Package 'isogeochem'

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Type Package

Title Tools For Carbonate Isotope Geochemistry

Version 0.0.0.9100

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Description This collection of functions makes working with stable oxygen and clumped isotope data simpler and more reproducible.

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

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.1

Suggests knitr,
rmarkdown

VignetteBuilder knitr

Imports shades,
graphics,
reconPlots (>= 0.1.0)

Remotes andrewheiss/reconPlots

R topics documented:

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a18_c_w *Calculate 18O/16O fractionation factor between CaCO3 and H2O*

Description

a18_c_w() calculates the 18O/16O oxygen isotope fractionation factor between calcium carbonate and water

Usage

```
a18_c_w(temp, min = "calcite", eq = "Daeron19")
```

Arguments

temp	Crystallization temperature, in degrees Celsius.
min	Mineralogy. Options are "calcite" (default), "aragonite", and "dolomite".
eq	Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between calcium carbonate and water. Options depend on mineralogy. For calcite choose from "Daeron19" (default), "Watkins13", "Coplen07", "KO97" , and "FO77". For aragonite and dolomite the eq need not be specified.

Value

Returns the 18O/16O oxygen isotope fractionation factor "alpha" and the corresponding isotope fractionation value "epsilon" (parts per mille).

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://www.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://www.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://www.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://www.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://www.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://www.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://www.doi.org/10.1130/g20992.1

See Also

d18O()

Examples

```
a18_c_w(25, "calcite")   # Returns 1.030249 and 30.25
a18_c_w(25, "aragonite") # Returns 1.000913 and 0.91
a18_c_w(25, "dolomite")  # Returns 1.031456 and 31.46
```

---

d17O *Triple oxygen isotope values*

Description

d17O() calculates calcite d18O, d17O, and D17O values for given temperatures.

Usage

```
d17O(temp, d18Ow_VSMOW, eq18 = "Daeron19", lambda = 0.528)
```

Arguments

temp	Calcite growth temperature in degrees Celsius.
d18Ow_VSMOW	Water d18O value expressed on the VSMOW scale (parts per mille).
eq18	Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between calcite and water. Options are "Daeron19" (default), "Watkins13", "Coplen07", "KO97" , and "FO77".
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 with the carbonate d18O, d17O, and D17O values expressed on the VSMOW scale (all in parts per mille).

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

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://www.doi.org/10.1038/s41467-019-08336-5

See Also

d18O()

Examples

```
d17O(10,-1) # Returns d18Oc = 32.44, d17Oc = 16.91, D17O = -0.084
d17O(10,-1)[,3] # Returns D17O = -0.084
prime(d17O(10,-1)[,2]) # Returns d'17O = 16.77
```

---

d18O *Equilibrium carbonate d18O value*

Description

d18O() calculates the d18O value of a carbonate grown at a given temperature in equilibrium with ambient water.

Usage

```
d18O(temp, d18Ow_VSMOW, min = "calcite", eq = "Daeron19")
```

Arguments

temp	Crystallization temperature in degrees Celsius.
d18Ow_VSMOW	Water d18O value expressed on the VSMOW scale (parts per mille).
min	Mineralogy. Options are "calcite" (default), "aragonite", and "dolomite".
eq	Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between calcium carbonate and water. Options depend on mineralogy. For calcite choose from "Daeron19" (default), "Watkins13", "Coplen07", "KO97" , and "FO77". For aragonite and dolomite the eq need not be specified.

Value

Returns the equilibrium carbonate d18O value expressed on the VSMOW scale (parts per mille).

Note

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

References

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://www.doi.org/10.1063/1.1671982

Friedman, I., & O'Neil, J. R. (1977). Compilation of stable isotope fractionation factors of geochemical interest. U.S. Geological Survey Professional Paper, 440-KK, 1-12. https://www.doi.org/10.3133/pp440KK

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://www.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://www.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://www.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://www.doi.org/10.1038/s41467-019-08336-5

See Also

d18Ow()

temp_d18O()

Examples

```
d18O(33.7, -13.54, eq="Coplen07") # Returns 14.58
VPDB(d18O(12, -6.94, min="aragonite")) # Returns -5.21
d18O(25, -10.96, min="dolomite") # Returns 20.15
```

---

d18Ow *Calculate water d18O value*

Description

d18Ow() calculates the d18O value of the ambient water from the d18O value of a carbonate and its crystallization temperature.

