Package ‘isogeochem’

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Type Package

Title Tools For Carbonate Isotope Geochemistry

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Description This toolbox makes working with stable oxygen, carbon, and clumped isotope data reproducible and straightforward.

License GPL (>= 3)

URL https://github.com/davidbajnai/isogeochem

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.1

Suggests shades,
knitr,
rmarkdown,
spelling

VignetteBuilder knitr

Imports stats,
graphics,
grDevices

Depends R (>= 2.10)

BugReports https://github.com/davidbajnai/isogeochem/issues

Language en-US

R topics documented:

`a18_CO2acid_c` *Acid fractionation factor: 18O/16O*

Description

`a18_CO2acid_c()` calculates the 18O/16O oxygen isotope fractionation factor between CO2 from acid digestion and carbonate.

Usage

```
a18_CO2acid_c(temp, min)
```

Arguments

`temp`	Acid digestion temperature (°C).
`min`	Mineralogy. Options are `"calcite"` and `"aragonite"`.

Value

Returns the 18O/16O oxygen isotope fractionation factor "alpha".

References

Sharma, T., & Clayton, R. N. (1965). Measurement of ratios of total oxygen of carbonates. Geochimica et Cosmochimica Acta, 29(12), 1347-1353. https://doi.org/10.1016/0016-7037(65)90011-6

Kim, S.-T., Mucci, A., & Taylor, B. E. (2007). Phosphoric acid fractionation factors for calcite and aragonite between 25 and 75 °C: Revisited. Chemical Geology, 246(3-4), 135-146. https://doi.org/10.1016/j.chemgeo.2007.08.005

Kim, S.-T., Coplen, T. B., & Horita, J. (2015). Normalization of stable isotope data for carbonate minerals: Implementation of IUPAC guidelines. Geochimica et Cosmochimica Acta, 158, 276-289. https://doi.org/10.1016/j.gca.2015.02.011

See Also

Other alpha: `a18_H2O_OH()`, `a18_c_H2O()`

Examples

```
a18_CO2acid_c(90, "calcite") # Returns 1.008146
```

`a18_c_H2O` *Calculate the 18O/16O fractionation factor between carbonate and water*

Description

`a18_c_H2O()` calculates the equilibrium 18O/16O fractionation factor between carbonate and water for a given temperature.

Usage

```
a18_c_H2O(temp, min, eq)
```

Arguments

`temp`	Crystallization temperature in degrees Celsius.
`min`	Mineralogy. Options are `"calcite"`, `"aragonite"`, and `"dolomite"`.
`eq`	Equation used for the calculations. Options for **calcite**: • `"Daeron19"`: the equation of Daëron et al. (2019) • `"Watkins13"`: the equation of Watkins et al. (2013) • `"Coplen07"`: the equation of Coplen (2007) • `"KO97"`: Kim and O'Neil (1997) • `"FO77"`: the equation of O'Neil et al. (1969) reprocessed by Friedman and O'Neil (1977) Options for **aragonite**: • `"Dettman99"`: the equation of Grossman and Ku (1986) reprocessed by Dettman et al. (1999) Options for **dolomite**: • `"Vasconcelos05"`: the equation of Vasconcelos et al. (2005)

Value

Returns the equilibrium 18O/16O fractionation factor "alpha".

References

Calcite:

O'Neil, J. R., Clayton, R. N., & Mayeda, T. K. (1969). Oxygen isotope fractionation in divalent metal carbonates. The Journal of Chemical Physics, 51(12), 5547-5558. https://doi.org/10.1063/1.1671982

Kim, S.-T., & O'Neil, J. R. (1997). Equilibrium and nonequilibrium oxygen isotope effects in synthetic carbonates. Geochimica et Cosmochimica Acta, 61(16), 3461-3475. https://doi.org/10.1016/S0016-7037(97)00169-5

Coplen, T. B. (2007). Calibration of the calcite–water oxygen-isotope geothermometer at Devils Hole, Nevada, a natural laboratory. Geochimica et Cosmochimica Acta, 71(16), 3948-3957. https://doi.org/10.1016/j.gca.2007.05.028

Watkins, J. M., Nielsen, L. C., Ryerson, F. J., & DePaolo, D. J. (2013). The influence of kinetics on the oxygen isotope composition of calcium carbonate. Earth and Planetary Science Letters, 375, 349-360. https://doi.org/10.1016/j.epsl.2013.05.054

