

Package ‘CIAAWconsensus’

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Type Package

Title Isotope Ratio Meta-Analysis

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Description Calculation of consensus values for atomic weights, isotope amount ratios, and isotopic abundances with the associated uncertainties using multivariate meta-regression approach for consensus building.

License Unlimited

LazyData yes

Imports mvtnorm, stringr, numDeriv, stats, Matrix

NeedsCompilation no

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abundances2ratios *Isotope ratios of a chemical element from isotopic abundances*

Description

This function calculates the isotope ratios of a chemical element from the given isotopic abundances and their uncertainties. The uncertainty evaluation is done using the propagation of uncertainty and the missing correlations between the isotopic abundances are reconstructed using Monte Carlo methods.

Usage

```
abundances2ratios(x, ux, ref=1, iterations=1e4)
```

Arguments

| | |
|------------|--|
| x | A vector of isotopic abundances of an element |
| ux | Standard uncertainties of x |
| ref | Index to specify the desired reference isotope for isotope amount ratios |
| iterations | Number of iterations for isotopic abundance correlation mapping |

Details

Situations are often encountered where isotopic abundances are reported but not the isotope ratios. In such cases we reconstruct the isotope ratios that are consistent with the abundances and their uncertainties. Given only the abundances and their uncertainties, for elements with four or more isotopes one cannot unambiguously infer the uncertainties of the ratios due to the unknown correlations between isotopic abundances. This missing information can be reconstructed by mapping all possible correlations between isotopic abundances.

Value

| | |
|-------|---|
| R | Isotope ratio vector, excluding the trivial ratio |
| R.u | Standard uncertainties of the isotope ratios |
| R.cov | Isotope ratio covariance matrix |
| N | Number of successful Monte Carlo iterations |

Author(s)

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References

J. Meija and Z. Mester (2008) **Atomic weight uncertainty calculation from isotopic composition of the elements**. *Metrologia*, 45, 459

J. Meija and A. Possolo (2017) **Data reduction framework for standard atomic weights and isotopic compositions of the elements**. *Metrologia*, 54, 229-238

JCGM 101:2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method

Examples

```
## Isotope ratios of zinc from the isotopic abundances
x = c(0.48630, 0.27900, 0.04100, 0.18750, 0.00620)
ux = c(0.00091, 0.00076, 0.00031, 0.00135, 0.00010)
abundances2ratios(x,ux,ref=2)

## The corresponding atomic weight can be obtained using at.weight(z$R,z$cov,"zinc","66Zn")
```

| | |
|-----------|--|
| at.weight | <i>Atomic weight and isotopic abundances of a chemical element from isotope ratios</i> |
|-----------|--|

Description

This function calculates the isotopic abundances and the atomic weight of a chemical element from the given isotope amount ratios and their uncertainties. The uncertainty evaluation is done using the Monte Carlo method and the relevant masses of the isotopes are extracted from the www.ciaaw.org.

Usage

```
at.weight(ratio, ratio.cov, element, ref.isotope, data=NULL)
```

Arguments

| | |
|-------------|---|
| ratio | A vector of nontrivial isotope amount ratios of an element |
| ratio.cov | A covariance matrix of ratio |
| element | A string consisting of the lowercase English name of the element. For example, "zinc" |
| ref.isotope | A string which specifies the reference isotope. For example, "64Zn" |
| data | Nuclide mass dataframe. Default dataframe is <code>ciaaw.mass.2016</code> |

Details

The isotopic composition of an element with N isotopes is characterized using a set of N-1 nontrivial isotope amount ratios. As an example, silicon has three stable isotopes (silicon-28, silicon-29, and silicon-30) and its isotope ratios can be reported against either of its stable isotopes in three distinct ways: (1) $^{29}\text{Si}/^{28}\text{Si}$ and $^{30}\text{Si}/^{28}\text{Si}$ or (2) $^{28}\text{Si}/^{29}\text{Si}$ and $^{30}\text{Si}/^{29}\text{Si}$, or (3) $^{28}\text{Si}/^{30}\text{Si}$ and $^{29}\text{Si}/^{30}\text{Si}$.