Usage

```
d18Ow(temp, d18Oc_VSMOW, min = "calcite", eq = "Daeron19")
```

Arguments

temp	Crystallization temperature, in degrees Celsius.
d18Oc_VSMOW	Carbonate d18O value expressed on the VSMOW scale (parts per mille).
min	Mineralogy. Options are "calcite" (default), "aragonite", and "dolomite".
eq	Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between calcium carbonate and water. Options depend on mineralogy. For calcite choose from "Daeron19" (default), "Watkins13", "Coplen07", "KO97" , and "FO77". For aragonite and dolomite the eq need not be specified.

Value

Returns the water d18O value expressed on the VSMOW scale (parts per mille).

Note

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

References

References are listed at a18_c_w().

See Also

a18_c_w()

d18O()

temp_d18O()

Examples

```
d18Ow(33.7, 14.58, "calcite", "Coplen07") # Returns -13.54
d18Ow(25, VSMOW(-7.47), "aragonite") # Returns -6.53
d18Ow(25, 20.43, "dolomite") # Returns -10.69
```

D47 *Carbonate D47 for given temperatures*

Description

D47() calculates carbonate D47 values for a given temperature.

Usage

```
D47(temp, eq = "Fiebig21")
```

Arguments

temp	Carbonate growth temperature in degrees Celsius.
eq	Equation used for the calculation. Options are "Fiebig21" (default) and "Petersen19". "Fiebig21" refers to the CDES90 calibration in Fiebig et al. (2021). "Petersen19" refers to the synthetic-only D47-RFACBr,WD "UNICAL" calibration of Petersen et al. (2019).

Value

Returns carbonate D47 values expressed on the CDES90 scale: referenced to 90°C acid digestion.

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()`

`D48()`

Examples

```
D47(33.7) # Returns 0.5713
```

D48 *Carbonate D48 at given temperature*

Description

`D48()` calculates carbonate D48 values for given temperatures.

Usage

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

Arguments

`temperature`	Carbonate growth temperature in degrees Celsius.
`eq`	Equation used for the calculation. Options are `"Fiebig21"` and `"Swart21"`. Default is `"Fiebig21"`, which refers to the CDES90 calibration in Fiebig et al. (2021). `"Swart21"` refers to the CDES90 "PBLM1" calibration in Swart et al. (2021).

Value

Returns carbonate D48 values expressed on the CDES90 scale: referenced to 90°C acid digestion.

References

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

D47()

Examples

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

---

mix_d17O *Mixing curves*

Description

Use mix_d17O() to produce mixing curves in 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 values of component A (parts per mille).
d17O_A	d17O values of component A (parts per mille).
d18O_B	d18O values of component B (parts per mille).
d17O_B	d17O values of component B (parts per mille).
lambda	Triple oxygen isotope reference slope. Default is 0.528.

Value

Returns a data frame that contains the d18O and d17O values of the mixture, from 100% A and 0% B to 0% A and 100% B.

See Also

d17O()

Examples

```
# Mixing between a Mesozoic marine carbonate and a diagentic carbonate
mix_d17O(d17O(10,-1)[1],d17O(10,-1)[2],d17O(100,0)[1],d17O(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 (parts per mille).

Details

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

Value

Returns the "delta prime" value (parts per mille).

See Also

unprime()

Examples

```
prime(10) # Returns 9.950331
```

temp_d18O *Carbonate growth temperature from d18O*

Description

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

Usage

```
temp_d18O(d18Oc_VSMOW, d18Ow_VSMOW, eq = "Daeron19")
```

Arguments

d18Oc_VSMOW	Carbonate d18O value expressed on the VSMOW scale (parts per mille).
d18Ow_VSMOW	Water d18O value expressed on the VSMOW scale (parts per mille).
eq	Equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between calcite and water. For calcite choose from "Daeron19" (default), "Watkins13", "Coplen07", "KO97" , and "FO77".

Value

Returns a single numeric value. The result is the carbonate growth temperature, in degrees Celsius.

Note

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

References

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://www.doi.org/10.1063/1.1671982

Friedman, I., & O'Neil, J. R. (1977). Compilation of stable isotope fractionation factors of geochemical interest. U.S. Geological Survey Professional Paper, 440-KK, 1-12. https://www.doi.org/10.3133/pp440KK

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://www.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://www.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://www.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://www.doi.org/10.1038/s41467-019-08336-5

See Also

`d18O()`

`d18Ow()`

Examples

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

`temp_D47` *Carbonate growth temperature from D47*

Description

`temp_D47()` calculates carbonate growth temperature from clumped isotope composition (D47).

Usage

