentration of CO2 is more than 0, and the modal calcite is present then Calcite is calculated.
digits	rounds the values to 'digits' after the decimal point. Default = 3, in order to keep their sum of rock oxides as close to 100 as possible.

Value

Calculate the CIPW Norm and others geochemical parameters.

Author(s)

Renee Gonzalez-Guzman <rguzman@cicese.edu.mx>

References

Cross, W., Iddings, J.P., Pirsson, L. V., Washington, Henry S. 1902, A quantitative chemico-mineralogical classification and nomenclature of igneous rocks: The Journal of Geology, v. 10, no. 6, pp. 555–690.

Verma, S.P., Torres-Alvarado, I.S., and Velasco-Tapia, F., 2003, A revised CIPW norm: Schweizerische Mineralogische und Petrographische Mitteilungen, v. 83, no. 2, pp. 197–216.

See Also

CIPW

Examples

```
#create a dataframe with major elements indicating the appropriate parameters of rocks
data(Andes)#example of dataframe
CIPW.trace(Andes)
##
```

MinWeight *The oxides molecular weights of normative minerals*

Description

Data frame with normative mineral names, chemical nomenclature, oxides molecular weights and theoretical density of minerals used in CIPW computations.

Usage

```
data(MinWeight)
```

Format

The format is a data frame with 36 rows and 6 columns, including the row names.

Details

This table is calculated from the 2011 table values after the IUPAC (International Union of Pure and Applied Chemistry), Commission on Isotopic Abundances and Atomic Weights. It is important to note that row names are the name of the normative minerals.

References

Wieser, M.E., and others. 2013. Pure and Applied Chemistry. International Union of Pure and Applied Chemistry (IUPAC). v. 78, no. 11, pp. 2051–2066.

See Also

AtomWeight,OxiWeight

Examples

```
data(MinWeight)
MinWeight['Quartz','ConsWeight']
##

MinWeight['Quartz','Density']
##
```

OxiWeight *The molecular weights*

Description

Data frame with chemical nomenclature and molecular weights used in CIPW computations.

Usage

```
data(OxiWeight)
```

Format

The format is a data frame with 26 rows and 3 columns, including the row names.

Details

This table is calculated from the 2011 table values after the IUPAC (International Union of Pure and Applied Chemistry), Commission on Isotopic Abundances and Atomic Weights. It is important to note that row names are the chemical nomenclature of the oxides and the third column is the oxide weight rounded.

References

Wieser, M.E., and others. 2013. Pure and Applied Chemistry. International Union of Pure and Applied Chemistry (IUPAC). v. 78, no. 11, pp. 2051–2066.

See Also

AtomWeight,MinWeight

Examples

```
data(OxiWeight)
OxiWeight ['SiO2','OWeight']
##
```

TASplot *TASplot*

Description

Plot the TAS diagram with automatical scales and adjusts. The TAS classification based on TAS diagram can be used to assign names to many common types of volcanic rocks based upon the relationships between the combined alkali content and the silica content. The Abbreviations in the plot mean; PB: Picrobasalt, B: Basalt, BA: Basaltic Andesite, A: Andesite, D: Dacite, R: Rhyolite, TB: Trachybasalt, BTA: Basaltictrachybasalt, TA: Trachyandesite, TD: Trachydacite, T: Trachyte, Ba: Basanite, Te: Tephrite, PT: Phonotephrite, TP: Tephriphonolite, P: Phonolite, F: Foidite.

Usage

```
TASplot(filename,color="blue",size=3,shape=1)
```

Arguments

filename	a whole rock major element chemical data.
color	color of the points. Default = "blue".
size	size of the points, in mm. Default = 3.
shape	shape of the points. Default = 1.

Author(s)

Renee Gonzalez Guzman <rguzman@cicese.edu.mx>

References

Le Bas, M.J., Le Maitre, R.W., Streckeisen, A. and Zanettin, B. (1986): A chemical classification of volcanic rocks on the total alkali vs silica diagram. Journal of Petrology. v 27, pp. 745–750.

Le Maitre, R.W et al. 2002. Igneous Rocks: A Classification and Glossary of Terms: Recommendations of the International Union of Geological Sciences, Subcommission on the Systematics of Igneous Rocks. Cambridge University Press, 2002, 252 pp.

Examples

```
data(Andes)
TASplot(Andes, color="blue")
##
```

TestTAS *Data collection of igneous rocks used in IUGSTAS software*

Description

Compilation of major elements data for 37 representative samples of volcanic rocks.

Usage

```
data(TestTAS)
```

Format

The format is a data frame with 37 rows and 20 columns.

Details

This data is available from the Cambridge University Press, as a part of IUGSTAS software.

References

Le Maitre, R.W et al. 2002. Igneous Rocks: A Classification and Glossary of Terms: Recommendations of the International Union of Geological Sciences, Subcommission on the Systematics of Igneous Rocks. Cambridge University Press, 2002, 252 pp.

See Also

Andes

Examples

```
data(TestTAS)
##
```

Index