Package 'seacarb'

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Description Calculates parameters of the seawater carbonate system and assists the design of ocean acidification perturbation experiments.

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R topics documented:

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alkalinity	*Example data file for function at*

Description

The variables are:

- volume: Volume of acid added to the sample in ml
- E: Potential measured during the titration in mV
- temperature: Temperature in degrees Celsius
- weight: Weight of the sample in g
- S: Salinity
- normality : Normality of the acid
- ETris: Potential used for the calibration of the electrode in mV
- pHTris: pH used for the calibration of the electrode with the TRIS buffer

Usage

```
alkalinity
```

Format

A data frame with 29 rows and 8 variables

Source

Data come from a potentiometric titration performed by Steeve Comeau.

---

amp	*pH value of the AMP buffer*

Description

pH value of the AMP buffer (on the total scale in mol/kg)

Usage

```
amp(S=35,T=25)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC

Details

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

AMP   pH value of the AMP buffer (on the total scale in mol/kg)

Author(s)

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

See Also

tris, pHslope, pH.

Examples

```
##Example from Dickson et al. (2007)
amp(S=35,T=25)
```

---

at   *Calculates total alkalinity from potentiometric titration data*

Description

Calculates total alkalinity from potentiometric titration data

Usage

```
at(S=35, T=25, C=0.1, d=1, pHTris=NULL, ETris=NULL, weight, E, volume)
```

Arguments

S   Salinity, default is 35. S must be a single value, not a vector.

T   Temperature in degrees Celsius, default is 25oC, can be given as a vector or as a single value.

C   Normality of the acid, default is 0.1. C must be a single value, not a vector.

d   Density of the acid, default is 1. d must be a single value, not a vector.

pHTris   pH used for the calibration of the electrode with the TRIS buffer. pHTris must be a single value, not a vector.

ETris	Potential used for the calibration of the electrode in mV. ETris must be a single value, not a vector.
weight	Weight of the sample in g. weight must be a single value, not a vector.
E	Potential measured during the titration in mV. E must be a vector.
volume	Volume of acid added to the sample in ml. volume must be a vector.

Details

Total alkalinity is estimated using the non-linear least-square procedure described by Dickson et al. (2007).

Value

AT	Total alkalinity in mol/kg)

Author(s)

Steeve Comeau, Heloise Lavigne and Jean-Pierre Gattuso

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

See Also

alkalinity

Examples

```
data(alkalinity)
data <- alkalinity
AT <- at(S=data$S[1], T=data$temperature, C=data$normality[1], pHTris=data$pHTris[1],
     ETris=data$ETris[1], E=data$E, weight=data$weight[1], volume=data$volume)
```

---

bjerrum	*Bjerrum plot*

Description

Plot the concentration of the various ionic forms of a molecule as a function of pH

Usage

```
bjerrum(K1=K1(), K2=NULL, K3=NULL, phmin=2, phmax=12, by=0.1, conc=1,
     type="l", col="black",  ylab="Concentration (mol/kg)", add=FALSE, ...)
```

Arguments

K1	First dissociation constant
K2	Second dissociation constant, default is NULL
K3	Third dissociation constant, default is NULL
phmin	Minimum pH value, default is 2
phmax	Maximum pH value, default is 12
by	Increment on the pH axis, default is 0.1
conc	concentration of molecule, default is 1
type	Type of plot, default is line
col	Color of plot, default is black
ylab	Label of Y axis, default is (mol/kg)
add	false:start new, true: add to current, default is false
...	Graphical parameters (see [par](#)) and any further arguments of plot, typically [plot.default](#), may also be supplied as arguments to this function. Hence, the high-level graphics control arguments described under [par](#) and the arguments to [title](#) may be supplied to this function.

Details

Note that the concentration is plotted in mol/kg only if conc is given is mol/kg

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl>

References

Zeebe, R. E. and Wolf-Gladrow D. A., 2001 *CO2 in seawater: equilibrium, kinetics, isotopes*. Amsterdam: Elsevier, 346 pp.

See Also

[matplot](#), [par](#), [speciation](#).

Examples

```
## Plot the bjerrum plot for the carbonate system using the default values
bjerrum(K1(),K2(),main="DIC speciation",lwd=2)
abline(v=-log10(K1()),col="grey")
mtext(side=3,at=-log10(K1()),"pK1")
abline(v=-log10(K2()),col="grey")
mtext(side=3,at=-log10(K2()),"pK2")
legend("left",lty=1:3,lwd=2,legend=c(expression(CO[2]),expression(HCO[3]^"-"),
expression(CO[3]^"2-")))

## Plot the bjerrum plot for phosphate using the default values
bjerrum(K1p(),K2p(),K3p(),main="phosphate speciation",lwd=2)
```

```
legend("left",lty=1:4,lwd=2,legend=c(expression(H[3]~PO[4]),
expression(H[2]~PO[4]^"-"),
expression(HPO[4]^"2-"),expression(PO[4]^"3-")))

## Plot the bjerrum plot for the carbonate system using the values other
## than the default ones, showing the effect of temperature
bjerrum(K1(T=25,S=35),K2(T=25,S=35),conc=1.3,main="effect of temperature" )
bjerrum(K1(T=0,S=35),K2(T=0,S=35),conc=1.3,add=TRUE,col="red")
legend("left",lty=1,col=c("black","red"),legend=c("T=25 oC","T=0 oC"))
legend("right",lty=1:3,legend=c(expression(CO[2]),expression(HCO[3]^"-"),
expression(CO[3]^"2-")))

## Plot the bjerrum plot for the carbonate system using the values other
## than the default ones, showing the effect of salinity
bjerrum(K1(T=25,S=35),K2(T=25,S=35),conc=1.3,main="effect of salinity" )
bjerrum(K1(T=25,S=5),K2(T=25,S=5),conc=1.3,add=TRUE,col="blue")
legend("left",lty=1,col=c("black","blue"),legend=c("S=35","S=5"))
legend("right",lty=1:3,legend=c(expression(CO[2]),expression(HCO[3]^"-"),
expression(CO[3]^"2-")))

## Plot the bjerrum plot for the carbonate system using the values other
## than the default ones, showing the effect of pressure
bjerrum(K1(P=0),K2(P=0),conc=1.3,main="effect of pressure" )
bjerrum(K1(P=300),K2(P=300),conc=1.3,add=TRUE,col="green")
legend("left",lty=1,col=c("black","green"),legend=c("P=0","P=300"),title="atm")
legend("right",lty=1:3,legend=c(expression(CO[2]),expression(HCO[3]^"-"),
expression(CO[3]^"2-")))
```

---

bor	*Total boron concentration (mol/kg)*

Description

total boron concentration ($mol\ kg^{-1}$)

Usage

```
bor(S, b)
```

Arguments

S	Salinity, default is 35
b	"l10" for using the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "u74"

Value

bor	total boron concentration ($mol\ kg^{-1}$))

Author(s)

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

DOE 1994 *Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water*. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.

Lee K., Tae-Wook K., Byrne R.H., Millero F.J., Feely R.A. and Liu Y-M, 2010 The universal ratio of the boron to chlorinity for the North Pacific and North Atlantoc oceans. *Geochimica et Cosmochimica Acta* **74** 1801-1811.

Uppstrom L.R., 1974 The boron/chlorinity ratio of the deep-sea water from the Pacific Ocean. *Deep-Sea Research I* **21** 161-162.

Examples

```
bor(35, "l10")
```

---

buffer   *Buffer parameters of the seawater carbonate system*

Description

Returns buffer parameters of the seawater carbonate system.

Usage

```
buffer(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0, k1k2="x",
kf="x", ks="d", pHscale="T", b="u74")
```

Arguments

flag   select the couple of variables available. The flags which can be used are:

                flag = 1 pH and CO2 given

                flag = 2 CO2 and HCO3 given

                flag = 3 CO2 and CO3 given

                flag = 4 CO2 and ALK given

                flag = 5 CO2 and DIC given

                flag = 6 pH and HCO3 given

                flag = 7 pH and CO3 given

                flag = 8 pH and ALK given

                flag = 9 pH and DIC given

                flag = 10 HCO3 and CO3 given

                flag = 11 HCO3 and ALK given

                flag = 12 HCO3 and DIC given

	flag = 13 CO3 and ALK given
	flag = 14 CO3 and DIC given
	flag = 15 ALK and DIC given
	flag = 21 pCO2 and pH given
	flag = 22 pCO2 and HCO3 given
	flag = 23 pCO2 and CO3 given
	flag = 24 pCO2 and ALK given
	flag = 25 pCO2 and DIC given
var1	enter value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	enter value of the second variable in mol/kg, except for pH
S	Salinity
T	Temperature in degrees Celsius
Patm	Surface atmospheric pressure in atm
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg; set to 0 if NA
Sit	Concentration of total silicate in mol/kg; set to 0 if NA
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.

- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag"pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

PhiD   PhiD, chemical buffer factor (dpH/d[DIC]); input/output of dissolved CO2 (unit pH per mol/kg)

BetaD   BetaD, homogeneous or Revelle buffer factor (dln(pCO2)/dln[DIC]); input/output of dissolved CO2

PiD	PiD, chemical buffer factor (dpCO2/d[DIC]); input/output of dissolved CO_2 (μatm per mol/kg)
PhiB	PhiB, chemical buffer factor (dpH/d[DIC]); from input/output of bicarbonate (unit pH per mol/kg)
BetaB	BetaB, homogeneous buffer factor (dln(pCO2)/dln[DIC]); input/output of bicarbonate
PiB	PiB, chemical buffer factor (dpCO2/d[DIC]); input/output of dissolved CO_2 (μatm per mol/kg)
PhiC	PhiC, chemical buffer factor (dpH/d[DIC]); input/output of carbonate (unit pH per mol/kg)
BetaC	BetaC, homogeneous buffer factor (dln(pCO2)/dln[DIC]); input/output of carbonate
PiC	PiC, chemical buffer factor (dpCO2/d[DIC]); input/output of carbonate (μatm per mol/kg)
PhiH	PhiH, chemical buffer factor (dpH/d[ALK]); input/output of strong acid (unit pH per mol/kg)
PiH	PiH, chemical buffer factor (dpCO2/d[ALK]); input/output of strong acid (μatm per mol/kg)

Author(s)

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: AgCI(s) + 1/2H2(g) = Ag(s) + HCI(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Khoo H. K., Ramette R. W., Culberson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40oC: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **49**, 29-34.

Frankignoulle M., 1994 A complete set of buffer factors for acid/base CO2 system in seawater. *Journal of Marine Systems* **5**, 111-118.

Lee K., Tae-Wook K., Byrne R.H., Millero F.J., Feely R.A. and Liu Y-M, 2010 The universal ratio of the boron to chlorinity for the North Pacific and North Atlantoc oceans. *Geochimica et Cosmochimica Acta* **74** 1801-1811.

Lueker T. J., Dickson A. G. and Keeling C. D., 2000 Ocean pCO2 calculated from dissolved inorganic carbon, alkalinity, and equations for K1 and K2: validation based on laboratory measurements of CO2 in gas and seawater at equilibrium. *Marine Chemistry* **70** 105-119.

Millero F. J., 2010 Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H. and Pierrot D., 2006 Dissociation constants of carbonic acid in seawateras a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

Perez F. F. and Fraga F., 1987 Association constant of fluoride and hydrogen ions in seawater. *Marine Chemistry* **21**, 161-168.

Roy R. N., Roy L. N., Vogel K. M., Porter-Moore C., Pearson T., Good C. E., Millero F. J. and Campbell D. M., 1993. The dissociation constants of carbonic acid in seawater at salinities 5 to 45 and temperatures 0 to 45oC. *Marine Chemistry* **44**, 249-267.

Uppstrom L.R., 1974 The boron/chlorinity ratio of the deep-sea water from the Pacific Ocean. *Deep-Sea Research I* **21** 161-162.

Examples

