

# Package ‘isogeochem’

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**Type** Package

**Title** Tools for Stable Isotope Geochemistry

**Version** 1.1.1

**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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**Author** David Bajnai [aut, cre] (ORCID: <https://orcid.org/0000-0002-4053-5056>), Julian Tödter [ctb]

**Maintainer** David Bajnai <david.bajnai@uni-goettingen.de>

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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>
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---

**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	<i>18O/16O fractionation factor between CO2(aq) and H2O(l)</i>
---------------	--

---

**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**

$$\alpha_{CO_2(g)/H_2O(l)}^{18} = (17.604 \times \frac{1}{T} - 0.01793) + 1$$

**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**

$$\alpha_{CO_3(2-)/H_2O}^{18} = e^{2.39 \times \frac{1000}{T^2} - 0.00270}$$

The equation above and in the function is the uncorrected equation in Beck et al. (2005). They experimentally determined the fractionation factor using BaCO<sub>3</sub> precipitation experiments. However, they applied the acid fractionation factor of calcite during the data processing and not that of BaCO<sub>3</sub>. The acid fractionation factor of BaCO<sub>3</sub> 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\(\)](#)

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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":

"O'Neil69": 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 CO<sub>2</sub>(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):

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

"Coplen07": Coplen (2007):

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

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

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

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

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

"Daeron19": Daëron et al. (2019):

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

Options for eq if min = "aragonite":

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

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

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

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

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

"Lécuyer10": Lécuyer et al. (2010):

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

Options for eq if min = "siderite":

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

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

Options for eq if min = "dolomite":

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

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

"Muller19": Müller et al. (2019):

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

## 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
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- 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., Storek, 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"> <li>Z20-X3LYP: the theoretical X3LYP/6-311+G(d,p) equation of Zeebe (2020).</li> <li>Z20-MP2: the theoretical MP2/aug-cc-pVDZ equation of Zeebe (2020).</li> </ul>

### 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 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\\_C02g\\_C02aq\(\)](#), [a18\\_C02acid\\_c\(\)](#), [a18\\_C02aq\\_H20\(\)](#), [a18\\_C02g\\_H20\(\)](#), [a18\\_C03\\_H20\(\)](#), [a18\\_H20\\_OH\(\)](#), [a18\\_c\\_H20\(\)](#), [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\\_H20\(\)](#), [a18\\_C02g\\_H20\(\)](#), [a18\\_C03\\_H20\(\)](#), [a18\\_H20\\_OH\(\)](#), [a18\\_HC03\\_H20\(\)](#), [a18\\_c\\_H20\(\)](#)

**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",
  eq17 = "Wostbrock20",
  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) and "aragonite".
eq17	Equation used to calculate the 17O/16O fractionation factor between carbonate and water. Options are "Wostbrock20" (default) and "GZ19".
eq18	Equation used to calculate the 18O/16O fractionation factor between carbonate and water. Options are like in <a href="#">a18_c_H2O()</a> . Default "Daeron19".
lambda	Triple oxygen isotope reference slope. Default 0.528.

### Details

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

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

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

"Wostbrock20": Wostbrock et al. (2020):

$$\theta_{\text{aragonite/water}} = \frac{-1.53}{T} + 0.5305$$

$$\theta_{\text{calcite/water}} = \frac{-1.39}{T} + 0.5305$$

"GZ19": Guo and Zhou (2019):

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

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

## 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

Wostbrock, J.A.G., Brand, U., Coplen, T.B., Swart, P.K., Carlson, S.J., Brearley, A.J., and Sharp, Z.D. (2020). Calibration of carbonate-water triple oxygen isotope fractionation: Seeing through diagenesis in ancient carbonates. *Geochimica et Cosmochimica Acta*, 288, 369-388. doi:10.1016/j.gca.2020.07.045

Guo, W., and Zhou, C. (2019). Triple oxygen isotope fractionation in the DIC-H<sub>2</sub>O-CO<sub>2</sub> 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\(\)](#), [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
```

---

d17O\_qz *Triple oxygen isotope values of quartz*

---

### Description

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

### Usage

d17O\_qz(temp, d18O\_H2O\_VSMOW, D17O\_H2O = 0, lambda = 0.528)

### Arguments

temp	Quartz 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.
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 SiO<sub>2</sub>-H<sub>2</sub>O system and applications to natural samples. *Geochimica et Cosmochimica Acta*, 186, 105-119. doi:10.1016/j.gca.2016.04.047

## Examples

```
d170_qz(temp = 10, d180_H2O_VSMOW = 0) # Returns the data frame (length = 3)
d170_qz(temp = 10, d180_H2O_VSMOW = 0)[, 3] # Returns the D170 value
```

---

d180_c	<i>Equilibrium carbonate d18O value</i>
--------	---

---

## Description

d180\_c() calculates the equilibrium d18O value of a carbonate grown at a given temperature.

## Usage

