

Package ‘isogeochem’

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Type Package

Title Tools for Stable Isotope Geochemistry

Version 1.1.0

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

License GPL (>= 3)

URL <https://davidbajnai.github.io/isogeochem/>

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

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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

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

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	<i>18O/16O acid fractionation factor</i>
---------------	--

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", "aragonite", and "dolomite".

Details

calcite (Kim et al. 2015):

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

aragonite (Kim et al. 2007):

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

dolomite (Rosenbaum & Sheppard 1986):

$$\alpha_{CO2acid/dolomite}^{18} = e^{(665 \times \frac{1}{T^2} + 0.00423)}$$

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

Rosenbaum, J. and Sheppard, S.M.F. (1986). An isotopic study of siderites, dolomites and ankerites at high temperatures. *Geochimica et Cosmochimica Acta*, 50, 1147-1150. doi:10.1016/0016-7037(86)903960

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

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

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

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

Value

Returns the 18O/16O fractionation factor.

References

Brennkmeijer, 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_HC03_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

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

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 1000lnα 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):

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

"K097-orig": Kim and O'Neil (1997):

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

NOTE: The "K097-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.

"K097": Kim and O'Neil (1997), reprocessed here to match the IUPAC-recommended AFF as in Kim et al. (2007, 2015):

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

"Coplen07": Coplen (2007):

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

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

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

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

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

"Daeron19": Daëron et al. (2019):

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

Options for eq if min = "aragonite":

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

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

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

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

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

"Lécuyer10": Lécuyer et al. (2010):

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

Options for eq if min = "siderite":

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

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

Options for eq if min = "dolomite":

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

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

"Muller19": Müller et al. (2019):

$$\alpha_{\text{dolomite}/\text{water}}^{18} = e^{(2.9923 \times \frac{1000}{T^2} + 0.0023592)}$$

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
- Müller, I.A., Rodriguez-Blanco, J.D., Storck, J.-C., do Nascimento, G.S., Bontognali, T.R.R., Vasconcelos, C., Benning, L.G. & Bernasconi, S.M. (2019). Calibration of the oxygen and clumped isotope thermometers for (proto-)dolomite based on synthetic and natural carbonates. *Chemical Geology*, 525, 1-17. doi:10.1016/j.chemgeo.2019.07.014

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", eq = "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. <ul style="list-style-type: none"> 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

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

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 1000ln α 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_C02g_C02aq(), a18_C02acid_c(), a18_C02aq_H2O(), a18_C02g_H2O(), a18_C03_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_C02g_C02aq\(\)](#), [a18_C02acid_c\(\)](#), [a18_C02aq_H2O\(\)](#), [a18_C02g_H2O\(\)](#), [a18_C03_H2O\(\)](#), [a18_H2O_OH\(\)](#), [a18_HC03_H2O\(\)](#), [a18_c_H2O\(\)](#)

Examples

a_A_B(A = 10, B = 12)

A_from_a	<i>Isotope delta from fractionation factor</i>
----------	--

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	<i>Isotope delta from fractionation factor</i>
----------	--

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(d180, d170, lambda = 0.528)

Arguments

d180	Isotope delta value (‰).
d170	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(d180 = -10, d170 = -5, lambda = 0.528)

d17O_c *Triple oxygen isotope values of carbonates*

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,
  D17O_H2O = 0,
  min = "calcite",
  eq18 = "Daeron19",
  lambda = 0.528
)
```

Arguments

temp	Calcite growth temperature (°C).
d18O_H2O_VSMOW	Water d18O value expressed on the VSMOW scale (‰).
D17O_H2O	D17O value of ambient water calculated using a lambda of 0.528. Default 0.
min	Mineralogy. Options are "calcite" (default), "aragonite", apatite, siderite, and "dolomite".
eq18	Equation used to calculate the 18O/16O fractionation factor between calcite and water. Options are like in a18_c_H2O() . Default "Daeron19".
lambda	Triple oxygen isotope reference slope. Default 0.528.

Details

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

$$\delta^{17}O_{H_2O,VSMOW} = \beta \times \delta^{18}O_{H_2O,VSMOW} + \gamma, \text{ where } \beta = 0.528 \text{ and } \gamma = 0$$

$$\Delta^{17}O_{CaCO_3,VSMOW} = \delta^{17}O_{CaCO_3,VSMOW} - \lambda \times \delta^{18}O_{CaCO_3,VSMOW}$$

NOTE: Due to a lack of experimental and theoretical data, the theta values for all carbonate mineralogies - except aragonite - are calculated with the calcite equation from Guo & Zhou (2019):

$$\theta_{aragonite/water} = \frac{78.1173}{T^2} - \frac{1.5152}{T} + 0.5299$$

$$\theta_{calcite/water} = \frac{59.1047}{T^2} - \frac{1.4089}{T} + 0.5297$$

Value

Returns a data frame:

1. d18O value of the carbonate expressed on the VSMOW scale (‰).
2. d17O 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](https://doi.org/10.1016/j.gca.2018.11.018)

See Also

Other equilibrium_carbonate: [D47\(\)](#), [D48\(\)](#), [d180_c\(\)](#)

Examples

