Package ‘isogeochem’

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Type Package

Title Tools for Carbonate Isotope Geochemistry

Version 1.0.8

Description This toolbox makes working with carbonate oxygen,
carbon, and clumped isotope data reproducible and straightforward.
Use it to quickly calculate isotope fractionation factors,
and apply paleothermometry equations.

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

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

Encoding UTF-8

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R topics documented:

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`a13_CO2g_CO2aq` *13C/12C fractionation factor between CO2(g) and CO2(aq)*

Description

`a13_CO2g_CO2aq()` calculates the 13C/12C fractionation factor between gaseous and dissolved CO2.

Usage

```
a13_CO2g_CO2aq(temp)
```

Arguments

`temp`	Temperature (°C).

Details

$$\alpha^{13}_{CO2(g)/CO2(aq)} = (\frac{-1.18 + 0.0041 \times (T - 273.15)}{1000} + 1)^{-1}$$

Value

Returns the 13C/12C fractionation factor.

References

Vogel, J. C., Grootes, P. M., & Mook, W. G. (1970). Isotopic fractionation between gaseous and dissolved carbon dioxide. Zeitschrift für Physik A: Hadrons and Nuclei, 230(3), 225-238. doi: 10.1007/Bf01394688

See Also

Other fractionation_factors: `a18_CO2acid_c()`, `a18_CO2aq_H2O()`, `a18_CO2g_H2O()`, `a18_CO3_H2O()`, `a18_H2O_OH()`, `a18_HCO3_H2O()`, `a18_c_H2O()`, `a_A_B()`

`a18_CO2acid_c` *18O/16O acid fractionation factor*

Description

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

Usage

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

Arguments

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

Details

calcite (Kim et al. 2015):

$$\alpha^{18}_{CO2acid/calcite} = e^{(3.48 \times \frac{1}{T} - 0.00147)}$$

aragonite (Kim et al. 2007):

$$\alpha^{18}_{CO2acid/aragonite} = e^{(3.39 \times \frac{1}{T} - 0.00083)}$$

Value

Returns the 18O/16O fractionation factor.

References

Sharma, T., and Clayton, R. N. (1965). Measurement of ratios of total oxygen of carbonates. Geochimica et Cosmochimica Acta, 29(12), 1347-1353. doi: 10.1016/00167037(65)900116

Kim, S.-T., Mucci, A., and 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. doi: 10.1016/j.chemgeo.2007.08.005

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

See Also

Other fractionation_factors: `a13_CO2g_CO2aq()`, `a18_CO2aq_H2O()`, `a18_CO2g_H2O()`, `a18_CO3_H2O()`, `a18_H2O_OH()`, `a18_HCO3_H2O()`, `a18_c_H2O()`, `a_A_B()`

Examples

```
a18_CO2acid_c(temp = 90, min = "calcite")
a18_CO2acid_c(temp = 72, min = "aragonite")
```

`a18_CO2aq_H2O` *18O/16O fractionation factor between CO2(aq) and H2O(l)*

Description

`a18_CO2_H2O()` calculates the 18O/16O fractionation factor between dissolved CO2 and liquid water.

Usage

```
a18_CO2aq_H2O(temp)
```

Arguments

`temp`	Temperature (°C).

Details

$$\alpha^{18}_{CO2(aq)/H2O(l)} = e^{2.52\times\frac{1000}{T^2}+0.01212}$$

Value

Returns the 18O/16O fractionation factor.

References

Beck, W. C., Grossman, E. L., & Morse, J. W. (2005). Experimental studies of oxygen isotope fractionation in the carbonic acid system at 15°, 25°, and 40°C. Geochimica et Cosmochimica Acta, 69(14), 3493-3503. doi: 10.1016/j.gca.2005.02.003

See Also

Other fractionation_factors: a13_CO2g_CO2aq(), a18_CO2acid_c(), a18_CO2g_H2O(), a18_CO3_H2O(), a18_H2O_OH(), a18_HCO3_H2O(), a18_c_H2O(), a_A_B()

---

a18_CO2g_H2O *18O/16O fractionation factor between CO2(g) and H2O(l)*

Description

a18_CO2_H2O() calculates the 18O/16O fractionation factor between gaseous CO2 and liquid water.