Daëron, M., Drysdale, R. N., Peral, M., Huyghe, D., Blamart, D., Coplen, T. B., et al. (2019). Most Earth-surface calcites precipitate out of isotopic equilibrium. Nature Communications, 10, 429. https://doi.org/10.1038/s41467-019-08336-5

Aragonite:

Dettman, D. L., Reische, A. K., & Lohmann, K. C. (1999). Controls on the stable isotope composition of seasonal growth bands in aragonitic fresh-water bivalves (unionidae). Geochimica et Cosmochimica Acta, 63(7-8), 1049-1057. https://doi.org/10.1016/s0016-7037(99)00020-4

Dolomite:

Vasconcelos, C., McKenzie, J. A., Warthmann, R., & Bernasconi, S. M. (2005). Calibration of the d18O paleothermometer for dolomite precipitated in microbial cultures and natural environments. Geology, 33(4), 317-320. https://doi.org/10.1130/g20992.1

See Also

Other alpha: a18_CO2acid_c(), a18_H2O_OH()

Examples

```
a18_c_H2O(25, "calcite", "Coplen07")   # Returns 1.030207
a18_c_H2O(25, "aragonite", "Dettman99") # Returns 1.029942
a18_c_H2O(25, "dolomite", "Vasconcelos05")  # Returns 1.031456
```

---

a18_H2O_OH — *Calculate the 18O/16O fractionation factor between water and hydroxide ion*

Description

a18_H2O_OH() calculates the 18O/16O oxygen isotope fractionation factor between H2O and aqueous hydroxide ion.

Usage

```
a18_H2O_OH(temp, eq = "Z21-X3LYP")
```

Arguments

temp	Temperature (°C).
eq	Equation used to calculate the fractionation factor. • Z20-X3LYP: the X3LYP/6-311+G(d,p) theoretical equation of Zeebe (2020). • Z20-MP2: the MP2/aug-cc-pVDZ theoretical equation of Zeebe (2020).

Value

Returns the 18O/16O oxygen isotope fractionation factor "alpha".

References

Zeebe, R. E. (2020). Oxygen isotope fractionation between water and the aqueous hydroxide ion. Geochimica et Cosmochimica Acta, 289, 182-195. https://doi.org/10.1016/j.gca.2020.08.025

See Also

Other alpha: a18_CO2acid_c(), a18_c_H2O()

Examples

```
a18_H2O_OH(90, "Z21-X3LYP") # Returns 1.008146
```

---

a_A_B *Isotope fractionation factor between A and B*

Description

a_A_B() calculates the isotope fractionation factor.

Usage

```
a_A_B(A, B)
```

Arguments

A	Delta value of A (‰).
B	Delta value of B (‰).

Details

$$\alpha^i E_{A/B} = \frac{\delta^i E_A + 1000}{\delta^i E_B + 1000}$$

Value

Returns the isotope fractionation factor "alpha".

See Also

B_from_a() calculates the delta value of B.

Examples

```
a_A_B(10, 12)
```

A_from_a *Isotope composition from fractionation factor*

Description

A_from_a() calculates the delta value of A from the isotope fractionation factor and the delta value of B.

Usage

```
A_from_a(a, B)
```

Arguments

a	Isotope fractionation factor between A/B "alpha".
B	Delta value of B (‰).

Value

Returns the delta value of B (‰).

See Also

a_A_B() calculates the isotope fractionation factor between A and B.

A_from_a() calculates the delta value of B.

Examples

```
A_from_a(1.033, -10)
```

B_from_a — *Isotope composition from fractionation factor*

Description

`B_from_a()` calculates the delta value of B using an isotope fractionation factor alpha.

Usage

```
B_from_a(a, A)
```

Arguments

`a`	Isotope fractionation factor between A/B.
`A`	Delta value of A (‰).

Value

Returns the delta value of B (‰).

See Also

`a_A_B()` calculates the isotope fractionation factor between A and B.

`A_from_a()` calculates the delta value of B.

Examples

```
B_from_a(1.033, 12)
```

d17O_c — *Triple oxygen isotope values*

Description

`d17O_c()` calculates equilibrium calcite d18O, d17O, and D17O values for a given temperature.