```
## Computation with a couple of variables
buffer(flag=8, var1=8.2, var2=0.00234, S=35, T=25, Patm=1, P=0, Pt=0,
Sit=0, pHscale="T", kf="pf", k1k2="l", b="u74")

## Using vectors as arguments
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649802, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
Sit <- c(0, 0, 0)
kf <- c("pf", "pf", "pf")
k1k2 <- c("l", "l", "l")
pHscale <- c("T", "T", "T")
b <- c("l10", "l10", "l10")
buffer(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt,
Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale, b=b)


## Test for all flags

flag <- c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 21, 22, 23, 24, 25)

var1 <- c(8.200000, 7.477544e-06, 7.477544e-06, 7.477544e-06, 7.477544e-06, 8.2,
8.2, 8.2, 8.2, 0.001685024, 0.001685024, 0.001685024,  0.0002888382,
0.0002888382, 0.002391252, 264.2008, 264.2008, 264.2008, 264.2008, 264.2008)

var2 <- c(7.477544e-06, 0.001685024, 0.0002888382, 0.002391252, 0.001981340,
0.001685024, 0.0002888382, 0.002391252, 0.001981340, 0.0002888382, 0.002391252,
0.001981340,  0.002391252, 0.001981340, 0.001981340, 8.2, 0.001685024,
0.0002888382, 0.002391252, 0.001981340)

buffer(flag=flag, var1=var1, var2=var2)
```

---

buffesm	*Buffer capacities of the seawater carbonate system as defined by Egleston et al. (2010)*

Description

Returns the six buffer factors of the seawater carbonate system as defined by Egleston, Sabine and Morel (2010), denoted here as ESM. Also returns the classic Revelle factor (relative change in pCO2 over that for DIC). In ESM, there are errors in the equations in Table 1 for S, Ω_{DIC}, and Ω_{Alk}. These errors have been corrected here. The results of this routine have been validated: they produce results that are identical to those shown in ESM's Fig. 2. This routine was inspired and adapted from seacarb's "buffer" function. Its input arguments are indentical to those in the "buffer" and "carb" functions of seacarb.

Usage

```
buffesm(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0, k1k2="x",
kf="x", ks="d", pHscale="T", b="u74")
```

Arguments

flag	select the couple of variables available. The flags which can be used are:
	flag = 1 pH and CO2 given
	flag = 2 CO2 and HCO3 given
	flag = 3 CO2 and CO3 given
	flag = 4 CO2 and ALK given
	flag = 5 CO2 and DIC given
	flag = 6 pH and HCO3 given
	flag = 7 pH and CO3 given
	flag = 8 pH and ALK given
	flag = 9 pH and DIC given
	flag = 10 HCO3 and CO3 given
	flag = 11 HCO3 and ALK given
	flag = 12 HCO3 and DIC given
	flag = 13 CO3 and ALK given
	flag = 14 CO3 and DIC given
	flag = 15 ALK and DIC given
	flag = 21 pCO2 and pH given
	flag = 22 pCO2 and HCO3 given
	flag = 23 pCO2 and CO3 given
	flag = 24 pCO2 and ALK given
	flag = 25 pCO2 and DIC given
var1	enter value of the first variable in mol/kg, except for pH and for pCO2 in μatm

var2	enter value of the second variable in mol/kg, except for pH
S	Salinity
T	Temperature in degrees Celsius
Patm	Surface atmospheric pressure in atm, default 1 atm
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg; set to 0 if NA
Sit	Concentration of total silicate in mol/kg; set to 0 if NA
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag? "pHscale".

For K0:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

gammaDIC	γ_{DIC}, ocean's capacity to buffer changes in [CO2] due to accumulation of CO2 from the atmosphere $(\partial ln[CO_2]/\partial DIC)^{-1}$ (units = mol/kg; multiply by 1000 to get mmol/kg, i.e., the units presented in Egleston et al., 2010)
betaDIC	β_{DIC}, ocean's capacity to buffer changes in [H+] due to accumulation of CO2 from the atmosphere $(\partial ln[H^+]/\partial DIC)^{-1}$ (units = mol/kg)
omegaDIC	Ω_{DIC}, ocean's capacity to buffer changes in $[CO_3^{2-}]$ due to accumulation of CO2 from the atmosphere $(\partial ln[CO_3^{2-}]/\partial DIC)^{-1}$; same as $(\partial ln\Omega_A/\partial DIC)^{-1}$ and $(\partial ln\Omega_C/\partial DIC)^{-1}$ (units= mol/kg)
gammaALK	γ_{Alk}, ocean's capacity to buffer changes in [CO2] due to changes in alkalinity $(\partial ln[CO_2]/\partial ALK)^{-1}$ (units = mol/kg)
betaALK	β_{Alk}, ocean's capacity to buffer changes in [H+] due to changes in alkalinity $(\partial ln[H^+]/\partial ALK)^{-1}$ (units = mol/kg)
omegaALK	Ω_{Alk}, ocean's capacity to buffer changes in $[CO_3^{2-}]$ due to changes in alkalinity $(\partial ln[CO_3^{2-}]/\partial ALK)^{-1}$; same as $(\partial ln\Omega_A/\partial ALK)^{-1}$ and $(\partial ln\Omega_C/\partial ALK)^{-1}$ (units = mol/kg)
R	Revelle factor, relative change in $[CO_2]$ or pCO_2 over the relative change in DIC $(\partial ln[CO_2]/\partial lnDIC)^{-1}$ (unitless)

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Uppstrom L.R., 1974 The boron/chlorinity ratio of the deep-sea water from the Pacific Ocean. *Deep-Sea Research I* **21** 161-162.

Examples

```
## Computation with a couple of variables
buffesm(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Pt=0,
Sit=0, pHscale="T", kf="pf", k1k2="l", b="u74")

## Using vectors as arguments
```

```
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649802, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
Sit <- c(0, 0, 0)
kf <- c("pf", "pf", "pf")
k1k2 <- c("l", "l", "l")
pHscale <- c("T", "T", "T")
b <- c("l10", "l10", "l10")
buffesm(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt,
Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale, b=b)

## Test for all flags
flag <- c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 21, 22, 23, 24, 25)

var1 <- c(8.200000, 7.477544e-06, 7.477544e-06, 7.477544e-06, 7.477544e-06, 8.2,
8.2, 8.2, 8.2, 0.001685024, 0.001685024, 0.001685024,  0.0002888382,
0.0002888382, 0.002391252, 264.2008, 264.2008, 264.2008, 264.2008, 264.2008)
var2 <- c(7.477544e-06, 0.001685024, 0.0002888382, 0.002391252, 0.001981340,
0.001685024, 0.0002888382, 0.002391252, 0.001981340, 0.0002888382, 0.002391252,
0.001981340,  0.002391252, 0.001981340, 0.001981340, 8.2, 0.001685024,
0.0002888382, 0.002391252, 0.001981340)
buffesm(flag=flag, var1=var1, var2=var2)

## Compute 2 additional factors of interest (ratios of relative changes)
be <- buffesm(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt,
Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale, b=b)
#      Ratio of gammaDIC/betaDIC = d ln [H+] / d ln pCO2
       Hfac <- (be$gammaDIC/be$betaDIC)                          #H+ factor
#      Ratio of gammaDIC/omegaDIC = d ln [CO32-] / d ln pCO2
       Satfac <- (be$gammaDIC/be$omegaDIC)                      #Saturation factor
```

---

carb   *Parameters of the seawater carbonate system*

Description

Returns parameters of the seawater carbonate system.

Usage

```
carb(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0,
        k1k2="x", kf="x", ks="d", pHscale="T", b="u74", gas="potential")
```

Arguments

flag	select the couple of variables available. The flags which can be used are:

flag = 1 pH and CO2 given

flag = 2 CO2 and HCO3 given

flag = 3 CO2 and CO3 given

flag = 4 CO2 and ALK given

flag = 5 CO2 and DIC given

flag = 6 pH and HCO3 given

flag = 7 pH and CO3 given

flag = 8 pH and ALK given

flag = 9 pH and DIC given

flag = 10 HCO3 and CO3 given

flag = 11 HCO3 and ALK given

flag = 12 HCO3 and DIC given

flag = 13 CO3 and ALK given

flag = 14 CO3 and DIC given

flag = 15 ALK and DIC given

flag = 21 pCO2 and pH given

flag = 22 pCO2 and HCO3 given

flag = 23 pCO2 and CO3 given

flag = 24 pCO2 and ALK given

flag = 25 pCO2 and DIC given

var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
S	Salinity
T	Temperature in degrees Celsius
Patm	Surface atmospheric pressure in atm, default is 1 atm
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg; set to 0 if NA
Sit	Concentration of total silicate in mol/kg; set to 0 if NA
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"

pHscale	"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"
gas	used to indicate the convention for INPUT pCO2, i.e., when it is an input variable (flags 21 to 25): "insitu" indicates it is referenced to in situ pressure and in situ temperature; "potential" indicates it is referenced to 1 atm pressure and potential temperature; and "standard" indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when pCO2 is not an input variable (flags 1 to 15). The default is "potential".

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

S	Salinity
T	Temperature in degrees Celsius
Patm	Surface atmospheric pressure in atm
P	Hydrostatic pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	"standard" pCO2, CO2 partial pressure computed at in situ temperature and atmospheric pressure (μatm)
fCO2	"standard" fCO2, CO2 fugacity computed at in situ temperature and atmospheric pressure (μatm)
pCO2pot	"potential" pCO2, CO2 partial pressure computed at potential temperature and atmospheric pressure (μatm)
fCO2pot	"potential" fCO2, CO2 fugacity computed at potential temperature and atmospheric pressure (μatm)
pCO2insitu	"in situ" pCO2, CO2 partial pressure computed at in situ temperature and total pressure (atm + hydrostatic) (μatm)
fCO2insitu	"in situ" fCO2, CO2 fugacity computed at in situ temperature and total pressure (atm + hydrostatic) (μatm)
HCO3	HCO3 concentration (mol/kg)
CO3	CO3 concentration (mol/kg)
DIC	DIC concentration (mol/kg)
ALK	ALK, total alkalinity (mol/kg)
OmegaAragonite	Omega aragonite, aragonite saturation state
OmegaCalcite	Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

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Examples