Usage

```
a18_CO2g_H2O(temp)
```

Arguments

temp	Temperature (°C).

Details

$$\alpha^{18}_{CO2(g)/H2O(l)} = (17.604 \times \frac{1}{T} - 0.01793) + 1$$

Value

Returns the 18O/16O fractionation factor.

References

Brenninkmeijer, C. A. M., Kraft, P., & Mook, W. G. (1983). Oxygen isotope fractionation between CO2 and H2O. Chemical Geology, 41, 181-190. doi: 10.1016/S00092541(83)800151

See Also

Other fractionation_factors: a13_CO2g_CO2aq(), a18_CO2acid_c(), a18_CO2aq_H2O(), a18_CO3_H2O(), a18_H2O_OH(), a18_HCO3_H2O(), a18_c_H2O(), a_A_B()

a18_CO3_H2O *18O/16O fractionation factor between CO3(2-) and H2O*

Description

`a18_CO3_H2O()` calculates the 18O/16O fractionation factor between carbonate ion CO3(2-) and water.

Usage

```
a18_CO3_H2O(temp)
```

Arguments

`temp`	Temperature (°C).

Details

$$\alpha^{18}_{CO3(2-)/H2O} = e^{2.39 \times \frac{1000}{T^2} - 0.00270}$$

The equation above and in the function is the uncorrected equation in Beck et al. (2005). They experimentally determined the fractionation factor using BaCO3 precipitation experiments. However, they applied the acid fractionation factor of calcite during the data processing and not that of BaCO3. The acid fractionation factor of BaCO3 is not known accurately, which may result in a bias of up to 1‰ in the calculated 1000lna values.

Value

Returns the 18O/16O fractionation factor.

References

Beck, W. C., Grossman, E. L., & Morse, J. W. (2005). Experimental studies of oxygen isotope fractionation in the carbonic acid system at 15°, 25°, and 40°C. Geochimica et Cosmochimica Acta, 69(14), 3493-3503. doi: 10.1016/j.gca.2005.02.003

See Also

Other fractionation_factors: `a13_CO2g_CO2aq()`, `a18_CO2acid_c()`, `a18_CO2aq_H2O()`, `a18_CO2g_H2O()`, `a18_H2O_OH()`, `a18_HCO3_H2O()`, `a18_c_H2O()`, `a_A_B()`

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

Description

`a18_c_H2O()` calculates the 18O/16O fractionation factor between carbonate and water.

Usage

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

Arguments

`temp`	Carbonate growth temperature (°C).
`min`	Mineralogy. Options are `"calcite"`, `"aragonite"`, `apatite`, `siderite`, and `"dolomite"`.
`eq`	Equation used for the calculations. See details.

Details

Options for eq if min = `"calcite"`:

`"ONeil69"`: O'Neil et al. (1969), modified by Friedman and O'Neil (1977):

$$\alpha^{18}_{calcite/water} = e^{(2.78 \times \frac{1000}{T^2} - 0.00289)}$$

`"KO97-orig"`: Kim and O'Neil (1997):

$$\alpha^{18}_{calcite/water} = e^{(18.03 \times \frac{1}{T} - 0.03242)}$$

NOTE: The "KO97-orig" equation should only be applied to data that considers a CO2(acid)/calcite AFF as in Kim & O'Neil (1997), i.e., 10.44 at 25 °C.

`"KO97"`: Kim and O'Neil (1997), reprocessed here to match the IUPAC-recommended AFF as in Kim et al. (2007, 2015):

$$\alpha^{18}_{calcite/water} = e^{(18.04 \times \frac{1}{T} - 0.03218)}$$

`"Coplen07"`: Coplen (2007):

$$\alpha^{18}_{calcite/water} = e^{(17.4 \times \frac{1}{T} - 0.0286)}$$

`"Tremaine11"`: Tremaine et al. (2011):

$$\alpha^{18}_{calcite/water} = e^{(16.1 \times \frac{1}{T} - 0.0246)}$$

`"Watkins13"`: Watkins et al. (2013):

$$\alpha^{18}_{calcite/water} = e^{(17.747 \times \frac{1}{T} - 0.029777)}$$

"Daeron19": Daëron et al. (2019):

$$\alpha^{18}_{calcite/water} = e^{(17.57\times\frac{1}{T}-0.02913)}$$

Options for eq if min = "aragonite":

"GK86": Grossman and Ku (1986), modified by Dettman et al. (1999):

$$\alpha^{18}_{aragonite/water} = e^{(2.559\times\frac{1000}{T^2}+0.000715)}$$

"Kim07": Kim et al. (2007):

$$\alpha^{18}_{aragonite/water} = e^{(17.88\times\frac{1}{T}-0.03114)}$$

Options for eq if min = "apatite". Apatite refers to apatite-bound carbonate.