Usage

```
d17O_c(temp, d18O_H2O_VSMOW, eq18 = "Daeron19", lambda = 0.528)
```

Arguments

`temp`	Calcite growth temperature (°C).
`d18O_H2O_VSMOW`	Water d18O value expressed on the VSMOW scale (‰).
`eq18`	Equation used to calculate the equilibrium 18O/16O fractionation factor between calcite and water. Options are as in `a18_c_H2O()` with `"Daeron19"` being here the default.
`lambda`	Triple oxygen isotope reference slope. Default is `0.528`.

Details

$$\theta_{A/B} = \frac{\alpha^{17}_{A/B}}{\alpha^{18}_{A/B}}$$

$$\delta'^{17}O_{w,VSMOW} = \beta \times \delta'^{18}O_{w,VSMOW} + \gamma \text{ where } \beta = 0.528 \text{ and } \gamma = 0$$

$$\Delta^{17}O = \delta'^{17}O_{c,VSMOW} - \lambda \times \delta'^{18}O_{c,VSMOW}$$

Value

Returns a data frame:

- d18O value of the carbonate expressed on the VSMOW scale (‰).
- d18O value of the carbonate expressed on the VSMOW scale (‰).
- D17O value of the carbonate expressed on the VSMOW scale (‰).

References

Guo, W., & Zhou, C. (2019). Triple oxygen isotope fractionation in the DIC-H2O-CO2 system: A numerical framework and its implications. Geochimica et Cosmochimica Acta, 246, 541-564. https://www.doi.org/10.1016/j.gca.2018.11.018

See Also

Other equilibrium_carbonate: `D47()`, `D48()`, `d18O_c()`

Examples

```
d17O_c(10,-1) # Returns d18O_c = 32.44, d17O_c = 16.91, D17O = -0.084
d17O_c(10,-1)[,3] # Returns D17O = -0.084
prime(d17O_c(10,-1)[,2]) # Returns d'17O = 16.77
```

---

d18O_c — *Equilibrium carbonate d18O value*

Description

`d18O_c()` calculates the equilibrium d18O value of a carbonate grown at a given temperature.

Usage

```
d18O_c(temp, d18O_H2O_VSMOW, min, eq)
```

Arguments

- `temp` Crystallization temperature (°C).
- `d18O_H2O_VSMOW` Water d18O value expressed on the VSMOW scale (‰).
- `min` Mineralogy. Options are `"calcite"` (default), `"aragonite"`, and `"dolomite"`.
- `eq` Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between carbonate and water. Options depend on mineralogy and listed in `a18_c_H2O()`.

Value

Returns the equilibrium carbonate d18O value expressed on the VSMOW scale (‰).

Note

Use `to_VSMOW()` and `to_VPDB()` to convert between the VSMOW and VPDB scales.

References

References are listed in the description of `a18_c_H2O()`.

See Also

`d18O_H2O()` calculates the d18O value of the ambient water from the d18O value of a carbonate and its growth temperature.

Other equilibrium_carbonate: `D47()`, `D48()`, `d17O_c()`

Examples

```
d18O_c(33.7, -13.54, min = "calcite", eq = "Coplen07") # Returns 14.58
to_VPDB(d18O_c(12, -6.94, min = "aragonite", eq = "Dettman99"))
# Returns -5.21
d18O_c(25, -10.96, min = "dolomite", eq = "Vasconcelos05")
# Returns 20.15
```

`d18O_H2O` *Calculate water d18O value*

Description

`d18O_H2O()` calculates the d18O value of the ambient water. from the d18O value of a carbonate and its growth temperature.

Usage

```
d18O_H2O(temp, d18O_c_VSMOW, min = "calcite", eq)
```

Arguments

`temp`	Crystallization temperature (°C).
`d18O_c_VSMOW`	Carbonate d18O value expressed on the VSMOW scale (‰).
`min`	Mineralogy. Options are `"calcite"` (default), `"aragonite"`, and `"dolomite"`.
`eq`	Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between carbonate and water. Options depend on mineralogy and listed in `a18_c_H2O()`.

Value

Returns the water d18O value expressed on the VSMOW scale (‰).

Note

Use `to_VSMOW()` and `to_VPDB()` to convert between the VSMOW and VPDB scales.