```
## With a couple of variables
carb(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
pHscale="T", kf="pf", k1k2="l", ks="d", b="u74")

## Using vectors as arguments
flag <- c(8, 2, 8)
var1 <- c(8.2, 7.477544e-06, 8.2)
var2 <- c(0.002343955, 0.001649802, 2400e-6)
S <- c(35, 35, 30)
T <- c(25, 25, 30)
P <- c(0, 0, 0)
Pt <- c(0, 0, 0)
Sit <- c(0, 0, 0)
kf <- c("pf", "pf", "pf")
k1k2 <- c("l", "l", "l")
pHscale <- c("T", "T", "T")
b <- c("l10", "l10", "l10")
carb(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P,
  Pt=Pt, Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale, b=b)

## Test with all flags
flag <- c((1:15), (21:25))
var1 <- c(8.200000, 7.308171e-06, 7.308171e-06, 7.308171e-06, 7.308171e-06,
8.2, 8.2, 8.2, 8.2, 0.001646857, 0.001646857, 0.001646857, 0.0002822957,
0.0002822957, 0.00234, 258.2164, 258.2164, 258.2164, 258.2164, 258.2164 )
var2 <- c(7.308171e-06, 0.001646857, 0.0002822957, 0.00234, 0.001936461,
0.001646857, 0.0002822957, 0.00234, 0.001936461, 0.0002822957,
0.00234, 0.001936461,  0.00234, 0.001936461, 0.001936461, 8.2,
0.001646857, 0.0002822957, 0.00234, 0.001936461)
carb(flag=flag, var1=var1, var2=var2)

## Test using a data frame
data(seacarb_test_P0) #test data set for P=0 (surface)
tab <- seacarb_test_P0[14:19,]

## method 1 using the column numbers
carb(flag=tab[[1]], var1=tab[[2]], var2=tab[[3]], S=tab[[4]], T=tab[[5]],
P=tab[[6]], Sit=tab[[8]], Pt=tab[[7]])

## method 2 using the column names
carb(flag=tab$flag, var1=tab$var1, var2=tab$var2, S=tab$S, T=tab$T,
P=tab$P, Sit=tab$Sit, Pt=tab$Pt)
```

---

carbb   *Parameters of the seawater carbonate system*

Description

Returns parameters of the seawater carbonate system.

Usage

```
carbb(flag, var1, var2, S=35, T=25, Patm=1, P=0, Pt=0, Sit=0,
        k1k2="x", kf="x", ks="d", pHscale="T", b="u74", gas="potential", badd=0)
```

Arguments

flag
: select the couple of variables available. The flags which can be used are:
  flag = 1 pH and CO2 given
  flag = 2 CO2 and HCO3 given
  flag = 3 CO2 and CO3 given
  flag = 4 CO2 and ALK given
  flag = 5 CO2 and DIC given
  flag = 6 pH and HCO3 given
  flag = 7 pH and CO3 given
  flag = 8 pH and ALK given
  flag = 9 pH and DIC given
  flag = 10 HCO3 and CO3 given
  flag = 11 HCO3 and ALK given
  flag = 12 HCO3 and DIC given
  flag = 13 CO3 and ALK given
  flag = 14 CO3 and DIC given
  flag = 15 ALK and DIC given
  flag = 21 pCO2 and pH given
  flag = 22 pCO2 and HCO3 given
  flag = 23 pCO2 and CO3 given
  flag = 24 pCO2 and ALK given
  flag = 25 pCO2 and DIC given

var1
: Value of the first variable in mol/kg, except for pH and for pCO2 in μatm

var2
: Value of the second variable in mol/kg, except for pH

S
: Salinity

T
: Temperature in degrees Celsius

Patm
: Surface atmospheric pressure in atm, default is 1 atm

P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg; set to 0 if NA
Sit	Concentration of total silicate in mol/kg; set to 0 if NA
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010) and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"
gas	used to indicate the convention for INPUT pCO2, i.e., when it is an input variable (flags 21 to 25): "insitu" indicates it is referenced to in situ pressure and in situ temperature; "potential" indicates it is referenced to 1 atm pressure and potential temperature; and "standard" indicates it is referenced to 1 atm pressure and in situ temperature. All three options should give identical results at surface pressure. This option is not used when pCO2 is not an input variable (flags 1 to 15). The default is "potential".
badd	Amount of boron added in mol/kg.

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.

- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.

- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.

- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.

- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

S	Salinity
T	Temperature in degrees Celsius
Patm	Surface atmospheric pressure in atm
P	Hydrostatic pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	"standard" pCO2, CO2 partial pressure computed at in situ temperature and atmospheric pressure (μatm)
fCO2	"standard" fCO2, CO2 fugacity computed at in situ temperature and atmospheric pressure (μatm)

pCO2pot	"potential" pCO2, CO2 partial pressure computed at potential temperature and atmospheric pressure (μatm)
fCO2pot	"potential" fCO2, CO2 fugacity computed at potential temperature and atmospheric pressure (μatm)
pCO2insitu	"in situ" pCO2, CO2 partial pressure computed at in situ temperature and total pressure (atm + hydrostatic) (μatm)
fCO2insitu	"in situ" fCO2, CO2 fugacity computed at in situ temperature and total pressure (atm + hydrostatic) (μatm)
HCO3	HCO3 concentration (mol/kg)
CO3	CO3 concentration (mol/kg)
DIC	DIC concentration (mol/kg)
ALK	ALK, total alkalinity (mol/kg)
OmegaAragonite	Omega aragonite, aragonite saturation state
OmegaCalcite	Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

Heloise Lavigne, James Orr and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

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Millero F. J., 1995. Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Millero F. J., 2010. Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H. and Pierrot D., 2006. Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

Orr J. C., Epitalon J.-M. and Gattuso J.-P., 2014. Comparison of seven packages that compute ocean carbonate chemistry. *Biogeosciences Discussions* **11**, 5327-5397.

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Roy R. N., Roy L. N., Vogel K. M., Porter-Moore C., Pearson T., Good C. E., Millero F. J. and Campbell D. M., 1993. The dissociation constants of carbonic acid in seawater at salinities 5 to 45 and temperatures 0 to 45oC. *Marine Chemistry* **44**, 249-267.

Uppstrom L.R., 1974 The boron/chlorinity ratio of the deep-sea water from the Pacific Ocean. *Deep-Sea Research I* **21** 161-162.

Weiss, R. F., 1974. Carbon dioxide in water and seawater: the solubility of a non-ideal gas, *Mar. Chem.*, **2**, 203-215.

Weiss, R. F. and Price, B. A., 1980. Nitrous oxide solubility in water and seawater, *Mar. Chem.*, **8**, 347-359.

Zeebe R. E. and Wolf-Gladrow D. A., 2001 *CO2 in seawater: equilibrium, kinetics, isotopes.* Amsterdam: Elsevier, 346 pp.

Examples

```
## With a couple of variables
carbb(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Patm=1.0, Pt=0, Sit=0,
pHscale="T", kf="pf", k1k2="l", ks="d", b="u74", badd=0)
```

---

d2p   *Converts depth in meters to pressure in dbar*

Description

Converts depth in meters to pressure in dbar

Usage

```
d2p(depth, lat=40)
```

Arguments

depth   Depth in meters

lat   Latitude in degrees, N and S is irrelevant, default is 40o

Value

pressure   Pressure corresponding to the depth given, in dbar

Author(s)

Heloise Lavigne and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Saunders P. M., 1981. Practical conversion of pressure to depth. *J. Phys. Oceanogr.* **11**: 573-574.

See Also

[p2d](#)

Examples

```
d2p(depth=7500, lat=30)
```

---

f2pCO2   *Converts the CO2 fugacity to CO2 partial pressure*

Description

Converts fCO2 (fugacity of CO2) into pCO2 (partial pressure in CO2)

Usage

```
f2pCO2(T = 25, Patm=1, P=0, fCO2)
```

Arguments

T   Temperature in degrees Celsius, default is 25oC

Patm   Surface atmospheric pressure in atm, default 1 atm

P   Hydrostatic pressure in bar, default is 0 bar (surface)

fCO2   Fugacity of CO2 in μatm, the same units as that for the pCO2 output

Value

pCO2   Partial pressure of CO2 in μatm, the same units as that for the fCO2 input

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

Heloise Lavigne, Jean-Pierre Gattuso, and James Orr <gattuso@obs-vlfr.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007. Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Orr J. C., Epitalon J.-M. and Gattuso J.-P., 2014. Comparison of seven packages that compute ocean carbonate chemistry. *Biogeosciences Discussions* **11**, 5327-5397.

Weiss, R. F. and Price, B. A., 1980. Nitrous oxide solubility in water and seawater, *Mar. Chem.*, **8**, 347-359, 1980.

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Weiss, R. F. and Price, B. A., 1980. Nitrous oxide solubility in water and seawater, *Mar. Chem.*, **8**, 347-359.

See Also

[p2fCO2](#).

Examples

```
f2pCO2(T=25, Patm=1.0, P=0, fCO2=380)
```

K0	*Henry's constant mol/(kg/atm)*

Description

Henry's constant mol/(kg/atm)

Usage

```
K0(S = 35, T = 25, P = 0, Patm = 1)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
Patm	Surface atmospheric pressure in atm, defaultis 1 atm

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between -1 and 45oC.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

K0   Henry's constant mol/(kg/atm)

Author(s)

Jean-Marie Epitalon, Aurelien Proye, and Jean-Pierre Gattuso `<gattuso@obs-vlfr.fr>`

References

Weiss R. F., 1974 Carbon dioxide in water and seawater: the solubility of a non-ideal gas. *Marine Chemistry* **2**, 203-215.

Examples

```
K0(S=35,T=25,P=0)
```

K1   *First dissociation constant of carbonic acid (mol/kg)*

Description

First dissociation constant of carbonic acid (mol/kg)

Usage

```
K1(S = 35, T = 25, P = 0, k1k2="x", pHscale="T", kSWS2scale=0, ktotal2SWS_P0=0)
```

Arguments

S   Salinity, default is 35

T   Temperature in degrees Celsius, default is 25oC

P   Hydrostatic pressure in bar (surface = 0), default is 0

k1k2   "l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".

pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale	Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. It is not required when k1k2 is "m10" or "w14" and the hydrostatic pressure is 0. If it is required and not given, it is computed, which slows down computations.
ktotal2SWS_P0	Conversion factor from the total scale to the SWS at an hydrostatic pressure of 0. It is only required when k1k2 is "l" or "r". If it is required and not given, it is computed, which slows down computations.