"Lecuyer10": Lécuyer et al. (2010):

$$\alpha^{18}_{apatite/water} = e^{(25.19\times\frac{1}{T}-0.05647)}$$

Options for eq if min = "siderite":

"vanDijk18": van Dijk et al. (2018):

$$\alpha^{18}_{siderite/water} = e^{(19.67\times\frac{1}{T}-0.03627)}$$

Options for eq if min = "dolomite":

"Vasconcelos05": Vasconcelos et al. (2005):

$$\alpha^{18}_{dolomite/water} = e^{(2.73\times\frac{1000}{T^2}+0.00026)}$$

Value

Returns the 18O/16O 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. doi: 10.1063/1.1671982

Grossman, E. L., & Ku, T. L. (1986). Oxygen and carbon isotope fractionation in biogenic aragonite: Temperature effects. Chemical Geology, 59(1), 59-74. doi: 10.1016/00092541(86)900446

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. doi: 10.1016/S0016-7037(97)001695

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. doi: 10.1016/s00167037(99)000204

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. doi: 10.1130/g20992.1

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. doi: 10.1016/j.chemgeo.2007.08.005

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. doi: 10.1016/j.gca.2007.05.028

Lécuyer, C., Balter, V., Martineau, F., Fourel, F., Bernard, A., Amiot, R., et al. (2010). Oxygen isotope fractionation between apatite-bound carbonate and water determined from controlled experiments with synthetic apatites precipitated at 10–37°C. Geochimica et Cosmochimica Acta, 74(7), 2072-2081. doi: 10.1016/j.gca.2009.12.024

Tremaine, D. M., Froelich, P. N., & Wang, Y. (2011). Speleothem calcite farmed in situ: Modern calibration of d18O and d13C paleoclimate proxies in a continuously-monitored natural cave system. Geochimica et Cosmochimica Acta, 75(17), 4929-4950. doi: 10.1016/j.gca.2011.06.005

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. doi: 10.1016/j.epsl.2013.05.054

van Dijk, J., Fernandez, A., Müller, I. A., Lever, M., & Bernasconi, S. M. (2018). Oxygen isotope fractionation in the siderite-water system between 8.5 and 62 °C. Geochimica et Cosmochimica Acta, 220, 535-551. doi: 10.1016/j.gca.2017.10.009

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. doi: 10.1038/s41467019083365

See Also

Other fractionation_factors: `a13_CO2g_CO2aq()`, `a18_CO2acid_c()`, `a18_CO2aq_H2O()`, `a18_CO2g_H2O()`, `a18_CO3_H2O()`, `a18_H2O_OH()`, `a18_HCO3_H2O()`, `a_A_B()`

Examples

```
a18_c_H2O(temp = 25, min = "calcite", eq = "Coplen07")
a18_c_H2O(temp = 25, min = "aragonite", "GK86")
```

`a18_H2O_OH` *18O/16O fractionation factor between water and hydroxide ion*

Description

`a18_H2O_OH()` calculates the 18O/16O fractionation factor between water and aqueous hydroxide ion.

Usage

```
a18_H2O_OH(temp, eq)
```

Arguments

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

Value

Returns the 18O/16O fractionation factor.

References

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

See Also

Other fractionation_factors: `a13_CO2g_CO2aq()`, `a18_CO2acid_c()`, `a18_CO2aq_H2O()`, `a18_CO2g_H2O()`, `a18_CO3_H2O()`, `a18_HCO3_H2O()`, `a18_c_H2O()`, `a_A_B()`

Examples

```
a18_H2O_OH(temp = 90, eq = "Z20-X3LYP")
```

`a18_HCO3_H2O` *18O/16O fractionation factor between HCO3(-) and H2O*

Description

`a18_HCO3_H2O()` calculates the 18O/16O fractionation factor between bicarbonate ion HCO3(-) and water.