References

References are listed in the description of `a18_c_H2O()`.

See Also

`d18O_c()` calculates the equilibrium d18O value of a carbonate grown at a given temperature.

`temp_d18O()` calculates growth temperatures from oxygen isotope data.

Examples

```
d18O_H2O(33.7, 14.58, "calcite", "Coplen07") # Returns -13.54
d18O_H2O(25, to_VSMOW(-7.47), "aragonite", "Dettman99") # Returns -6.53
d18O_H2O(25, 20.43, "dolomite", "Vasconcelos05") # Returns -10.69
```

`D47` *Carbonate D47 for a given temperature*

Description

`D47()` calculates the equilibrium carbonate D47 value for a given temperature.

Usage

```
D47(temp, eq)
```

Arguments

`temp`	Carbonate growth temperature (°C).
`eq`	Equation used for the calculation. • `"Fiebig21"`: the CDES90 calibration of Fiebig et al. (2021). • `"Petersen19"`: the synthetic-only IUPAC parameter "UNICAL" calibration of Petersen et al. (2019).

Value

Returns the carbonate D47 value expressed on the CDES90 scale (‰).

References

Petersen, S. V., Defliese, W. F., Saenger, C., Daëron, M., Huntington, K. W., John, C. M., et al. (2019). Effects of improved 17O correction on interlaboratory agreement in clumped isotope calibrations, estimates of mineral-specific offsets, and temperature dependence of acid digestion fractionation. Geochemistry, Geophysics, Geosystems, 20(7), 3495-3519. https://www.doi.org/10.1029/2018GC008127

Fiebig, J., Daëron, M., Bernecker, M., Guo, W., Schneider, G., Boch, R., et al. (2021). Calibration of the dual clumped isotope thermometer for carbonates. Geochimica et Cosmochimica Acta. https://www.doi.org/10.1016/j.gca.2021.07.012

See Also

`temp_D47()` calculates growth temperature from a D47 value.

Other equilibrium_carbonate: `D48()`, `d17O_c()`, `d18O_c()`

Examples

```
D47(33.7, "Petersen19") # Returns 0.580016
```

`D48` *Carbonate D48 for a given temperature*

Description

`D48()` calculates the equilibrium carbonate D48 value for a given temperature.

Usage

```
D48(temperature, eq = "Fiebig21")
```

Arguments

`temperature`	Carbonate growth temperature (°C).
`eq`	Equation used for the calculation. • `"Fiebig21"`: the CDES90 calibration of Fiebig et al. (2021). • `"Swart21"`: the CDES90 "PBLM1" calibration in Swart et al. (2021).

Value

Returns the carbonate equilibrium D48 value expressed on the CDES90 scale (‰).

References

Bajnai, D., Guo, W., Spötl, C., Coplen, T. B., Methner, K., Löffler, N., et al. (2020). Dual clumped isotope thermometry resolves kinetic biases in carbonate formation temperatures. Nature Communications, 11, 4005. https://doi.org/10.1038/s41467-020-17501-0

Fiebig, J., Daëron, M., Bernecker, M., Guo, W., Schneider, G., Boch, R., et al. (2021). Calibration of the dual clumped isotope thermometer for carbonates. Geochimica et Cosmochimica Acta. https://www.doi.org/10.1016/j.gca.2021.07.012

Swart, P. K., Lu, C., Moore, E., Smith, M., Murray, S. T., & Staudigel, P. T. (2021). A calibration equation between D48 values of carbonate and temperature. Rapid Communications in Mass Spectrometry, 35(17), e9147. https://www.doi.org/10.1002/rcm.9147

See Also

Other equilibrium_carbonate: `D47()`, `d17O_c()`, `d18O_c()`

Examples

```
D48(33.7, eq = "Fiebig21") # Returns 0.237
D48(33.7, eq = "Swart21") # Returns 0.239
```

`devilshole` *Devils Hole carbonate d18O time series*

Description

A dataset containing the d18O values of the "original" Devils Hole cores.

Usage

```
devilshole
```

Format

A data frame with 442 rows and 4 variables:

age Interpolated uranium-series age of the sample expressed as thousands of years before present (ka).

d18O_VSMOW Carbonate d18O value relative to VSMOW (per mille).

d18O_error Standard deviation on the d18O value.

core Name of the core (DHC2-8, DHC2-3, DH-11).