Details

The Lueker et al. (2000) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.

- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.

- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.

- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

- Waters et al.(2014): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

The pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

K1	First dissociation constant of carbonic acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

DOE 1994 *Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water*. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.

Lueker T. J., Dickson A. G., and Keeling C. D., 2000 Ocean pCO2 calculated from dissolved inorganic carbon, alkalinity, and equations for K1 and K2: validation based on laboratory measurements of CO2 in gas and seawater at equilibrium. *Marine Chemistry* **70** 105-119.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H., and Pierrot D., 2006 Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

Millero F. J., 2010 Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Roy R. N., Roy L. N., Vogel K. M., Porter-Moore C., Pearson T., Good C. E., Millero F. J. and Campbell D. M., 1993. The dissociation constants of carbonic acid in seawater at salinities 5 to 45 and temperatures 0 to 45oC. *Marine Chemistry* **44**, 249-267.

Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

See Also

K2.

Examples

```
K1(S=35,T=25,P=0,k1k2="l",pHscale="T")
```

K1p   *First dissociation constant of phosphoric acid (mol/kg)*

Description

First dissociation constant of phosphoric acid (mol/kg)

Usage

```
K1p(S = 35, T = 25, P = 0, pHscale = "T", kSWS2scale = 0)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	Choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale	Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45oC.

The pressure correction was applied on the seawater scale. Hence, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

K1p	First dissociation constant of phosphoric acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

See Also

K2p, K3p.

Examples

```
K1p(35,25,0)
```

K2   *Second dissociation constant of carbonic acid (mol/kg)*

Description

Second dissociation constant of carbonic acid (mol/kg)

Usage

```
K2(S = 35, T = 25, P = 0, k1k2 = "x", pHscale = "T", kSWS2scale=0, ktotal2SWS_P0=0)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale	Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. It is not required when k1k2 is "m10" or "w14" and the hydrostatic pressure is 0. If it is required and not given, it is computed, which slows down computations.
ktotal2SWS_P0	Conversion factor from the total scale to the SWS at an hydrostatic pressure of 0. It is only required when k1k2 is "l" or "r". If it is required and not given, it is computed, which slows down computations.

Details

The Lueker et al. (2000) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

- Waters et al.(2014): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

The pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

K2   Second dissociation constant of carbonic acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

The Lueker et al. (2000) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). The Roy et al. (1993) constants is recommended by DOE (1994).

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

DOE 1994 *Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water*. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.

Lueker T. J., Dickson A. G. and Keeling C. D., 2000 Ocean pCO2 calculated from dissolved inorganic carbon, alkalinity, and equations for K1 and K2: validation based on laboratory measurements of CO2 in gas and seawater at equilibrium. *Marine Chemistry* **70** 105-119.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H. and Pierrot D., 2006 Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

Millero F. J., 2010 Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Roy R. N., Roy L. N., Vogel K. M., Porter-Moore C., Pearson T., Good C. E., Millero F. J. and Campbell D. M., 1993. The dissociation constants of carbonic acid in seawater at salinities 5 to 45 and temperatures 0 to 45oC. *Marine Chemistry* **44**, 249-267.

Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

See Also

K1.

Examples

```
K2(35,25,0)
```

K2p   *Second dissociation constant of phosphoric acid (mol/kg)*

Description

Second dissociation constant of phosphoric acid (mol/kg)

Usage

```
K2p(S = 35, T = 25, P = 0, pHscale = "T", kSWS2scale = 0)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale	Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45oC.

The pressure correction was applied on the seawater scale. Hence, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

K2p	Second dissociation constant of phosphoric acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso `<gattuso@obs-vlfr.fr>`

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

See Also

K1p, K3p.

Examples

```
K2p(35,25,0)
```

K3p	*Third dissociation constant of phosphoric acid (mol/kg)*

Description

Third dissociation constant of phosphoric acid (mol/kg)

Usage

```
K3p(S = 35, T = 25, P = 0, pHscale = "T", kSWS2scale = 0)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale	Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45oC.

The pressure correction was applied on the seawater scale. Hence, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

K3p   Third dissociation constant of phosphoric acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso `<gattuso@obs-vlfr.fr>`

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

See Also

K1p, K2p.

Examples

```
K3p(35,25,0)
```

Kb   *Dissociation constant of boric acid (mol/kg)*

Description

Dissociation constant of boric acid (mol/kg)

Usage

```
Kb(S = 35, T = 25, P = 0, pHscale="T", kSWS2scale=0, ktotal2SWS_P0=0)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale	Conversion factor from SWS pH scale to chosen scale at chosen pressure; if needed and not given, it is computed; if given, computation speed is increased
ktotal2SWS_P0	Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. It is not required when the selected pH scale is SWS and the hydrostatic pressure is 0. If it is required and not given, it is computed, which slows down computations.

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 5 and 45 and T ranging between 0 and 45oC.

The pressure correction is applied on the seawater scale. Hence, values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

Kb	Dissociation constant of boric acid (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Thermodynamics of the dissociation of boric acid in synthetic seawater from 273.15 to 318.15 K. *Deep-Sea Research* **375**, 755-766.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

DOE 1994 *Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water*. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Examples

```
Kb(S=35,T=25,P=0,pHscale="T")
```

---

kconv	*Conversion factors to change the pH scale of dissociation constants*

Description

Conversion factors from the total scale to the free and seawater scales

Usage

```
kconv(S=35,T=25, P=0, kf, Ks, Kff)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994); if the fonction Kf was used previously, the default value is the value given for the argument kf in the fonction Kf. If the Kf function was not used previously, the default value is "pf", except if T is outside the range 9 to 33oC or of S is outside the range 10 to 40. In these cases, the default is "dg".
Ks	Stability constant of hydrogen sulfate (mol/kg) at given S, T and P, optional; if not given, it will be computed, if given, it allows for speed optimisation
Kff	Stability constant of hydrogen fluoride (mol/kg) on free pH scale at given S, T and P, optional; if not given, it will be computed, if given, it allows for speed optimisation and kf parameter is then ignored

Details

It is critical to consider that each formulation is valid in specific ranges of temperature and salinity:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

Note that kconv may be called in many functions (i.e. K1, K2, K1P, K2P, K3P, Kw, Ksi, etc...) without user controls it. To force a particular formulation for Kf, it is recommended to call kconv() first then pass the resulting conversion factors to these functions.

Value

The function returns a list with 3 conversion factors :

ktotal2SWS	to convert from the total scale to seawater scale
ktotal2free	to convert from the total scale to the free scale
kfree2SWS	to convert from the free scale to the seawater scale

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl>

References

Dickson A.G. and F.J. Millero, 1987 A comparison of the equilibrium constants for the dissociation of carbonic acid in seawater media. *Deep-Sea Research* **34**:1733-1743.

See Also

[pHconv]().

Examples

```
##To convert dissociation constants from the total scale to the free scale
## (at salinity=35, temperature=25oC and atmospheric pressure):
kconv(35,25,0)
conv <- kconv()
 c(K1_total=K1(),K1_SWS=K1()*conv$ktotal2SWS,K1_free=K1()*conv$ktotal2free)
```

Kf	*Equilibrium constant of hydrogen fluoride (mol/kg)*

Description

Stability constant of hydrogen fluoride (mol/kg)

Usage

```
Kf(S = 35, T = 25, P = 0, kf = "x", pHscale="T", Ks_p0=0, Ks_p=0)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
kf	"pf" for using Kf from Perez and Fraga (1987) "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994), default is "pf". Attention do not use a vector for this argument.

pHscale	choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
Ks_p0	Stability constant of hydrogen sulfate (mol/kg) at pressure zero; needed if kf = "pf" ; if needed and not given, it is computed; if given, computation speed is increased
Ks_p	Stability constant of hydrogen sulfate (mol/kg) at chosen pressure if not given, it is computed; if given, computation speed is increased

Details

The Perez and Fraga (1987) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). The Dickson and Riley (1979 in Dickson and Goyet, 1994) constant is recommended by DOE (1994).

It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

The pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

Kf	Stability constant of hydrogen fluoride (mol/kg)

Author(s)

Jean-Marie Epitalon and Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G. and Riley J. P., 1979 The estimation of acid dissociation constants in seawater media from potentiometric titrations with strong base. I. The ionic product of water. *Marine Chemistry* **7**, 89-99.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

DOE 1994 *Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water*. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Perez F. F. and Fraga F., 1987 Association constant of fluoride and hydrogen ions in seawater. *Marine Chemistry* **21**, 161-168.

Examples

```
Kf(S=35,T=25,P=0,kf="pf",pHscale="T")
```

---

kfg   *variable for internal use*

Description

nothing

Khs   *Dissociation constant of hydrogen sulfide (mol/kg)*

Description

Dissociation constant of hydrogen sulfide (mol/kg)

Usage

```
Khs(S=35, T=25, P=0, pHscale="T")
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45oC.

The pressure correction is applied on the seawater scale. Hence, the values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value is transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

Khs   Dissociation constant of hydrogen sulfide

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl> and Heloise Lavigne

References

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* 59: 661-677.

Examples

```
Khs(S=35,T=25,P=0, pHscale="T")
```

Kn   *Dissociation constant of ammonium (mol/kg)*

Description

Dissociation constant of ammonium on the total scale (mol/kg)

Usage

```
Kn(S=35, T=25, P=0, pHscale="T")
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45oC.

The pressure correction is applied on the seawater scale. Hence, values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value is transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

Kn   Dissociation constant of ammonium (mol/kg)

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl> and Heloise Lavigne

References

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Examples

```
Kn(S=35,T=25,P=0, pHscale="T")
```

Ks   *Stability constant of hydrogen sulfate (mol/kg)*

Description

Stability constant of hydrogen sulfate (mol/kg)

Usage

```
Ks(S = 35, T = 25, P = 0, ks="d")
```

Arguments

S   Salinity, default is 35
T   Temperature in degrees Celsius, default is 25oC
P   Hydrostatic pressure in bar (surface = 0), default is 0
ks   "d" for using Ks from Dickson (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

Details

The Dickson (1990) constant is recommended by Guide to Best Practices for Ocean CO2 Measurements (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

The pressure correction is applied on the free scale.

Value

Ks   Stability constant of hydrogen sulfate (mol/kg), pHscale = free scale

Author(s)

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: $AgCI(s) + 1/2H2(g) = Ag(s) + HCI(aq)$, and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Khoo H. K., Ramette R. W., Culberson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40oC: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **22**, vol49 29-34.

Examples

    Ks(S=35,T=25,P=0, ks="d")

Ksi   *Dissociation constant of Si(OH)4*

Description

Dissociation constant of Si(OH)4 on total scale (mol/kg)

Usage

    Ksi(S=35, T=25, P=0, pHscale="T", kSWS2scale=0)

Arguments

S   Salinity, default is 35

T   Temperature in degrees Celsius, default is 25oC

P   Hydrostatic pressure in bar (surface = 0), default is 0

pHscale   choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale

kSWS2scale   Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45oC.

The pressure correction is applied on the seawater scale. Hence, values are first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value is transformed back to the required scale (T, F or SWS).

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

Ksi   Dissociation constant of Si(OH)4 (mol/kg)

Author(s)

Karline Soetaert <K.Soetaert@nioo.knaw.nl> and Heloise Lavigne

References

DOE 1994 *Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water*. ORNL/CDIAC-74. Oak Ridge,Tenn.: Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Examples