Usage

```
a18_HCO3_H2O(temp)
```

Arguments

`temp`	Temperature (°C).

Details

$$\alpha^{18}_{HCO3(-)/H2O} = e^{2.59 \times \frac{1000}{T^2} + 0.00189}$$

The equation above and in the function is the uncorrected equation in Beck et al. (2005). They experimentally determined the fractionation factor using BaCO3 precipitation experiments. However, they applied the acid fractionation factor of calcite during the data processing and not that of BaCO3. The acid fractionation factor of BaCO3 is not known accurately, which may result in a bias of up to 1‰ in the calculated 1000lna values.

Value

Returns the 18O/16O fractionation factor.

References

Beck, W. C., Grossman, E. L., & Morse, J. W. (2005). Experimental studies of oxygen isotope fractionation in the carbonic acid system at 15°, 25°, and 40°C. Geochimica et Cosmochimica Acta, 69(14), 3493-3503. doi: 10.1016/j.gca.2005.02.003

See Also

Other fractionation_factors: `a13_CO2g_CO2aq()`, `a18_CO2acid_c()`, `a18_CO2aq_H2O()`, `a18_CO2g_H2O()`, `a18_CO3_H2O()`, `a18_H2O_OH()`, `a18_c_H2O()`, `a_A_B()`

---

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	Isotope delta value of A (‰).
B	Isotope delta value of B (‰).

Details

$$\alpha^i E_{A/B} = \frac{\delta^i E_A + 1}{\delta^i E_B + 1}$$

Value

Returns the isotope fractionation factor.

See Also

`A_from_a()` calculates the isotope delta value of A.

`B_from_a()` calculates the isotope delta value of B.

Other fractionation_factors: `a13_CO2g_CO2aq()`, `a18_CO2acid_c()`, `a18_CO2aq_H2O()`, `a18_CO2g_H2O()`, `a18_CO3_H2O()`, `a18_H2O_OH()`, `a18_HCO3_H2O()`, `a18_c_H2O()`

Examples

```
a_A_B(A = 10, B = 12)
```

`A_from_a` *Isotope delta from fractionation factor*

Description

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

Usage

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

Arguments

`a`	Isotope fractionation factor between A and B.
`B`	Isotope delta value of B (‰).

Value

Returns the isotope delta value of B (‰).

See Also

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

`B_from_a()` calculates the isotope delta value of B.

Examples

```
A_from_a(a = 1.033, B = -10)
```

`B_from_a` *Isotope delta from fractionation factor*

Description

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

Usage

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

Arguments

`a`	Isotope fractionation factor between A and B.
`A`	Isotope delta value of A (‰).

Value

Returns the Isotope delta value of B (‰).

See Also

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

A_from_a() calculates the isotope delta value of A.

Examples

```
B_from_a(a = 1.033, A = 10)
```

D17O — *Triple oxygen isotope value*

Description

D17O() calculates the D17O value.

Usage

```
D17O(d18O, d17O, lambda = 0.528)
```

Arguments

d18O	Isotope delta value (‰).
d17O	Isotope delta value (‰).
lambda	Triple oxygen isotope reference slope. Default 0.528.

Details

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

Value

Returns the D17O value (‰).

Examples

```
D17O(d18O = -10, d17O = -5, lambda = 0.528)
```

d17O_c *Triple oxygen isotope values*

Description

d17O_c() calculates the equilibrium d18O, d17O, and D17O values of a calcite grown at 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 18O/16O fractionation factor between calcite and water. Options are like those for calcite in a18_c_H2O() with "Daeron19" being here the default.
lambda	Triple oxygen isotope reference slope. Default 0.528.