Source

https://doi.org/10.3133/ofr20111082

References

Winograd, I. J., Landwehr, J. M., Coplen, T. B., Sharp, W. D., Riggs, A. C., Ludwig, K. R., & Kolesar, P. T. (2006). Devils Hole, Nevada, d18O record extended to the mid-Holocene. Quaternary Research, 66(2), 202-212. https://doi.org/10.1016/j.yqres.2006.06.003

See Also

Other "datasets": `GTS2020`, `LR04`

`GTS2020` *Oxygen isotope stratigraphy from the Geologic Time Scale 2020: macrofossils*

Description

A dataset containing a compilation of d18O and d13C values of various macrofossils (bivalves, gastropods, belemnites, ammonites) together with information on their age, shell mineralogy, and the climate zone they represent. This dataset is a condensed version of the entire dataset presented in the Geologic Time Scale 2020. Specifically, the full dataset was filtered for those "select" d18O and d13C values that also have age information.

Usage

```
GTS2020
```

Format

A data frame with 9676 rows and 8 variables:

age Age of the sample expressed as millions of years before present (Ma).

d18O_VPDB Carbonate d18O value relative to VPDB (per mille).

d13C_VPDB Carbonate d13C value relative to VPDB (per mille).

mineralogy The mineralogy of the carbonate hard part.

group The fossil group (bivalve, gastropod, belemnite, ammonite).

clim_zone The climate zone the fossil represents.

Source

`https://download.pangaea.de/dataset/930093/files/GTS2020-App_10.2A.xlsx`

References

Grossman, E. L., & Joachimski, M. M. (2020). Oxygen isotope stratigraphy. In F. M. Gradstein, J. G. Ogg, M. D. Schmitz, & G. M. Ogg (Eds.), Geologic Time Scale 2020: Volume 1 (pp. 279-307): Elsevier. `https://doi.org/10.1016/B978-0-12-824360-2.00010-3`

See Also

Other "datasets": `LR04`, `devilshole`

LR04 — *A Pliocene-Pleistocene benthic foraminifera d18O stack*

Description

A dataset containing the LR04 benthic d18O stack.

Usage

```
LR04
```

Format

A data frame with 2115 rows and 3 variables:

age Age of the sample expressed as thousands of years before present (ka).

d18O_VPDB Carbonate d18O value relative to VPDB (per mille).

d18O_error Standard error on the d18O value.

Source

https://lorraine-lisiecki.com/stack.html

References

Lisiecki, L. E., & Raymo, M. E. (2005). A Pliocene-Pleistocene stack of 57 globally distributed benthic d18O records. Paleoceanography, 20(1), PA1003. https://doi.org/10.1029/2004pa001071

See Also

Other "datasets": GTS2020, devilshole

mix_d17O — *Mixing curves in triple oxygen isotope space*

Description

`mix_d17O()` produces mixing curves between two endmembers (A and B) in triple oxygen isotope space (d18O vs. D17O).

Usage

```
mix_d17O(d18O_A, d17O_A, d18O_B, d17O_B, lambda = 0.528)
```

Arguments

d18O_A	d18O value of component A (‰).
d17O_A	d17O value of component A (‰).
d18O_B	d18O value of component B (‰).
d17O_B	d17O value of component B (‰).
lambda	Triple oxygen isotope reference slope. Default `0.528`.

Value

Returns a data frame:

- d18O value of the mixture at x% mixing (‰).
- d18O value of the mixture x% mixing (‰).
- relative amount of component B in the mixture (%): from 100% A and 0% B to 0% A and 100% B.

See Also

`d17O_c()` calculates equilibrium calcite d18O, d17O, and D17O values for a given temperature.

Examples

```
# Mixing between a Mesozoic marine carbonate and a diagentic carbonate
mix_d17O(d17O_c(10, -1)[1],d17O_c(10, -1)[2],
  d17O_c(100,0)[1], d17O_c(100, 0)[2])
```

`prime` *Converting delta to delta prime*

Description

`prime()` converts "classical delta" values to "delta prime" values.

Usage

```
prime(classical)
```

Arguments

`classical`	"Classical delta" values to be converted (‰).