```
Ksi(S=35, T=25, P=0, pHscale="T")
```

Kspa   *Solubility product of aragonite (mol/kg)*

Description

Solubility product of aragonite (mol/kg)

Usage

```
Kspa(S = 35, T = 25, P = 0)
```

Arguments

S   Salinity, default is 35
T   Temperature in degrees Celsius, default is 25oC
P   Hydrostatic pressure in bar (surface = 0), default is 0

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 5 and 44 and T ranging between 5 and 40oC.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

Kspa   Solubility product of aragonite (mol2/kg)

Author(s)

Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Mucci A., 1983 The solubility of calcite and aragonite in seawater at various salinities, temperature, and one atmosphere total pressure. *American Journal of Science* **283**: 780-799.

See Also

[Kspc](#).

Examples

```
Kspa(S=35,T=25,P=0)
```

Kspc   *Solubility product of calcite (mol/kg)*

Description

Solubility product of calcite (mol/kg)

Usage

```
Kspc(S = 35, T = 25, P = 0)
```

Arguments

S   Salinity, default is 35
T   Temperature in degrees Celsius, default is 25oC
P   Hydrostatic pressure in bar (surface = 0), default is 0

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 5 and 44 and T ranging between 5 and 40oC.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

Kspc   Solubility product of calcite (mol2/kg)

Author(s)

Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Mucci A., 1983 The solubility of calcite and aragonite in seawater at various salinities, temperature, and one atmosphere total pressure. *American Journal of Science* **283**: 780-799.

See Also

Kspa.

Examples

    Kspc(S=35,T=25,P=0)

Kw   *Ion product of water (mol2/kg2)*

Description

Ion product of water (mol2/kg2)

Usage

    Kw(S = 35, T = 25, P = 0, pHscale = "T", kSWS2scale=0)

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
kSWS2scale	Conversion factor from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated. If it is required and not given, it is computed, which slows down computations.

Details

This formulation is only valid for specific ranges of temperature and salinity:

- S ranging between 0 and 45 and T ranging between 0 and 45oC.

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

Kw	Ion product of water (mol2/kg2)

Author(s)

Heloise Lavigne, Aurelien Proye and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica et Cosmochimica Acta* **59** 661-677.

Examples

```
Kw(S=35,T=25,P=0,pHscale="T")
```

---

oa	*Perturbation of the seawater carbonate system*

Description

Describes the various approaches that can be used to alter the seawater carbonate system. Its main purpose is to assist the design of ocean acidification perturbation experiments.

Usage

```
oa(flag, var1, var2, pCO2f, pCO2s=1e6, S=35, T=25, P=0,
Pt=0, Sit=0, k1k2='x', kf='x', ks="d", pHscale="T", plot=FALSE, b="u74")
```

Arguments

flag	select the couple of variables available to describe the initial seawater. The flags which can be used are:
	flag = 1 pH and CO2 given
	flag = 2 CO2 and HCO3 given
	flag = 3 CO2 and CO3 given
	flag = 4 CO2 and ALK given
	flag = 5 CO2 and DIC given
	flag = 6 pH and HCO3 given
	flag = 7 pH and CO3 given
	flag = 8 pH and ALK given
	flag = 9 pH and DIC given
	flag = 10 HCO3 and CO3 given
	flag = 11 HCO3 and ALK given
	flag = 12 HCO3 and DIC given
	flag = 13 CO3 and ALK given
	flag = 14 CO3 and DIC given
	flag = 15 ALK and DIC given
	flag = 21 pCO2 and pH given
	flag = 22 pCO2 and HCO3 given
	flag = 23 pCO2 and CO3 given
	flag = 24 pCO2 and ALK given
	flag = 25 pCO2 and DIC given
var1	Value of the first variable available to describe the initial seawater, in mol/kg except for pH and for pCO2 in uatm
var2	Value of the second variable available to describe the initial seawater, in mol/kg except for pH
pCO2f	pCO2 target value, in uatm

pCO2s	pCO2s is the pCO2, in uatm, of the "high-CO2" seawater that will be mixed with "normal seawater". The default value is 10^6 uatm, that is seawater bubbled with pure CO2 gas and saturated with CO2.
S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25
P	Hydrostatic pressure in bar (surface = 0), default is 0
Pt	Concentration of total phosphate in mol/kg, default is 0
Sit	Concentration of total silicate in mol/kg, default is 0
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
plot	A plot of the different perturbation methods can be plotted in a DIC vs ALK field with pCO2 isoclines are drawn in the back. Default is false.
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.

- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.

- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.

- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.

- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a list built as follows:

description	A table describing in plain English the various ways to reach the target pCO2. Note that if a vector is given in argument only the first value is used.
perturbation	Table providing key parameters for the following methods:
	CO2 bubbling: high-CO2 air is bubbled in seawater. The first parameter is the value of the pCO2 in the air required to bubble the seawater (in uatm).
	SW mixing: mixing of "normal" and "high-CO2" seawater. The fist parameter, "Weight fraction high-CO2 SW" or wf, is the weight fraction of the high-CO2 seawater per kg seawater.
	Addition of acid: strong acid is added to seawater. Note that this method is not recommended because it does not closely mimic natural ocean acidification (Gattuso and Lavigne, 2009). The first parameter, H+ (mol/kg), is the amount of

H+ that must be added (mol/kg). The acid must be fortified with NaCl in order to have the same salinity than seawater.

Addition of HCO3 and acid: bicarbonate (HCO3) and a strong acid are added. The first parameter, HCO3, is the amount of HCO3 that must be added (mol/kg). The second parameter, H+, is the quantity of H+ that must be added (mol/kg). The acid must be fortified with NaCl in order to have the same salinity than seawater.

Addition of CO3 and acid: carbonate, CO3, and a strong acid are added. The first parameter, HCO3, is the quantity of CO3 that must be added (mol/kg). The second parameter, H+, is the quantity of H+ that must be added (mol/kg).

summary   Table summarizing the carbonate chemistry before and after applying each per-turbation: pCO2 bubbling, mixing with high-CO2 seawater, addition of strong acid, and addition of bicarbonate/carbonate and strong acid.

Warnings

- It is recommended to use concentrated solutions of acid or base in order to add small volumes.

- The addition of strong acid does not simulate well natural ocean acidification (higher concentration of dissolved inorganic carbon at constant total alkalinity) since it generates a decrease in total alkalinity while dissolved inorganic carbon is kept constant.

- Other important advice is provided in Gattuso and Lavigne (2009), Schulz et al. (2009) and in the "Guide for Best Practices on Ocean Acidification Research and Data Reporting" (http://www.epoca-project.eu/index.php/Home/Guide-to-OA-Research/)

Author(s)

Heloise Lavigne and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., 1990 Standard potential of the reaction: AgCI(s) + 1/2H2(g) = Ag(s) + HCI(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Khoo H. K., Ramette R. W., Culberson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40oC: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **49**, 29-34.

Gattuso J.-P. and Lavigne H., 2009 Technical note: approaches and software tools to investigate the impact of ocean acidification. *Biogeosciences* **21**, 6:2121-2133.

Lueker T. J., Dickson A. G. and Keeling C. D., 2000 Ocean pCO2 calculated from dissolved inorganic carbon, alkalinity, and equations for K1 and K2: validation based on laboratory measurements of CO2 in gas and seawater at equilibrium. *Marine Chemistry* **70** 105-119.

Lee K., Tae-Wook K., Byrne R.H., Millero F.J., Feely R.A. and Liu Y-M, 2010 The universal ratio of the boron to chlorinity for the North Pacific and North Atlantoc oceans. *Geochimica et Cosmochimica Acta* **74** 1801-1811.

Millero F. J., 2010 Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H. and Pierrot D., 2006. Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

Perez F. F. and Fraga F., 1987 Association constant of fluoride and hydrogen ions in seawater. *Marine Chemistry* **21**, 161-168.

Roy R. N., Roy L. N., Vogel K. M., Porter-Moore C., Pearson T., Good C. E., Millero F. J. and Campbell D. M., 1993 The dissociation constants of carbonic acid in seawater at salinities 5 to 45 and temperatures 0 to 45oC. *Marine Chemistry* **44**, 249-267.

Schulz K. G., Barcelos e Ramos J., Zeebe R. E. and Riebesell U., 2009 CO2 perturbation experiments: similarities and differences between dissolved inorganic carbon and total alkalinity manipulations. *Biogeosciences* **6**, 2145-2153.

Uppstrom L.R., 1974 The boron/chlorinity ratio of the deep-sea water from the Pacific Ocean. *Deep-Sea Research I* **21** 161-162.

Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

Zeebe R. E. and Wolf-Gladrow D. A., 2001 *CO2 in seawater: equilibrium, kinetics, isotopes*. Amsterdam: Elsevier, 346 pp.

See Also

[carb](), [pgas](), [pmix](), [ppH](), [pTA]().

Examples

```
oa(flag=24, var1=384, var2=2325e-6, pCO2s=1e6, pCO2f=793, S=34.3, T=16,
P=0, pHscale="T", kf="pf", k1k2="l", ks="d", plot=TRUE, b="u74")
```

Om   *Carbonate saturation state for magnesian calcites*

Description

Calculates the calcium carbonate saturation state for magnesian calcite

Usage