Details

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

$$\delta'^{17}O_{H2O,VSMOW} = \beta \times \delta'^{18}O_{H2O,VSMOW} + \gamma \text{ , where } \beta = 0.528 \text{ and } \gamma = 0$$

$$\Delta^{17}O_{CaCO3,VSMOW} = \delta'^{17}O_{CaCO3,VSMOW} - \lambda \times \delta'^{18}O_{CaCO3,VSMOW}$$

Value

Returns a data frame:

1. d18O value of the carbonate expressed on the VSMOW scale (‰).
2. d18O value of the carbonate expressed on the VSMOW scale (‰).
3. 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. doi: 10.1016/j.gca.2018.11.018

See Also

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

Examples

```
d17O_c(temp = 10, d18O_H2O_VSMOW = -1) # Returns the data frame (length = 3)
prime(d17O_c(temp = 10, d18O_H2O_VSMOW = -1)[, 2]) # Returns the d'17O value
d17O_c(temp = 10, d18O_H2O_VSMOW = -1)[, 3] # Returns the D17O value
```

---

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`	Carbonate growth temperature (°C).
`d18O_H2O_VSMOW`	Water d18O value expressed on the VSMOW scale (‰).
`min`	Mineralogy. Options are as in `a18_c_H2O()`.
`eq`	Equation used for the calculations. Options depend on mineralogy and are 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")
to_VPDB(d18O_c(temp = 12, d18O_H2O_VSMOW = -6.94,
               min = "aragonite", eq = "GK86"))
```

d18O_H2O *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, eq)
```

Arguments

`temp`	Carbonate growth temperature (°C).
`d18O_c_VSMOW`	Carbonate d18O value expressed on the VSMOW scale (‰).
`min`	Mineralogy. Options are `"calcite"`, `"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(temp = 33.7, d18O_c_VSMOW = 14.58,
         min = "calcite", eq = "Coplen07")
d18O_H2O(temp = 25, d18O_c_VSMOW = to_VSMOW(-7.47),
         min = "aragonite", eq = "GK86")
```

D47 *Equilibrium carbonate D47 value*

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.

- `"Petersen19"`: the synthetic-only composite IUPAC-parameter calibration of Petersen et al. (2019).
- `"Anderson21"`: the I-CDES90 calibration of Anderson et al. (2021).
- `"Fiebig21"`: the CDES90 calibration of Fiebig et al. (2021).

Details

"Petersen19":

$$\Delta_{47,CDES90} = 0.0383 \times \frac{10^6}{T^2} + 0.170$$

"Anderson21":

$$\Delta_{47,I-CDES90} = 0.0391 \times \frac{10^6}{T^2} + 0.154$$

"Fiebig21":

$$\Delta_{47,CDES90} = 1.038 \times (-5.897 \times \frac{1}{T} - 3.521 \times \frac{10^3}{T^2} + 2.391 \times \frac{10^7}{T^3} - 3.541 \times \frac{10^9}{T^4}) + 0.1856$$

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. doi: 10.1029/2018GC008127

Anderson, N. T., Kelson, J. R., Kele, S., Daëron, M., Bonifacie, M., Horita, J., et al. (2021). A unified clumped isotope thermometer calibration (0.5–1100°C) using carbonate-based standardization. Geophysical Research Letters, 48(7), e2020GL092069. doi: 10.1029/2020gl092069

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. doi: 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(temp = 33.7, eq = "Petersen19") # Returns 0.577
D47(temp = 33.7, eq = "Fiebig21") # Returns 0.571
```

D48 — *Equilibrium carbonate D47 value*

Description

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

Usage

```
D48(temp, eq)
```

Arguments

`temp`	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).

Details

"Fiebig21":

$$\Delta_{48,CDES90} = 1.028 \times (6.002 \times \frac{1}{T} - 1.299 \times \frac{10^4}{T^2} + 8.996 \times \frac{10^6}{T^3} - 7.423 \times \frac{10^8}{T^4}) + 0.1245$$

"Swart21":

$$\Delta_{48,CDES90} = 0.0142 \times \frac{10^6}{T^2} + 0.088$$

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. doi: 10.1038/s41467020175010

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. doi: 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. doi: 10.1002/rcm.9147

See Also

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

Examples

```
D48(temp = 33.7, eq = "Fiebig21") # Returns 0.237
D48(temp = 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 expressed on the VSMOW scale (‰).

d18O_error Standard deviation on the d18O value.

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

Source

doi: 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. doi: 10.1016/j.yqres.2006.06.003

See Also

Other "datasets": GTS2020, LR04

`epsilon` *Isotope fractionation value*

Description

`epsilon()` converts isotope fractionation factors to isotope fractionation values.

Usage

```
epsilon(alpha)
```

Arguments

alpha	Isotope fractionation factor

Details

$$\epsilon^{i}E_{A/B} = \alpha^{i}E_{A/B} - 1$$

Value

Returns the isotope fractionation value (‰).

See Also

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

Examples