```
d170_c(temp = 10, d180_H2O_VSMOW = -1) # Returns the data frame (length = 3)
prime(d170_c(temp = 10, d180_H2O_VSMOW = -1)[, 2]) # Returns the d'17O value
d170_c(temp = 10, d180_H2O_VSMOW = -1)[, 3] # Returns the D17O value
```

d170_qz

Triple oxygen isotope values of quartz

Description

d170_qz() calculates the equilibrium d18O, d17O, and D17O values of quartz grown at a given temperature.

Usage

```
d170_qz(temp, d180_H2O_VSMOW, D170_H2O = 0, lambda = 0.528)
```

Arguments

temp	Quartz growth temperature (°C).
d180_H2O_VSMOW	Water d18O value expressed on the VSMOW scale (‰).
D170_H2O	D17O value of ambient water calculated using a lambda of 0.528. Default 0.
lambda	Triple oxygen isotope reference slope. Default 0.528.

Details

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

$$\delta^{17}O_{H_2O,VSMOW} = \beta \times \delta^{18}O_{H_2O,VSMOW} + \gamma, \text{ where } \beta = 0.528 \text{ and } \gamma = 0$$

$$\Delta^{17}O_{SiO_2,VSMOW} = \delta^{17}O_{SiO_2,VSMOW} - \lambda \times \delta^{18}O_{SiO_2,VSMOW}$$

NOTE:

$$\theta_{quartz/water} = -\frac{1.85}{T} + 0.5305$$

$$\alpha_{quartz/water}^{18} = e^{\left(\frac{4280}{T^2} - \frac{3.5}{T}\right)}$$

Value

Returns a data frame:

1. d18O value of the quartz expressed on the VSMOW scale (%■).
2. d17O value of the quartz expressed on the VSMOW scale (%■).
3. D17O value of the quartz expressed on the VSMOW scale (%■).

References

Sharp, Z.D., Gibbons, J.A., Maltsev, O., Atudorei, V., Pack, A., Sengupta, S., Shock, E.L. and Knauth, L.P. (2016). A calibration of the triple oxygen isotope fractionation in the SiO₂-H₂O system and applications to natural samples. *Geochimica et Cosmochimica Acta*, 186, 105-119. [doi:10.1016/j.gca.2016.04.047](https://doi.org/10.1016/j.gca.2016.04.047)

Examples

```
d17O_qz(temp = 10, d18O_H2O_VSMOW = 0) # Returns the data frame (length = 3)
d17O_qz(temp = 10, d18O_H2O_VSMOW = 0)[, 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\(\)](#), [d170_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	<i>Water d18O value</i>
----------	-------------------------

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. <ul style="list-style-type: none"> "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":

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

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()`, `d170_c()`, `d180_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

- | | |
|-------------------|---|
| <code>temp</code> | Carbonate growth temperature (°C). |
| <code>eq</code> | Equation used for the calculation. <ul style="list-style-type: none"> "Fiebig21": the CDES90 calibration of Fiebig et al. (2021). "Swart21": the CDES90 "PBLM1" calibration in Swart et al. (2021). |

Details**"Fiebig21":**

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

"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()`, `d170_c()`, `d180_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).

d180_VSMOW Carbonate d18O value expressed on the VSMOW scale (‰).

d180_error Standard deviation on the d18O value.

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

Source

[doi:10.3133/ofr20111082](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. [doi:10.1016/j.yqres.2006.06.003](https://doi.org/10.1016/j.yqres.2006.06.003)

See Also

Other "datasets": [GTS2020](#), [LR04](#), [meteoric_water](#)

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](#), [meteoric_water](#)

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).

d180_VPDB Carbonate d18O value expressed on the VPDB scale (‰).

d180_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](#), [meteoric_water](#)

meteoric_water

Oxygen isotope values for meteoric waters

Description

A dataset containing a compilation of d17O and d17O values of various meteoric waters.

Usage

meteoric_water

Format

A data frame with 156 rows and 4 variables:

Sample Sample ID as in the original publication.

d17O Water d17O value expressed on the VSMOW scale (‰).

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

Reference Abbreviated reference for the data point.

