Package 'isogeochem'

August 31, 2021

Type Package

Title Tools For Carbonate Isotope Geochemistry

Version 0.0.0.9000

Description This package contains a collection of functions, which are especially useful when working with stable oxygen or clumped isotope data. Please cite the original refernces listed after each function.

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Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.1

Suggests knitr,
rmarkdown

VignetteBuilder knitr

Imports reconPlots (>= 0.1.0)

Remotes andrewheiss/reconPlots

R topics documented:

`alpha18_cc_water` *Calculate 18O/16O fractionation factor*

Description

`alpha18_cc_water()` calculates the d18O value of the ambient water from the d18O value of a carbonate and its crystallization temperature.

Usage

```
alpha18_cc_water(temperature, eq = "Daeron19")
```

Arguments

`temperature`	Crystallization temperature, in degrees Celsius.
`eq`	Defines the equation used for the calculation. Options are *"KO97"*, *"Coplen07"*, *"Watkins13"*, and *"Daeron19"*. Default is *"Daeron19"*.

Value

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

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

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()`

Examples

```
alpha18_cc_water(33.7,"Coplen07") # Returns -13.54
```

d17O *Triple oxygen isotope values*

Description

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

Usage

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

Arguments

temperature	Carbonate growth temperature in degrees Celsius.
d18Ow_VSMOW	Water d18O value expressed on the VSMOW scale (parts per mille).
eq18	Defines the equation used to calculate the equilibrium 18O/16O oxygen isotope fractionation factor between water and calcium carbonate. Options are *"KO97"*, *"Coplen07"*, *"Watkins13"*, and *"Daeron19"*. Default is *"Daeron19"*. See also alpha18_cc_water().
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, d17Oand 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(temperature, d18O_water_VSMOW, eq = "Daeron19")
```

Arguments

temperature	Crystallization temperature in degrees Celsius.
d18O_water_VSMOW	Water d18O value expressed on the VSMOW scale (parts per mille).
eq	Defines the equation used for the calculation. Options are *"FO77"*, *"KO97"*, *"Coplen07"*, *"Watkins13"*, and *"Daeron19"*. Default is *"Daeron19"*.

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,"Coplen07") # Returns 14.58
```

---

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(temperature, d18O_carbonate_VSMOW, eq = "Daeron19")
```

Arguments

temperature	Crystallization temperature, in degrees Celsius.
d18O_carbonate_VSMOW	Carbonate d18O value expressed on the VSMOW scale (parts per mille).
eq	Defines the equation used for the calculation. Options are *"FO77"*, *"KO97"*, *"Coplen07"*, *"Watkins13"*, and *"Daeron19"*. Default is *"Daeron19"*.

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

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() temp_d18O()

Examples

```
d18Ow(33.7,14.58,"Coplen07") # Returns -13.54
```

D47 *Carbonate D47 for given temperatures*

Description

D47() calculates carbonate D47 values for given temperatures.

Usage

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

Arguments

temperature	Carbonate growth temperature in degrees Celsius.
eq	Defines the equation used for the calculation. Options are *"Petersen19"* and *"Fiebig21"*. Default is *"Fiebig21"*, which 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	Defines the equation used for the calculation. Options are *"Swart21"* and *"Fiebig21"*. 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 d18O to d'18O*

Description

`prime()` converts d18O values to d'18O

Usage

```
prime(d18O)
```

Arguments

d18O	d18O values to be converted (parts per mille).

Value

Returns the d'18O value (parts per mille).

See Also

`unprime()`

Examples

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

`temp_d18O` *Carbonate growth temperature from d18O*

Description

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

Usage

```
temp_d18O(d18O_carbonate_VSMOW, d18O_water_VSMOW, eq = "Daeron19")
```

Arguments

`d18O_carbonate_VSMOW`	Carbonate d18O value expressed on the VSMOW scale (parts per mille).
`d18O_water_VSMOW`	Water d18O value expressed on the VSMOW scale (parts per mille).
`eq`	Defines the equation used for the calculation. Options are *"FO77"*, *"KO97"*, *"Coplen07"*, *"Watkins13"*, and *"Daeron19"*. Default is *"Daeron19"*.

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	Defines the equation used for the calculation. Options are *"Kele15"* and *"Petersen19"*. Default is *"Petersen19"*, which 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()

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, kinetic_slope)
```

Arguments

D47_CDES90	Carbonate D47 values expressed on the CDES90 scale.
D48_CDES90	Carbonate D48 values expressed on the CDES90 scale.
kinetic_slope	Kinetic slope. Either -0.6 or +1.

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
```

---

unprime *Converting d'18O to d18O*

Description

unprime() converts d'18O values to d18O.

Usage

```
unprime(d18O_prime)
```

Arguments

d18O_prime	d18O values to be converted (parts per mille).

Value

Returns the d18O 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	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"*.

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"*.

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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