```
epsilon(a18_H2O_OH(25, "Z20-X3LYP"))
```

`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 expressed on the VPDB scale (‰).

d13C_VPDB Carbonate d13C value expressed on the VPDB scale (‰).

mineralogy The mineralogy of the carbonate hard part.

group Taxonomic group of the sample (bivalve, gastropod, belemnite, ammonite).

clim_zone The climate zone the sample 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. doi: 10.1016/B9780128243602.000103

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 expressed on the VPDB scale (‰).

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. doi: 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:

1. d18O value of the mixture at x% mixing (‰).
2. d18O value of the mixture x% mixing (‰).
3. 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

```
mix_d17O(d18O_A = d17O_c(10, -1)[1], d17O_A = d17O_c(10, -1)[2],
         d18O_B = d17O_c(100,0)[1], d17O_B = 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, min, eq)
```

Arguments

`d18O_c_VSMOW`	Carbonate d18O value expressed on the VSMOW scale (‰).
`d18O_H2O_VSMOW`	Water d18O value expressed on the VSMOW scale (‰).
`min`	Mineralogy. Options are as in `a18_c_H2O()`.
`eq`	Equation used for the calculations. 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(d18O_c_VSMOW = 14.58, d18O_H2O_VSMOW = -13.54,
          min = "calcite", eq = "Coplen07")
```

`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. Options are as in `D47()`.

Details

The D47 vs temperature equations are listed at `D47()`.

Value

Returns the carbonate growth temperature (°C). If `D47_error` is specified `temp_D47()` returns a data frame.

References

References are listed at `D47()`.

See Also

`D47()` calculates the equilibrium carbonate D47 value.

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

Examples

```
temp_D47(D47_CDES90 = 0.577, eq = "Petersen19")
```

`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 = "black",
  pch = 19
)
```

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 `temp_D47()` function and the equilibrium D47_CDES90 vs temperature equation of Fiebig et al. (2021).

Value

Returns the carbonate growth temperature (°C). If both `D47_error` and `D48_error` are specified `temp_D48()` returns a data frame.

Contributors

The source code of this function contains elements from the reconPlots package, available at https://github.com/andrewheiss/reconPlots

References

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

See Also

`D47()` calculates the equilibrium carbonate D47 value. `D48()` calculates the equilibrium carbonate D48 value.

Other thermometry: `temp_D47()`, `temp_d18O()`

Examples

```
temp_D48(0.617, 0.139, ks = -0.6)
temp_D48(0.546, 0.277, ks = -1)
```

`to_VPDB` *Converting isotope delta from VSMOW to VPDB*

Description

`to_VPDB()` convert d18O value 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)
to_VPDB(0, eq = "Coplen83")
```

`to_VSMOW` *Converting isotope delta from VPDB to VSMOW*

Description

`to_VSMOW()` converts d18O value 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. doi: 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. doi: 10.1515/pac20131023

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. doi: 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)
to_VSMOW(0, eq = "Coplen83")
```

`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
```

`X_absorption` *Relative rates of CO2 absorption reactions*

Description

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

Usage

```
X_absorption(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 or ‰).

Details

X_hydration = ((kCO2 / (kCO2 + kOHxKw / aH)) * 100), where

- kCO2 is the rate constant for CO2 hydration from Johnson (1982)
- kOHxKw is the rate constant for CO2 hydroxylation x Kw from Schulz et al. (2006).
- aH is 10^(-pH)

Value

Returns a data frame with the relative rates of CO2 absorption reactions:

- Relative rate of CO2 hydration (%).
- Relative rate of CO2 hydroxylation (%).

References

Johnson, K. S. (1982). Carbon dioxide hydration and dehydration kinetics in seawater. Limnology and Oceanography, 27(5), 894-855. doi: 10.4319/lo.1982.27.5.0849

Schulz, K. G., Riebesell, U., Rost, B., Thoms, S., & Zeebe, R. E. (2006). Determination of the rate constants for the carbon dioxide to bicarbonate inter-conversion in pH-buffered seawater systems. Marine Chemistry, 100(1-2), 53-65. doi: 10.1016/j.marchem.2005.11.001

Examples

```
X_absorption(temp = 25, pH = 7, S = 30)
```

`X_DIC` *Dissolved inorganic carbon species*

Description

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

Usage

```
X_DIC(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 or ‰).