References

Luz, B., & Barkan, E. (2010). Variations of $^{17}\text{O}/^{16}\text{O}$ and $^{18}\text{O}/^{16}\text{O}$ in meteoric waters. *Geochimica et Cosmochimica Acta*, 74(22), 6276–6286. doi:10.1016/j.gca.2010.08.016

Aron, P. G., Levin, N. E., Beverly, E. J., Huth, T. E., Passey, B. H., Pelletier, E. M., Poulsen, C. J., Winkelstern, I. Z., & Yarian, D. A. (2021). Triple oxygen isotopes in the water cycle. *Chemical Geology*, 565, 116770. doi:10.1016/j.chemgeo.2020.120026

See Also

Other "datasets": [GTS2020](#), [LR04](#), [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(  
  d180_A,  
  d170_A,  
  D170_A,  
  d180_B,  
  d170_B,  
  D170_B,  
  lambda = 0.528,  
  step = 10  
)
```

Arguments

d180_A	d18O value of component A (%■).
d170_A	d17O value of component A (%■).
D170_A	Alternatively, the D17O value of component A (%■).
d180_B	d18O value of component B (%■).
d170_B	d17O value of component B (%■).
D170_B	Alternatively, the D17O value of component B (%■).
lambda	Triple oxygen isotope reference slope. Default 0.528.
step	Output resolution, i.e., step size. Default 10%.

Details

If both d17O and D17O values are specified for a component, the function uses the d17O values for the calculations.

Value

Returns a data frame:

1. d18O value of the mixture at x% mixing (%■).
2. D17O value of the mixture at x% mixing (%■).
3. relative amount of component B in the mixture (%): from 100% A and 0% B to 0% A and 100% B.
4. d17O value of the mixture at x% mixing (%■).

See Also

[d170_c\(\)](#) calculates equilibrium calcite d18O, d17O, and D17O values for a given temperature.

Examples

```
# The two functions below yield the same output.
mix_d170(d180_A = d170_c(10, -1)[1], d170_A = d170_c(10, -1)[2],
         d180_B = d170_c(100,0)[1], d170_B = d170_c(100, 0)[2])
mix_d170(d180_A = d170_c(10, -1)[1], D170_A = d170_c(10, -1)[3],
         d180_B = d170_c(100,0)[1], D170_B = d170_c(100, 0)[3])
```

prime	<i>Converting delta to delta prime</i>
-------	--

Description

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

Usage

```
prime(classical)
```

Arguments

classical "Classical delta" values to be converted (%■).

Details

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

Value

Returns the "delta prime" value (%■).

See Also

[unprime\(\)](#) converts "delta prime" values to "classical delta" values.

Examples

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

temp_d180	<i>Oxygen isotope thermometry</i>
-----------	-----------------------------------

Description

temp_d180() calculates carbonate growth temperature from oxygen isotope data.

Usage

```
temp_d180(d180_c_VSMOW, d180_H2O_VSMOW, min, eq)
```

Arguments

d180_c_VSMOW	Carbonate d18O value expressed on the VSMOW scale (‰).
d180_H2O_VSMOW	Water d18O value expressed on the VSMOW scale (‰).
min	Mineralogy. Options are as in a18_c_H20() .
eq	Equation used for the calculations. Options depend on mineralogy and listed in a18_c_H20() .

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_H20\(\)](#).

See Also

[d180_c\(\)](#) calculates the equilibrium d18O value of a carbonate grown at a given temperature.

[d180_H20\(\)](#) 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_d180(d180_c_VSMOW = 14.58, d180_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_d180\(\)](#)

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_d180\(\)](#)

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(d180_VSMOW, eq = "IUPAC")
```

Arguments

d180_VSMOW	d18O values expressed on the VSMOW scale (%■).
eq	Equation used for the conversion. <ul style="list-style-type: none"> • "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. <ul style="list-style-type: none"> • "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	<i>Converting delta prime to delta</i>
---------	--

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	<i>Relative rates of CO2 absorption reactions</i>
--------------	---

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

$X_{\text{hydration}} = ((k_{\text{CO2}} / (k_{\text{CO2}} + k_{\text{OHxKw}} / a_{\text{H}})) * 100)$, where

- k_{CO2} is the rate constant for CO2 hydration from Johnson (1982)
- k_{OHxKw} is the rate constant for CO2 hydroxylation x K_{w} from Schulz et al. (2006).
- a_{H} is $10^{(-\text{pH})}$

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

<code>temp</code>	The temperature of the solution (°C).
<code>pH</code>	The pH of the solution.
<code>S</code>	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

<code>x</code>	vector of x values.
<code>y</code>	vector of y values. Has to be same the length as x.
<code>x_err</code>	Error on the x values. Has to be same the length as x.
<code>y_err</code>	Error on the y values. Has to be same the length as x.
<code>r</code>	Correlation coefficient of <code>x_err</code> and <code>y_err</code> 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.

c1	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](https://doi.org/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,  
  c1 = 0.98)
```

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