```
Om(x, flag, var1, var2, k1k2='x', kf='x', ks="d", pHscale="T", b="u74")
```

Arguments

x	mole fraction of magnesium ions, note that the function is only valid for x ranging between 0 and 0.25
flag	select the couple of variables available. The flags which can be used are:

flag = 1 pH and CO2 given

flag = 2 CO2 and HCO3 given

flag = 3 CO2 and CO3 given

flag = 4 CO2 and ALK given

flag = 5 CO2 and DIC given

flag = 6 pH and HCO3 given

flag = 7 pH and CO3 given

flag = 8 pH and ALK given

flag = 9 pH and DIC given

flag = 10 HCO3 and CO3 given

flag = 11 HCO3 and ALK given

flag = 12 HCO3 and DIC given

flag = 13 CO3 and ALK given

flag = 14 CO3 and DIC given

flag = 15 ALK and DIC given

flag = 21 pCO2 and pH given

flag = 22 pCO2 and HCO3 given

flag = 23 pCO2 and CO3 given

flag = 24 pCO2 and ALK given

flag = 25 pCO2 and DIC given

var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickson (1990) and "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

It is important to note that this function is **only valid** for:

- Salinity = 35
- Temperature = 25 degrees Celsius
- Hydrostatic pressure = 0 bar (surface)
- Concentration of total phosphate = 0 mol/kg
- Concentration of total silicate = 0 mol/kg

Note that the stoichiometric solubility products with respect to Mg-calcite minerals have not been determined experimentally. The saturation state with respect to Mg-calcite minerals is therefore calculated based on ion activities, i.e.,

$$\Omega_x = \frac{\{Ca^{2+}\}^{1-x}\{Mg^{2+}\}^{x}\{CO_3\}^{2-}}{K_x}$$

The ion activity {a} is calculated based on the observed ion concentrations [C] multiplied by the total ion activity coefficient, γ_T, which has been determined experimentally or from theory (e.g. Millero & Pierrot 1998): {a}=γ_T[C]. Because a true equilibrium cannot be achieved with respect to Mg-calcite minerals, K_x represents a metastable equilibrium state obtained from what has been referred to as stoichiometric saturation (Thorstenson & Plummer 1977; a term not equivalent to the definition of the stoichiometric solubility product, see for example Morse et al. (2006) and references therein). In the present calculation calcium and magnesium concentrations were calculated based on salinity. Total ion activity coefficients with respect to Ca^{2+}, Mg^{2+}, and CO_3^{2-} were adopted from Millero & Pierrot (1998).

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.

- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a list with

`OmegaMgCa_biogenic`
> Mg-calcite saturation state for minimally prepared biogenic Mg-calcite.

`OmegaMgCa_biogenic_cleaned`
> Mg-calcite saturation state for cleaned and annealed biogenic Mg-calcite.

Author(s)

Heloise Lavigne, Andreas J. Andersson and Jean-Pierre Gattuso `<gattuso@obs-vlfr.fr>`

References

Only the references related to the saturation state of magnesian calcite are listed below; the other references are listed under the carb function.

Andersson A. J., Mackenzie F. T., Nicholas R. B., 2008, Life on the margin: implications of ocean acidification on Mg-calcite, high latitude and cold-water marine calcifiers. *Marine Ecology Progress Series* **373**, 265-273.

Bischoff W. D., Bertram M. A., Mackenzie F. T. and Bishop F.C., 1993 Diagenetic stabilization pathways of magnesian calcites. *Carbonates and Evaporites* **8**, 82-89.

Millero F. J. and Pierrot D., 1998. A chemical equilibrium model for natural waters. *Aquatic Geochemistry* **4**, 153-199.

Morse J. W., Andersson A. J. and Mackenzie F. T., 2006. Initial responses of carbonate-rich shelf sediments to rising atmospheric pCO2 and ocean acidification: Role of high Mg-calcites. *Geochimica et Cosmochimica Acta* **70**, 5814-5830.

Thorstenson D.C. and Plummer L.N., 1977. Equilibrium criteria for two component solids reacting with fixed composition in an aqueous phase-example: the magnesian calcites. *American Journal of Science* **277**, 1203-1233.

Examples

```
Om(x=seq(0.01, 0.252, 0.01), flag=8, var1=8.2, var2=0.00234,
  k1k2='x', kf='x', ks="d", pHscale="T", b="u74")
```

---

p2d   *Converts pressure in dbar to depth in meters*

Description

Converts pressure in dbar to depth in meters

Usage

```
p2d(pressure, lat=40)
```

Arguments

pressure	Pressure in dbar
lat	Latitude in degrees, N and S is irrelevant, default is 40o

Value

depth	Depth corresponding to the pressure given, in meters

Author(s)

Heloise Lavigne and Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Saunders P. M., 1981. Practical conversion of pressure to depth. *J. Phys. Oceanogr.* **11**: 573-574.

See Also

[d2p](#)

Examples

```
p2d(pressure=7686, lat=30)
```

---

p2fCO2   *Converts pCO2 (partial pressure in CO2) into fCO2 (fugacity of CO2)*

Description

Converts pCO2 (partial pressure in CO2) into fCO2 (fugacity of CO2)

Usage

```
p2fCO2(T = 25, Patm=1, P=0, pCO2)
```

Arguments

T	Temperature in degrees Celsius, default is 25oC
Patm	Surface atmospheric pressure in atm, default is 1 atm
P	Hydrostatic pressure in bar, default is 0 bar (surface)
pCO2	Partial pressure in CO2 in μatm, the same units as that for the fugacity output

Value

fCO2	Fugacity of CO2 in μatm, the same units as that for the pCO2 input.

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

Heloise Lavigne, Jean-Pierre Gattuso, and James Orr `<gattuso@obs-vlfr.fr>`

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Orr J. C., Epitalon J.-M. and Gattuso J.-P., 2014. Comparison of seven packages that compute ocean carbonate chemistry. *Biogeosciences Discussions* **11**, 5327-5397.

Weiss, R. F., 1974. Carbon dioxide in water and seawater: the solubility of a non-ideal gas, *Mar. Chem.*, **2**, 203-215.

Weiss, R. F. and Price, B. A., 1980. Nitrous oxide solubility in water and seawater, *Mar. Chem.*, **8**, 347-359.

See Also

f2pCO2.

Examples

```
p2fCO2(T=25, Patm=0.97, P=0, pCO2=380)
```

---

p2xCO2	*Converts partial pressure of CO2 to mole fraction of CO2*

Description

Converts pCO2 (partial pressure of CO2) into xCO2 (mole fraction of CO2)

Usage

```
p2xCO2(S=35, T=25, Patm=1, pCO2)
```

Arguments

S	Salinity on the practical salinity scale, default is 35
T	Temperature in degrees Celsius, default is 25oC
Patm	Atmospheric pressure in atmospheres, default is 1.0 (this is not the hydrostatic pressure)
pCO2	Partial pressure of CO2 in μatm

Details

The xCO2 (ppm) is computed from pCO2 (μatm) using the following equation: $xCO2 = pCO2/(Patm - pH2O)$, where pH20 is the vapor pressure of seawater computed following best practices (Dickson et al., 2007). That computed pH20 is identical, when rounded to the 4th decimal place, with that computed by the equation from Weiss and Price (1980).

Value

xCO2	Mole fraction of CO2 in ppm.

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

James Orr <james.orr@lsce.ipsl.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R. (2007) Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Orr J. C., Epitalon J.-M. and Gattuso J.-P., 2014. Comparison of seven packages that compute ocean carbonate chemistry. *Biogeosciences Discussions* **11**, 5327-5397.

Weiss, R. F. (1974) Carbon dioxide in water and seawater: the solubility of a non-ideal gas, Mar. Chem., **2**, 203-215.

Weiss, R. F. and Price, B. A. (1980) Nitrous oxide solubility in water and seawater, Mar. Chem., **8**, 347-359.

See Also

[x2pCO2](x2pCO2) and vapress

Examples

```
## Convert atmospheric pressure from mbar to atm
   Patm_mbar = 1052                 # in millibar
   Patm      = Patm_mbar / 1013.25  # in atm
## Compute xCO2 from pCO2
   pCO2 = 380
   xCO2 = p2xCO2(T=25, S=35, Patm=Patm, pCO2=pCO2)
   print(xCO2)
## The result is 377.1546 ppm
```

---

pCa   *pCa*

Description

Calculates the changes in the saturation states of aragonite and calcite resulting from the manipulation of the calcium concentration

Usage

```
pCa(flag, var1, var2, Ca, S=35, T=20, P=0, Pt=0, Sit=0, k1k2="x",
kf="x", ks="d", pHscale="T", b="u74")
```

Arguments

flag   select the couple of variables available. The flags which can be used are:

                flag = 1 pH and CO2 given

                flag = 2 CO2 and HCO3 given

                flag = 3 CO2 and CO3 given

                flag = 4 CO2 and ALK given

                flag = 5 CO2 and DIC given

	flag = 6 pH and HCO3 given
	flag = 7 pH and CO3 given
	flag = 8 pH and ALK given
	flag = 9 pH and DIC given
	flag = 10 HCO3 and CO3 given
	flag = 11 HCO3 and ALK given
	flag = 12 HCO3 and DIC given
	flag = 13 CO3 and ALK given
	flag = 14 CO3 and DIC given
	flag = 15 ALK and DIC given
	flag = 21 pCO2 and pH given
	flag = 22 pCO2 and HCO3 given
	flag = 23 pCO2 and CO3 given
	flag = 24 pCO2 and ALK given
	flag = 25 pCO2 and DIC given
var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
Ca	Calcium concentration in mol/kg
S	Salinity
T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

`comment`	The initial or final state water
`S`	Salinity
`T`	Temperature in degrees Celsius
`P`	Pressure in bar
`pH`	pH
`CO2`	CO2 concentration (mol/kg)
`pCO2`	pCO2, CO2 partial pressure (μatm)
`fCO2`	fCO2, CO2 fugacity (μatm)
`HCO3`	HCO3 concentration (mol/kg)
`CO3`	CO3 concentration (mol/kg)
`DIC`	DIC concentration (mol/kg)
`ALK`	ALK, total alkalinity (mol/kg)
`OmegaAragonite`	Omega aragonite, aragonite saturation state
`OmegaCalcite`	Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2015)

Author(s)

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References

Ben-Yaakov S. and Goldhaber M. B., 1973 The influence of sea water composition on the apparent constants of the carbonate system. *Deep-Sea Research* **20**, 87-99.

Dickson A. G., 1990 Standard potential of the reaction: AgCI(s) + 1/2H2(g) = Ag(s) + HCI(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Gattuso J.-P. and Lavigne H, 2009 Perturbation experiments to investigate the impact of ocean acidification: approaches and software tools. *Biogeosciences* **6**, 4413-4439.

Khoo H. K., Ramette R. W., Culberson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40oC: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **49**, 29-34.

Lee K., Tae-Wook K., Byrne R.H., Millero F.J., Feely R.A. and Liu Y-M, 2010 The universal ratio of the boron to chlorinity for the North Pacific and North Atlantoc oceans. *Geochimica et Cosmochimica Acta* **74** 1801-1811.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

Millero F. J., 2010 Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H. and Pierrot D., 2006. Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

Orr J. C., Epitalon J.-M. and Gattuso J.-P., 2014. Comparison of seven packages that compute ocean carbonate chemistry. *Biogeosciences Discussions* **11**, 5327-5397.

Uppstrom L.R., 1974 The boron/chlorinity ratio of the deep-sea water from the Pacific Ocean. *Deep-Sea Research I* **21** 161-162.

Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

Examples