```
temp_D47(D47_CDES90, eq = "Petersen19")
```

Arguments

D47_CDES90	Carbonate D47 values expressed on the CDES90 scale: referenced to 90°C acid digestion.
eq	Equation used for the calculation. Options are "Petersen19" (default) and "Kele15". "Petersen19" refers to the synthetic-only IUPAC-reprocessed "Br "UNICAL" calibration of Petersen et al. (2019). "Kele14" refers to the Kele et al. (2015) calibration reprocessed by Bernasconi et al. (2020) using the IUPAC parameters.

Value

Returns the carbonate growth temperature in degrees Celsius.

References

Kele, S., Breitenbach, S. F. M., Capezzuoli, E., Meckler, A. N., Ziegler, M., Millan, I. M., et al. (2015). Temperature dependence of oxygen- and clumped isotope fractionation in carbonates: a study of travertines and tufas in the 6–95 °C temperature range. Geochimica et Cosmochimica Acta, 168, 172-192. https://www.doi.org/10.1016/j.gca.2015.06.032

Bernasconi, S. M., Müller, I. A., Bergmann, K. D., Breitenbach, S. F. M., Fernandez, A., Hodell, D. A., et al. (2018). Reducing uncertainties in carbonate clumped isotope analysis through consistent carbonate-based standardization. Geochemistry, Geophysics, Geosystems, 19(9), 2895-2914. https://www.doi.org/10.1029/2017gc007385

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

See Also

temp_d18O()

temp_D48()

Examples

```
temp_D47(0.580) # Returns 33.7
```

---

temp_D48 *Dual clumped isotope thermometry*

Description

temp_D48() calculates growth temperatures from D47 and D48 values.

Usage

```
temp_D48(D47_CDES90, D48_CDES90, ks, add = F)
```

Arguments

D47_CDES90	Carbonate D47 values expressed on the CDES90 scale.
D48_CDES90	Carbonate D48 values expressed on the CDES90 scale.
ks	Kinetic slope. Either -0.6 or -1. Has to be negative!
add	Add kinetic slope to an already existing plot?

Details

The function calculates a D47 value as an intersect of two curves:

- the equilibrium D47 vs D48 curve from Fiebig et al. (2021)
- the kinetic slope

The resulting D47 value is then converted to temperature using the D47() function, i.e., by default the equation of Petersen et al. (2019). This is not consistent and I will fix it in a later version. In any case, the resulting discrepancy is smaller than the temperature error.

Value

Returns the carbonate growth temperature in degrees Celsius.

References

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

D48()

temp_D47()

Examples

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

---

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 (parts per mille).

Details

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

Value

Returns the "classical delta" value (parts per mille).

See Also

`prime()`

Examples

```
unprime(9.950331) # Returns 10
```

VPDB *Converting between VSMOW and VPDB scales*

Description

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

Usage

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

Arguments

`d18O_VSMOW`	d18O values expressed on the VSMOW scale (parts per mille).
`eq`	Equation used for the conversion. Options are `"IUPAC"`, and `"Coplen83"`. The default is `"IUPAC"`: the IUPAC recommended equation listed in Brand et al. (2014) and Kim et al. (2015). To use the equation listed in Coplen et al. (1983) and the Hoefs book, set the parameter to `"Coplen83"`.

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 d18O values expressed on the VPDB scale (parts per mille).

References

Coplen, T. B., Kendall, C., & Hopple, J. (1983). Comparison of stable isotope reference samples. Nature, 302, 236-238. https://www.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://www.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://www.doi.org/10.1016/j.gca.2015.02.011

See Also

VSMOW()

Examples

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

VSMOW *Converting between VPDB and VSMOW scales*

Description

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

Usage

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

Arguments

d18O_VPDB	d18O values expressed on the VPDB scale (parts per mille).
eq	Defines the equation used for the conversion. Options are "IUPAC", and "Coplen83". The default is "IUPAC": the IUPAC recommended equation listed in Brand et al. (2014) and Kim et al. (2015). To use the equation listed in Coplen et al. (1983) and the Hoefs book, set the parameter to "Coplen83".

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 d18O values expressed on the VSMOW scale (parts per mille).

References

Coplen, T. B., Kendall, C., & Hopple, J. (1983). Comparison of stable isotope reference samples. Nature, 302, 236-238. https://www.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://www.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://www.doi.org/10.1016/j.gca.2015.02.011

See Also

VPDB()

Examples

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

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