Value

| | |
|----------------|---|
| aw | Atomic weight |
| aw.u | Standard uncertainty of the atomic weight |
| aw.U95 | Expanded uncertainty of the atomic weight corresponding to 95% confidence |
| abundances | Isotopic abundances |
| abundances.u | Standard uncertainty of the isotopic abundances |
| abundances.U95 | Expanded uncertainty of the isotopic abundances corresponding to 95% confidence |
| abundances.cov | Covariance matrix of the isotopic abundances |

Author(s)

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References

- J.Meija and Z. Mester (2008) **Uncertainty propagation of atomic weight measurement results**. *Metrologia*, 45, 53-62
- J. Meija and A. Possolo (2017) **Data reduction framework for standard atomic weights and isotopic compositions of the elements**. *Metrologia*, 54, 229-238
- JCGM 101:2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method

Examples

```
## Atomic weight and isotopic abundances of iridium which correspond
## to the isotope ratio 191Ir/193Ir = 0.59471(13)
at.weight(0.59471, matrix(0.00013^2), "iridium", "193Ir")

## Atomic weight and isotopic abundances of silicon which correspond
## to isotope ratios 28Si/29Si = 1.074(69) and 30Si/29Si = 260(11)
## with a correlation of 0.80 between the two isotope ratios
ratios = c(1.074,260)
r.cov = matrix(c(0.069^2,0.80*0.069*11,0.80*0.069*11,11^2),ncol=2,byrow=TRUE)
at.weight(ratios, r.cov, "silicon", "29Si")
```

ciaaw.mass.2003

Atomic masses of isotopes (IUPAC/CIAAW 2003)

Description

This data set gives the atomic masses and uncertainties of all polyisotopic nuclides as they are used by the IUPAC/CIAAW.

Usage

ciaaw.mass.2003

Format

A data frame with 268 rows and 4 variables:

- isotope: Symbol of the isotope
- element: Name of the element (lowercase english)
- mass: Atomic mass of the isotope in daltons
- uncertainty: Uncertainty of the atomic mass of the isotope as used by the IUPAC-CIAAW

Source

AME2003, <http://www.ciaaw.org/>

ciaaw.mass.2012

Atomic masses of isotopes (IUPAC/CIAAW 2012)

Description

This data set gives the atomic masses and uncertainties of all polyisotopic nuclides as they are used by the IUPAC/CIAAW.

Usage

ciaaw.mass.2012

Format

A data frame with 268 rows and 4 variables:

- isotope: Symbol of the isotope
- element: Name of the element (lowercase english)
- mass: Atomic mass of the isotope in daltons
- uncertainty: Uncertainty of the atomic mass of the isotope as used by the IUPAC-CIAAW

Source

AME2012 <https://doi.org/10.1088/1674-1137/41/3/030003>, <http://www.ciaaw.org/>

ciaaw.mass.2016 *Atomic masses of isotopes (IUPAC/CIAAW 2016)*

Description

This data set gives the atomic masses and uncertainties of all polyisotopic nuclides as they are used by the IUPAC/CIAAW.

Usage

ciaaw.mass.2016

Format

A data frame with 268 rows and 4 variables:

- isotope: Symbol of the isotope
- element: Name of the element (lowercase english)
- mass: Atomic mass of the isotope in daltons
- uncertainty: Uncertainty of the atomic mass of the isotope as used by the IUPAC-CIAAW

Source

AME2016 <https://doi.org/10.1088/1674-1137/41/3/030003>, <http://www.ciaaw.org/>

iridium.data *Iridium isotope ratio data from various studies*

Description

This data set gives the iridium isotope ratios as reported by various studies. These data are used by the IUPAC/CIAAW to determine the standard atomic weight of iridium.

Usage

iridium.data

Format

A data frame.

Source

IUPAC/CIAAW 2018

Description

This function provides meta-analysis of multivariate correlated data using the marginal method of moments with working independence assumption as described by Chen et al (2016). As such, the meta-analysis does not require correlations between the outcomes within each dataset.

Usage

```
mmm(y, uy, knha = TRUE, verbose = TRUE)
```

Arguments

| | |
|---------|---|
| y | A matrix of results from each of the n laboratories (rows) where each study reports m isotope ratios (columns) |
| uy | A matrix with uncertainties of the results given in y |
| knha | (Logical) Allows for the adjustment of consensus uncertainties using the Birge ratio (Knapp-Hartung adjustment) |
| verbose | (Logical) Requests annotated summary output of the results |

Details

The marginal method of moments delivers the inference for correlated effect sizes using multiple univariate meta-analyses.