```
d180_c(temp, d180_H2O_VSMOW, min, eq)
```

## Arguments

temp	Carbonate growth temperature (°C).
d180_H2O_VSMOW	Water d18O value expressed on the VSMOW scale (‰).
min	Mineralogy. Options are as in <a href="#">a18_c_H2O()</a> .
eq	Equation used for the calculations. Options depend on mineralogy and are listed in <a href="#">a18_c_H2O()</a> .

## 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

[d180\\_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**

```
d180_c(33.7, -13.54, min = "calcite", eq = "Coplen07")
to_VPDB(d180_c(temp = 12, d180_H2O_VSMOW = -6.94,
              min = "aragonite", eq = "GK86"))
```

---

d180_H2O	<i>Water d18O value</i>
----------	-------------------------

---

**Description**

d180\_H2O() calculates the d18O value of the ambient water from the d18O value of a carbonate and its growth temperature.

**Usage**

```
d180_H2O(temp, d180_c_VSMOW, min, eq)
```

**Arguments**

temp	Carbonate growth temperature (°C).
d180_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 <a href="#">a18_c_H2O()</a> .

**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**

[d180\\_c\(\)](#) calculates the equilibrium d18O value of a carbonate grown at a given temperature.  
[temp\\_d180\(\)](#) calculates growth temperatures from oxygen isotope data.

**Examples**

```
d180_H2O(temp = 33.7, d180_c_VSMOW = 14.58,
          min = "calcite", eq = "Coplen07")
d180_H2O(temp = 25, d180_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"> <li>"Petersen19": the synthetic-only composite IUPAC-parameter calibration of Petersen et al. (2019).</li> <li>"Anderson21": the I-CDES90 calibration of Anderson et al. (2021).</li> <li>"Fiebig21": the CDES90 calibration of Fiebig et al. (2021).</li> </ul>

**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"> <li>"Fiebig21": the CDES90 calibration of Fiebig et al. (2021).</li> <li>"Swart21": the CDES90 "PBLM1" calibration in Swart et al. (2021).</li> </ul> |

**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](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 *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**

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

**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 *Oxygen isotope thermometry*

---

**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 <a href="#">a18_c_H20()</a> .
eq	Equation used for the calculations. Options depend on mineralogy and listed in <a href="#">a18_c_H20()</a> .

**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 <a href="#">D47()</a> .

**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 (%o).
D48_CDES90	Carbonate D48 values expressed on the CDES90 scale (%o).
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(d18O_VSMOW, eq = "IUPAC")
```

**Arguments**

d18O_VSMOW	d18O values expressed on the VSMOW scale (‰).
eq	Equation used for the conversion. <ul style="list-style-type: none"> <li>• "IUPAC" (default): the IUPAC recommended equation listed in Brand et al. (2014) and Kim et al. (2015).</li> <li>• "Coplen83": the equation listed in Coplen et al. (1983) and the Hoefs book.</li> </ul>

**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(d180_VPDB, eq = "IUPAC")
```

**Arguments**

d180_VPDB	d18O values expressed on the VPDB scale (‰).
eq	Equation used for the conversion. <ul style="list-style-type: none"> <li>• "IUPAC" (default): the IUPAC recommended equation listed in Brand et al. (2014) and Kim et al. (2015).</li> <li>• "Coplen83": the equation listed in Coplen et al. (1983) and the Hoefs book.</li> </ul>

**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 (%o).

**Details**

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

**Value**

Returns the "classical delta" value (%o).

**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

$X_{\text{hydration}} = ((k_{\text{CO}_2} / (k_{\text{CO}_2} + k_{\text{OH}} \times K_w / a_{\text{H}})) * 100)$ , where

- $k_{\text{CO}_2}$  is the rate constant for CO<sub>2</sub> hydration from Johnson (1982)
- $k_{\text{OH}} \times K_w$  is the rate constant for CO<sub>2</sub> hydroxylation x  $K_w$  from Schulz et al. (2006).
- $a_{\text{H}}$  is  $10^{(-\text{pH})}$

### Value

Returns a data frame with the relative rates of CO<sub>2</sub> absorption reactions:

- Relative rate of CO<sub>2</sub> hydration (%).
- Relative rate of CO<sub>2</sub> 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 CO<sub>2</sub> (%).
- Relative abundance of bicarbonate ion (%).
- Relative abundance of carbonate ion (%).

### References

Harned, H. S., and Scholes, S. R. (1941). The ionization constant of HCO<sub>3</sub><sup>-</sup> 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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