```
pCa(flag=15, var1=2302e-6, var2=2050e-6, Ca=0.01028, S=35, T=20, P=0,
Pt=0, Sit=0, pHscale="T", kf="pf", k1k2="l", ks="d", b="u74") # with normal Ca concentration
pCa(flag=15, var1=2302e-6, var2=2050e-6, Ca=0.01028/2, S=35, T=20, P=0,
Pt=0, Sit=0, pHscale="T", kf="pf", k1k2="l", ks="d", b="u74") # with 0.5 * Ca concentration
```

Pcoeffs   *Coefficients used for pressure-correcting the equilibrium constants*

Description

Pressure corrections are based on the following equations:

$$\ln \frac{K_i^P}{K_i^0} = -\frac{\Delta V_i}{RT}.P + 0.5\frac{\Delta K_i}{RT}.P^2$$

with

$$\Delta V_i = a_0 + a_1 T + a_2 T^2$$

and

$$\Delta K_i = b_0 + b_1 T + b_2 T^2$$

The variables are:

- K indicating the type of equilibrium constant
- coefficient a_0
- coefficient a_1
- coefficient a_2
- coefficient b_0
- coefficient b_1
- coefficient b_2

Usage

```
Pcoeffs
```

Format

A data frame with 14 rows and 7 variables

Details

For Kb, to be consistent with Millero (1979) a2 was changed to -2.608e-3 instead of 2.608e-3 (value given in Millero, 1995) For Kw, coefficients are from Millero (1983).

Source

Millero F. J., 1979 The thermodynamics of the carbonate system in seawater. *Geochemica et Cosmochemica Acta* **43**: 1651-1661.

Millero F. J., 1983 Influence of pressure on chemical processes in the sea. pp. 1-88. In J. P. Riley and R. Chester (eds.), Chemical Oceanography. Academic Press, New York.

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica Cosmochimica Acta* **59**: 661-677.

See Also

Pcorrect

Pcorrect	*Pressure correction of equilibrium constants*

Description

Computes the pressure correction of the equilibrium constants

Usage

```
Pcorrect(Kvalue, Ktype, T=25, S=35, P=0, pHscale="T",
  kconv2ScaleP0=0, kconv2Scale=0)
```

Arguments

Kvalue   Value of the constant at P=0 (hydrostatic pressure in bar, surface = 0)

Ktype   Name of the constant,

- K1 First dissociation constant of carbonic acid (mol/kg)
- K2 Second dissociation constant of carbonic acid (mol/kg)
- Kb Dissociation constant of boric acid (mol/kg)
- Kw Ion product of water (mol2/kg2)
- Ks Stability constant of hydrogen sulfate (mol/kg)

- Kf Stability constant of hydrogen fluoride (mol/kg)
- Kspc Solubility product of calcite (mol/kg)
- Kspa Solubility product of aragonite (mol/kg)
- K1p First dissociation constant of phosphoric acid (mol/kg)
- K2p Second dissociation constant of phosphoric acid (mol/kg)
- K3p Third dissociation constant of phosphoric acid (mol/kg)
- Khs Dissociation constant of hydrogen sufide(mol/kg)
- Kn Dissociation constant of ammonium (mol/kg)
- Ksi Dissociation constant of Si(OH)4 (mol/kg)

T	Temperature in degrees Celsius, default is 25oC
S	Salinity, default is 35
P	Hydrostatic pressure in bar (surface = 0), default is 0
pHscale	pHscale of the constant given in Kvalue
kconv2ScaleP0	Conversion factor from the pH scale selected to the SWS (or free for Kf) scale at pressure zero. It is computed if it is not given, which significantly slows down the computation
kconv2Scale	Conversion factor from the pH scale selected to the SWS (or free for Kf) scale at the hydrostatic pressure value indicated. It is computed if it is not given, which significantly slows down the computation

Details

- The pressure correction is applied on the seawater scale for K1, K2, K1p, K2p, K3p, Kb, Khs, Kn, Ksi and Kw. Hence the K value is first converted on the seawater scale if needed. After pressure correction, the constant is converted back to the initial pH scale.
- The pressure correction is applied on the free scale for Kf.
- There is no issue of pH scale for Ks, Kspa and Kspc.

Value

The equilibrium constant given in argument but after pressure correction

Author(s)

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References

Millero F. J., 1995 Thermodynamics of the carbon dioxide system in the oceans. *Geochimica et Cosmochimica Acta* **59** 661-677.

See Also

Pcoeffs

Examples

```
k10 <- K1(T=25, P=0, S=35)
Pcorrect(Kvalue=k10, Ktype="K1", P=300, T=25, S=35, pHscale="T")
```

---

pgas	*pgas*

Description

Calculates the carbonate chemistry after changes in pCO2 generated by gas bubbling

Usage

```
pgas(flag, var1, var2, pCO2g, S=35, T=20, P=0, Pt=0, Sit=0, k1k2="x",
kf="x", ks="d", pHscale="T", b="u74")
```

Arguments

flag
: select the couple of variables available. The flags which can be used are:
: flag = 1 pH and CO2 given
: flag = 2 CO2 and HCO3 given
: flag = 3 CO2 and CO3 given
: flag = 4 CO2 and ALK given
: flag = 5 CO2 and DIC given
: flag = 6 pH and HCO3 given
: flag = 7 pH and CO3 given
: flag = 8 pH and ALK given
: flag = 9 pH and DIC given
: flag = 10 HCO3 and CO3 given
: flag = 11 HCO3 and ALK given
: flag = 12 HCO3 and DIC given
: flag = 13 CO3 and ALK given
: flag = 14 CO3 and DIC given
: flag = 15 ALK and DIC given
: flag = 21 pCO2 and pH given
: flag = 22 pCO2 and HCO3 given
: flag = 23 pCO2 and CO3 given
: flag = 24 pCO2 and ALK given
: flag = 25 pCO2 and DIC given

var1
: Value of the first variable in mol/kg, except for pH and for pCO2 in μatm

var2
: Value of the second variable in mol/kg, except for pH

pCO2g
: CO2 partial pressure of the gas used for bubbling in μatm

S
: Salinity

T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.

- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

comment	The initial or final state water
S	Salinity
T	Temperature in degrees Celsius
P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure (μatm)
fCO2	fCO2, CO2 fugacity (μatm)
HCO3	HCO3 concentration (mol/kg)
CO3	CO3 concentration (mol/kg)
DIC	DIC concentration (mol/kg)
ALK	ALK, total alkalinity (mol/kg)
OmegaAragonite	Omega aragonite, aragonite saturation state
OmegaCalcite	Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

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References

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Millero F. J., 2010 Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H. and Pierrot D., 2006. Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

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Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

Examples

```
pgas(flag=15, var1=2302e-6, var2=2050e-6, pCO2g=750, S=35, T=20, P=0,
Pt=0, Sit=0, pHscale="T", kf="pf", k1k2="l", ks="d", b="u74")
```

---

pH   *Potentiometric pH*

Description

Calculation of potentiometric pH

Usage

```
pH(Ex=-67,Etris=-72.4,S=35,T=25)
```

Arguments

Ex	e.m.f. of the seawater sample in mV, default is 67
Etris	e.m.f. of the TRIS buffer in mV, default is -72.4
S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC

Details

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

pH	Potentiometric pH (in mol/kg on the total scale)

Author(s)

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

See Also

tris, amp, pHslope.

Examples

```
##Example from Dickson et al. (2007)
pH(Ex=-67,Etris=-72.4,S=35,T=25)
```

---

pHconv   *Conversion of pH*

Description

Converts pH from one scale to another one chosen between the total scale, the free scale and the seawater scale

Usage

```
pHconv(flag=1, pH=8.10, S=35, T=25, P=0, ks="d")
```

Arguments

flag   choice of the type of conversion : flag=1: seawater scale to total scale flag=2: free scale to total scale flag=3: total scale to seawater scale flag=4: total scale to free scale flag=5: seawater scale to free scale flag=6: free scale to seawater scale default is flag=1

pH   Enter the value of pH which need to be converted, default is 8.100

S   Salinity, default is 35

T   Temperature in degrees Celsius, default is 25oC

P   Hydrostatic pressure in bar (surface = 0), default is 0

ks   "d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

Details

The Dickson (1990) constant is recommended by the Guide to Best Practices for Ocean CO2 Measurements (2007). It is critical to consider that each formulation is valid in specific ranges of temperature and salinity:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Value

The function returns the values of pH converted

Author(s)

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References

Dickson A.G. and F.J. Millero, 1987 A comparison of the equilibrium constants for the dissociation of carbonic acid in seawater media. *Deep-Sea Research* **34**:1733-1743.

Dickson A. G., 1990 Standard potential of the reaction: AgCI(s) + 1/2H2(g) = Ag(s) + HCI(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Khoo H. K., Ramette R. W., Culberson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40oC: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **49**, 29-34.

See Also

kconv.

Examples

```
##To convert pH=8.10 from the seawater scale to the total scale
##at salinity=35, temperature=25oC and atmospheric pressure:

  pHc <- pHconv(flag=1, pH=8.10, S=35, T=25, P=0, ks="d")

##note that pHc is the value of the pH converted in total scale

## By using vectors
## to convert the pH values : 8, 8.05, 8.10, 8.15, 8.20
## from the free to the total scale

pH <- c(8, 8.05, 8.10, 8.15, 8.20)
pHc <- pHconv(flag=2, pH=pH, S=35, T=25, P=0, ks="d")

## note that pHc is a vector containing the value of the pH converted
## to the total scale
```

---

pHinsi   *pH at in situ temperature*

Description

pH at in situ temperature

Usage

```
pHinsi(pH=8.2, ALK=2.4e-3, Tinsi=20, Tlab=25, S=35, Pt=0, Sit=0, k1k2 = "x",
kf = "x", ks="d", pHscale = "T", b="u74")
```

Arguments

pH	pH measured in the laboratory
ALK	ALK, total alkalinity (mol/kg)
Tinsi	In situ temperature in degrees Celsius
Tlab	Measurement temperature in degrees Celsius
S	Salinity
Pt	value of the concentration of total phosphate in mol/kg
Sit	the value of the total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	"l10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

pH   pH at in situ temperature

Author(s)

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References

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Millero F. J., 2010 Carbonate constant for estuarine waters. *Marine and Freshwater Research* **61**: 139-142.

Millero F. J., Graham T. B., Huang F., Bustos-Serrano H. and Pierrot D., 2006. Dissociation constants of carbonic acid in seawater as a function of salinity and temperature. *Marine Chemistry* **100**, 80-84.

Uppstrom L.R., 1974 The boron/chlorinity ratio of the deep-sea water from the Pacific Ocean. *Deep-Sea Research I* **21** 161-162.

Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

Examples

```
pHinsi(pH=8.2,ALK=2.4e-3,Tinsi=25,Tlab=25,S=35,Pt=0,Sit=0)
```

---

pHslope   *Slope of the calibration curve of a pH electrode*

Description

Slope of the calibration curve of a pH electrode (percent of theoretical slope)

Usage

```
pHslope(Etris=-72.4,Eamp=4.9,S=35,T=25)
```

Arguments

Etris	e.m.f. of the TRIS buffer in mV, default is -72.4
Eamp	e.m.f. of the AMP buffer in mV, default is 4.9
S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC

Details

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

pHslope	Slope of the calibration curve (in percent of theoretical slope)

Author(s)

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

See Also

[tris](), [amp](), [pH]().

Examples