Value

| | |
|----------|---|
| studies | The number of independent studies |
| beta | The consensus estimates for all outcomes |
| beta.u | Standard uncertainties of the consensus estimates |
| beta.U95 | Expanded uncertainties of the consensus estimates corresponding to 95% confidence |
| beta.cov | Covariance matrix of the consensus estimates |
| beta.cor | Correlation matrix of the consensus estimates |
| H | Birge ratios (Knapp-Hartung adjustment) which were applied to adjust the standard uncertainties of each consensus outcome |
| I2 | Relative total variability due to heterogeneity (in percent) for each outcome |

Author(s)

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References

- Y. Chen, Y. Cai, C. Hong, and D. Jackson (2016) [Inference for correlated effect sizes using multiple univariate meta-analyses](#). *Statistics in Medicine*, 35, 1405-1422
- J. Meija and A. Possolo (2017) [Data reduction framework for standard atomic weights and isotopic compositions of the elements](#). *Metrologia*, 54, 229-238

Examples

```
## Consensus isotope amount ratios for platinum
df=normalize.ratios(platinum.data, "platinum", "195Pt")
mmm(df$R, df$u.R)
```

| | |
|------------------|--|
| normalize.ratios | <i>Normalize isotope amount ratios to a common reference isotope</i> |
|------------------|--|

Description

This function converts the isotope amount ratios of an element from various studies to a single common reference isotope so that all isotope ratios can be directly compared to one another. The conversion involves a direct application of the law of propagation of uncertainty and this function discards the possible covariances between the isotope ratios.

Usage

```
normalize.ratios(dat, element, ref.isotope, expand = FALSE)
```

Arguments

| | |
|-------------|---|
| dat | A data frame of results from each study where each study reports one or more isotope ratios (outcomes). The data frame must include the following named columns: Study, Year, Author, Outcome, Value, Unc, k_extra (see Details). |
| element | Lowercase english name of the element, e.g., "antimony" |
| ref.isotope | Desired reference isotope, e.g., "121Sb" |
| expand | (Logical) Specification of whether or not to expand the isotope ratio uncertainties using the values of dat\$k_extra |

Details

The isotope ratio vector R is transformed to the reference isotope R_{ref} by dividing each element of the set to the chosen reference isotope. The covariances of the transformed isotope ratios are obtained using the Law of Propagation of Uncertainty. This function assumes all isotope ratios reported by a given study as uncorrelated. While this is not strictly true in practice, such assumption is made largely because of the lack of reported correlations in the literature.

The format of dat data frame for a simple dataset is as follows:

| Study | Year | Author | Outcome | Value | Unc | k_extra |
|-------|------|--------|---------|-------|-----|---------|
|-------|------|--------|---------|-------|-----|---------|

| | | | | | | |
|---|------|---------|-------------|---------|---------|---|
| 1 | 1954 | Howard | 191Ir/193Ir | 0.5949 | 0.0025 | 9 |
| 2 | 1991 | Creaser | 191Ir/193Ir | 0.5948 | 0.0001 | 9 |
| 3 | 1992 | Chang | 191Ir/193Ir | 0.59399 | 0.00103 | 6 |
| 4 | 1993 | Walczyk | 191Ir/193Ir | 0.59418 | 0.00037 | 9 |
| 5 | 2017 | Zhu | 191Ir/193Ir | 0.59290 | 0.00021 | 6 |

Value

| | |
|-------|--|
| R | A list of the normalized isotope amount ratios |
| u.R | A list of standard uncertainties for R |
| cov.R | A list of covariance matrices for R (forced to zero covariances) |

Author(s)

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References

- J. Meija and Z. Mester (2008) [Uncertainty propagation of atomic weight measurement results](#). *Metrologia*, 45, 53-62
- J. Meija and A. Possolo (2017) [Data reduction framework for standard atomic weights and isotopic compositions of the elements](#). *Metrologia*, 54, 229-238

Examples

```
## Normalize all platinum isotope data to platinum-195
normalize.ratios(platinum.data, "platinum", "195Pt")
```

| | |
|---------------|---|
| platinum.data | <i>Platinum isotope ratio data from various studies</i> |
|---------------|---|

Description

This data set gives the platinum isotope ratios as reported by various studies. These data are used by the IUPAC/CIAAW to determine the standard atomic weight of platinum.

Usage

```
platinum.data
```

Format

A data frame.

Source

IUPAC/CIAAW 2016

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