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 (%).

References

Harned, H. S., and Scholes, S. R. (1941). The ionization constant of HCO3- from 0 to 50°. J. Am. Chem. Soc., 63(6), 1706-1709. doi: 10.1021/ja01851a058

Harned, H. S., and Davis, R. (1943). The ionization constant of carbonic acid in water and the solubility of carbon dioxide in water and aqueous salt solutions from 0 to 50°. J. Am. Chem. Soc., 65(10), 2030-2037. doi: 10.1021/ja01250a059

Millero, F. J., Graham, T. B., Huang, F., Bustos-Serrano, H., et al. (2006). Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. Mar. Chem., 100(1-2), 80-94. doi: 10.1016/j.marchem.2005.12.001

Examples

```
X_DIC(temp = 25, pH = 7, S = 30)
```

york_fit *Error-considering linear regression*

Description

`york_fit()` calculates the regression parameters of an error-considering linear regression.

Usage

```
york_fit(x, y, x_err, y_err, r = 0)
```

Arguments

`x`	vector of x values.
`y`	vector of y values. Has to be same the length as x.
`x_err`	Error on the x values. Has to be same the length as x.
`y_err`	Error on the y values. Has to be same the length as x.
`r`	Correlation coefficient of x_err and y_err at each data point. Default: `0` (independent errors). Has to be same the length as x. Optional.

Details

Regression fitting method according to York et al. (2004). The algorithm is described in the appendix of Wacker et al. (2014).

Value

A list with regression parameters:

- slope and its standard error
- intercept and its standard error
- weights of the points (normalized to 1)
- residual standard error (sigma)
- R2
- p-value (two-tailed t-test).

Contributors

Julian Tödter

References

York, D., Evensen, N. M., López Martínez, M., & De Basabe Delgado, J. (2004). Unified equations for the slope, intercept, and standard errors of the best straight line. American Journal of Physics, 72(3), 367-375. doi: 10.1119/1.1632486

Wacker, U., Fiebig, J., Tödter, J., Schöne, B. R., Bahr, A., Friedrich, O., et al. (2014). Empirical calibration of the clumped isotope paleothermometer using calcites of various origins. Geochimica et Cosmochimica Acta, 141, 127-144. doi: 10.1016/j.gca.2014.06.004

Examples

```
york_fit(
  x = c(1, 2, 3),
  y = c(1.1, 1.9, 3.2),
  x_err = c(0.1, 0.2, 0.1),
  y_err = c(0.2, 0.1, 0.2))
```

---

york_plot *Regression confidence intervals*

Description

york_plot() calculates and optionally plots the confidence intervals of an (error-considering) linear regression.

Usage

```
york_plot(
  x,
  slope,
  slope_se,
  intercept,
  intercept_se,
  cl = 0.95,
  weights = -1,
  add = FALSE,
  col = "black"
)
```

Arguments

x	x values of the data points.
slope	regression slope.
slope_se	Standard error of the slope.
intercept	regression intercept.
intercept_se	Standard error of the intercept.
cl	Confidence level. Default: 0.95.
weights	Weights of the data points. If given, mean & SD of x are computed with the weights. Has to be same the length as x. Optional.
add	Add graphics to an already existing plot? Default: FALSE.
col	Graphical parameter. Optional.

Details

The algorithm is described in the appendix of Wacker et al. (2014).

Value

A list with regression parameters:

- slope and its standard error
- intercept and its standard error
- weights of the points (normalized to 1)
- residual standard error (sigma)
- R2
- p-value (two-tailed t-test).

Contributors

Julian Tödter

References

Wacker, U., Fiebig, J., Tödter, J., Schöne, B. R., Bahr, A., Friedrich, O., et al. (2014). Empirical calibration of the clumped isotope paleothermometer using calcites of various origins. Geochimica et Cosmochimica Acta, 141, 127-144. doi: 10.1016/j.gca.2014.06.004

Examples

```
york_plot(
  x = c(1, 2, 3),
  slope = 1.06,
  slope_se = 1.60,
  intercept = -0.05,
  intercept_se = 0.34,
  cl = 0.98)
```

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