Details

$$\delta'^{17}O = 1000 \times \ln(\frac{\delta^{17}O}{1000} + 1)$$

Value

Returns the "delta prime" value (‰).

See Also

`unprime()` converts "delta prime" values to "classical delta" values.

Examples

```
prime(10) # Return 9.950331
```

`temp_d18O` *Oxygen isotope thermometry*

Description

`temp_d18O()` calculates carbonate growth temperature from oxygen isotope data.

Usage

```
temp_d18O(d18O_c_VSMOW, d18O_H2O_VSMOW, eq = "Daeron19")
```

Arguments

`d18O_c_VSMOW`	Carbonate d18O value expressed on the VSMOW scale (‰).
`d18O_H2O_VSMOW`	Water d18O value expressed on the VSMOW scale (‰).
`eq`	Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between carbonate and water. Options depend on mineralogy and listed in `a18_c_H2O()`.

Value

Returns the carbonate growth temperature (°C).

Note

Use `to_VSMOW()` and `to_VPDB()` to convert between the VSMOW and VPDB scales.

References

References are listed in the description of `a18_c_H2O()`.

See Also

`d18O_c()` calculates the equilibrium d18O value of a carbonate grown at a given temperature.

`d18O_H2O()` calculates the d18O value of the ambient water from the d18O value of a carbonate and its growth temperature.

Other thermometry: `temp_D47()`, `temp_D48()`

Examples

```
temp_d18O(14.58, -13.54, "Coplen07") # Returns 33.7
```

`temp_D47` *Clumped isotope thermometry*

Description

`temp_D47()` calculates carbonate growth temperature from D47 value.

Usage

```
temp_D47(D47_CDES90, D47_error, eq)
```

Arguments

`D47_CDES90`	Carbonate D47 values expressed on the CDES90 scale (‰).
`D47_error`	Error on the D47 value. Optional.
`eq`	Equation used for the calculation. • `"Petersen19"`: the synthetic-only IUPAC parameter "UNICAL" calibration of Petersen et al. (2019). • `"Kele14"`: the Kele et al. (2015) calibration reprocessed by Bernasconi et al. (2020) using the IUPAC parameters.

Value

Returns the carbonate growth temperature (°C), and — if `D47_error` is specified — also the error.

References

References are listed at `D47()`.

See Also

`D47()` calculates the equilibrium carbonate D47 value for a given temperature.

Other thermometry: `temp_D48()`, `temp_d18O()`

Examples

```
temp_D47(D47_CDES90 = 0.580, eq = "Petersen19") # Returns 33.7
temp_D47(D47_CDES90 = 0.580, D47_error = 0.004,
  eq = "Petersen19") # Returns 33.7 and 1.5
```

temp_D48 *Dual clumped isotope thermometry*

Description

`temp_D48()` calculates carbonate growth temperature from D47 and D48 values.

Usage

```
temp_D48(
  D47_CDES90,
  D48_CDES90,
  D47_error,
  D48_error,
  ks,
  add = FALSE,
  col,
  pch
)
```

Arguments

`D47_CDES90`	Carbonate D47 values expressed on the CDES90 scale (‰).
`D48_CDES90`	Carbonate D48 values expressed on the CDES90 scale (‰).
`D47_error`	Error on the D47 value. Optional.
`D48_error`	Error on the D48 value. Optional.
`ks`	Kinetic slope. Has to be negative!
`add`	Add graphics to an already existing plot? Default `FALSE`.
`col`	Graphical parameter. Optional.
`pch`	Graphical parameter. Optional.

Details

The function calculates a D47 value as an intersect of two curves: the equilibrium D47 vs D48 curve from Fiebig et al. (2021) and the kinetic slope. The resulting D47 value is then converted to temperature using the `D47()` function and the equation of Petersen et al. (2019). This is not consistent and I will fix it in a later patch. In any case, the resulting discrepancy is smaller than the temperature error.

Value

Returns the carbonate growth temperature (‰).

References

References are listed at `D48()` and `D47()`.

See Also

D47() calculates the equilibrium carbonate D47 value for a given temperature.

D48() calculates the equilibrium carbonate D48 value for a given temperature.

Other thermometry: temp_D47(), temp_d18O()

Examples

```
temp_D48(0.617, 0.139, ks = -0.6) # Returns 44
temp_D48(0.546, 0.277, ks = -1)   # Returns 33
```

---

to_VPDB — *Converting between VSMOW and VPDB scales*

Description

`to_VPDB()` converts d18O values expressed on the VSMOW scale to the VPDB scale.

Usage

```
to_VPDB(d18O_VSMOW, eq = "IUPAC")
```

Arguments

d18O_VSMOW	d18O values expressed on the VSMOW scale (‰).
eq	Equation used for the conversion. • "IUPAC" (default): the IUPAC recommended equation listed in Brand et al. (2014) and Kim et al. (2015). • "Coplen83": the equation listed in Coplen et al. (1983) and the Hoefs book.

Details

The IUPAC recommended equation to convert between the scales is:

$$\delta^{18}O_{VPDB} = 0.97001 \times \delta^{18}O_{VSMOW} - 29.99$$

Value

Returns the d18O value expressed on the VPDB scale (‰).

References

References are listed at to_VSMOW().

See Also

to_VSMOW() converts d18O values expressed on the VPDB scale to the VSMOW scale.

Examples

```
to_VPDB(0) # Returns -29.99
to_VPDB(0, eq = "Coplen83") # Returns -29.98
```

`to_VSMOW` *Converting between VPDB and VSMOW scales*

Description

`to_VSMOW()` converts d18O values expressed on the VPDB scale to the VSMOW scale.

Usage

```
to_VSMOW(d18O_VPDB, eq = "IUPAC")
```

Arguments

`d18O_VPDB`	d18O values expressed on the VPDB scale (‰).
`eq`	Equation used for the conversion. • `"IUPAC"` (default): the IUPAC recommended equation listed in Brand et al. (2014) and Kim et al. (2015). • `"Coplen83"`: the equation listed in Coplen et al. (1983) and the Hoefs book.

Details

The IUPAC recommended equation to convert between the scales is:

$$\delta^{18}O_{VSMOW} = 1.03092 \times \delta^{18}O_{VPDB} + 30.92$$

Value

Returns the d18O value expressed on the VSMOW scale (‰).

References

Coplen, T. B., Kendall, C., & Hopple, J. (1983). Comparison of stable isotope reference samples. Nature, 302, 236-238. https://doi.org/10.1038/302236a0

Brand, W. A., Coplen, T. B., Vogl, J., Rosner, M., & Prohaska, T. (2014). Assessment of international reference materials for isotope-ratio analysis (IUPAC Technical Report). Pure and Applied Chemistry, 86(3), 425-467. https://doi.org/10.1515/pac-2013-1023

Kim, S.-T., Coplen, T. B., & Horita, J. (2015). Normalization of stable isotope data for carbonate minerals: Implementation of IUPAC guidelines. Geochimica et Cosmochimica Acta, 158, 276-289. https://doi.org/10.1016/j.gca.2015.02.011

See Also

`to_VPDB()` converts d18O values expressed on the VSMOW scale to the VPDB scale.

Examples

```
to_VSMOW(0) # Returns 30.92
to_VSMOW(0, eq = "Coplen83") # Returns 30.91
```

`unprime` *Converting delta prime to delta*

Description

`unprime()` converts "delta prime" values to "classical delta" values.

Usage

```
unprime(prime)
```

Arguments

`prime`	"Delta prime" values to be converted (‰).

Details

$$\delta^{17}O = 1000 \times e^{(\frac{\delta'^{17}O}{1000}+1)}$$

Value

Returns the "classical delta" value (‰).

See Also

`prime()` converts "classical delta" values to "delta prime" values.

Examples

```
unprime(9.950331) # Return 10
```

`xDIC` *Dissolved inorganic carbon species*

Description

`xDIC()` calculates the relative abundance of the DIC species as a function of solution temperature, pH, and salinity.

Usage

```
xDIC(temp, pH, S)
```

Arguments

`temp`	The temperature of the solution (°C).
`pH`	The pH of the solution.
`S`	The salinity of the solution (g/kg, ‰).

Value

Returns a data frame with the relative abundance of the DIC species:

- Relative abundance of dissolved CO2 (%).
- Relative abundance of bicarbonate ion (%).
- Relative abundance of carbonate ion (%).

Examples

```
xDIC(25, 7, 30)
```

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