```
##Example from Dickson et al. (2007)
pHslope(Etris=-72.4,Eamp=4.9,S=35,T=25)
```

---

pmix *pmix*

Description

Calculates the carbonate chemistry after mixing of two water samples with different pCO2

Usage

```
pmix(flag, var1, var2, pCO2s, wf, S=35, T=20, P=0, Pt=0, Sit=0, k1k2="x",
kf="x", ks="d", pHscale="T", b="u74")
```

Arguments

flag   select the couple of variables available. The flags which can be used are:

flag = 1 pH and CO2 given

flag = 2 CO2 and HCO3 given

flag = 3 CO2 and CO3 given

flag = 4 CO2 and ALK given

flag = 5 CO2 and DIC given

flag = 6 pH and HCO3 given

flag = 7 pH and CO3 given

flag = 8 pH and ALK given

flag = 9 pH and DIC given

flag = 10 HCO3 and CO3 given

flag = 11 HCO3 and ALK given

flag = 12 HCO3 and DIC given

flag = 13 CO3 and ALK given

flag = 14 CO3 and DIC given

flag = 15 ALK and DIC given

flag = 21 pCO2 and pH given

flag = 22 pCO2 and HCO3 given

	flag = 23 pCO2 and CO3 given
	flag = 24 pCO2 and ALK given
	flag = 25 pCO2 and DIC given
var1	Value of the first variable in mol/kg except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg except for pH
pCO2s	Partial pressure of the high CO2 component in μatm
wf	Weight fraction of the high CO2 seawater per kg seawater
S	Salinity
T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

comment	The initial or final state water
S	Salinity
T	Temperature in degrees Celsius
P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure (μatm)
fCO2	fCO2, CO2 fugacity (μatm)

HCO3	HCO3 concentration (mol/kg)
CO3	CO3 concentration (mol/kg)
DIC	DIC concentration (mol/kg)
ALK	ALK, total alkalinity (mol/kg)
OmegaAragonite	Omega aragonite, aragonite saturation state
OmegaCalcite	Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

Jean-Pierre Gattuso and Heloise Lavigne<gattuso@obs-vlfr.fr>

References

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Examples

```
pmix(flag=24, var1=384, var2=2302e-6, pCO2s=1e6, wf=0.003, S=34.3,
T=16, P=0, pHscale="T", kf="pf", k1k2="l", ks="d", b="u74")
```

---

ppH	*ppH*

Description

Calculates the carbonate chemistry after pH manipulations through addition of acid or base

Usage

```
ppH(flag, sys, var1, var2, pCO2a, vol, N, S=35, T=20, P=0, Pt=0,
Sit=0, pHscale="T", k1k2="x", kf="x", ks="d")
```

Arguments

flag   Select the couple of variables available. The flags which can be used are:

flag = 1 pH and CO2 given

flag = 2 CO2 and HCO3 given

flag = 3 CO2 and CO3 given

flag = 4 CO2 and ALK given

flag = 5 CO2 and DIC given

flag = 6 pH and HCO3 given

flag = 7 pH and CO3 given

flag = 8 pH and ALK given

flag = 9 pH and DIC given

flag = 10 HCO3 and CO3 given

flag = 11 HCO3 and ALK given

flag = 12 HCO3 and DIC given

flag = 13 CO3 and ALK given

flag = 14 CO3 and DIC given

flag = 15 ALK and DIC given

flag = 21 pCO2 and pH given

flag = 22 pCO2 and HCO3 given

flag = 23 pCO2 and CO3 given

flag = 24 pCO2 and ALK given

flag = 25 pCO2 and DIC given

sys	0 if the manipulation is carried out in a system closed to the atmosphere or 1 if its is carried out in a system open to the atmosphere
var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
pCO2a	CO2 partial pressure in the atmosphere pCO2 in μatm. It is only used in systems open to the atmosphere (i.e. when sys=1)
vol	Volume of acid or base added in liter. By convention, it is given a negative sign for acid additions and a positive sign for base additions. The acid must be fortified with NaCl in order to have the same salinity than seawater.
N	Normality of the acid or base in mol/kg
S	Salinity
T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	choice of pH scale: "T" for using the total scale, "F" for using the free scale and "SWS" for using the seawater scale, default is total scale

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.

- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.

- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.

- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

comment	The initial or final state water
S	Salinity
T	Temperature in degrees Celsius
P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure (μatm)

fCO2	fCO2, CO2 fugacity (μatm)
HCO3	HCO3 concentration (mol/kg)
CO3	CO3 concentration (mol/kg)
DIC	DIC concentration (mol/kg)
ALK	ALK, total alkalinity (mol/kg)
OmegaAragonite	Omega aragonite, aragonite saturation state
OmegaCalcite	Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

Jean-Pierre Gattuso and Heloise Lavigne<gattuso@obs-vlfr.fr>

References

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Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

See Also

buffer.

Examples

```
ppH(flag=24, sys=0, var1=384, var2=2302e-6, pCO2a=384, vol=-12e-3,
N=0.01, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="l", ks="d")

ppH(flag=24, sys=1, var1=384, var2=2302e-6, pCO2a=384, vol=-12e-3,
N=0.01, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="l", ks="d")
```

---

psi	*Molar ratio of CO2 released vs CaCO3 precipitated*

Description

Returns the molar ratio of CO2 released vs CaCO3 precipitated described by Frankignoulle et al. (1994).

Usage

```
psi(flag, var1, var2, S=35, T=20, Patm, P=0, Pt=0, Sit=0, pHscale="T",
kf="x", k1k2="x", ks="d")
```

Arguments

flag   select the couple of variables available. The flags which can be used are:

                         flag = 1 pH and CO2 given

                         flag = 2 CO2 and HCO3 given

                         flag = 3 CO2 and CO3 given

                         flag = 4 CO2 and ALK given

                         flag = 5 CO2 and DIC given

                         flag = 6 pH and HCO3 given

                         flag = 7 pH and CO3 given

                         flag = 8 pH and ALK given

                         flag = 9 pH and DIC given

                         flag = 10 HCO3 and CO3 given

                         flag = 11 HCO3 and ALK given

                         flag = 12 HCO3 and DIC given

                         flag = 13 CO3 and ALK given

                         flag = 14 CO3 and DIC given

                         flag = 15 ALK and DIC given

                         flag = 21 pCO2 and pH given

                         flag = 22 pCO2 and HCO3 given

                         flag = 23 pCO2 and CO3 given

                         flag = 24 pCO2 and ALK given

                         flag = 25 pCO2 and DIC given

var1   enter value of the first variable in mol/kg, except for pH and for pCO2 in μatm

var2	enter value of the second variable in mol/kg, except for pH
S	Salinity
T	Temperature in degrees Celsius
Patm	Surface atmospheric pressure in atm, default is 1 atm
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg; set to 0 if NA
Sit	Concentration of total silicate in mol/kg; set to 0 if NA
pHscale	choice of pH scale: "T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.

- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.

- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.

- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For Kf:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.

- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.

- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

psi   ratio of CO2 released vs CaCO3 precipitated (mol/mol)

Author(s)

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References

Dickson A. G., 1990 Standard potential of the reaction: AgCI(s) + 1/2H2(g) = Ag(s) + HCI(aq), and the standard acidity constant of the ion HSO4 in synthetic sea water from 273.15 to 318.15 K. *Journal of Chemical Thermodynamics* **22**, 113-127.

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Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

See Also

speciation.

Examples

```
## Calculation using the numerical example given in Frankignoulle et al. (1994)
psi(flag=24, var1=350, var2=2400e-6, S=35, T=25, P=0, Pt=0,
Sit=0, pHscale="T", kf="pf", k1k2="l", ks="d")
```

---

pTA   *pTA*

Description

Calculates the carbonate chemistry following addition of CO_3^{2-} or HCO_3^-

Usage

```
pTA(flag, sys=0, var1, var2, pCO2a, co3, hco3, S=35, T=20, P=0,
Pt=0, Sit=0, k1k2="x", kf="x", ks="d", pHscale="T", b="u74")
```

Arguments

flag   select the couple of variables available. The flags which can be used are:

                  flag = 1 pH and CO2 given

                  flag = 2 CO2 and HCO3 given

                  flag = 3 CO2 and CO3 given

                  flag = 4 CO2 and ALK given

                  flag = 5 CO2 and DIC given

                  flag = 6 pH and HCO3 given

                  flag = 7 pH and CO3 given

                  flag = 8 pH and ALK given

                  flag = 9 pH and DIC given

flag = 10 HCO3 and CO3 given

flag = 11 HCO3 and ALK given

flag = 12 HCO3 and DIC given

flag = 13 CO3 and ALK given

flag = 14 CO3 and DIC given

flag = 15 ALK and DIC given

flag = 21 pCO2 and pH given

flag = 22 pCO2 and HCO3 given

flag = 23 pCO2 and CO3 given

flag = 24 pCO2 and ALK given

flag = 25 pCO2 and DIC given

sys	0 if the manipulation is carried out in a system closed to the atmosphere or 1 if its is carried out in a system open to the atmosphere
var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
pCO2a	CO2 partial pressure in the atmosphere pCO2 in μatm. It is only used in systems open to the atmosphere (i.e. when sys=1)
co3	Amount of CO_3^{2-} added in $mol\ kg^{-1}$
hco3	Amount of HCO_3^{2-} added in $mol\ kg^{-1}$
S	Salinity
T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. (2000), "m06" from Millero et al. (2006), "m10" from Millero (2010), "w14" from Waters et al. (2014), and "r" from Roy et al. (1993). "x" is the default flag; the default value is then "l", except if T is outside the range 2 to 35oC and/or S is outside the range 19 to 43. In these cases, the default value is "m10".
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Riley (1979 in Dickson and Goyet, 1994). "x" is the default flag; the default value is then "pf", except if T is outside the range 9 to 33oC and/or S is outside the range 10 to 40. In these cases, the default is "dg".
ks	"d" for using Ks from Dickon (1990), "k" for using Ks from Khoo et al. (1977), default is "d"
pHscale	"T" for the total scale, "F" for the free scale and "SWS" for using the seawater scale, default is "T" (total scale)
b	Concentration of total boron. "l10" for the Lee et al. (2010) formulation or "u74" for the Uppstrom (1974) formulation, default is "u74"

Details

The Lueker et al. (2000) constants for K1 and K2, the Perez and Fraga (1987) constant for Kf and the Dickson (1990) constant for Ks are recommended by Dickson et al. (2007). It is, however, critical to consider that each formulation is only valid for specific ranges of temperature and salinity:

For K1 and K2:

- Roy et al. (1993): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Lueker et al. (2000): S ranging between 19 and 43 and T ranging between 2 and 35oC.
- Millero et al. (2006): S ranging between 0.1 and 50 and T ranging between 1 and 50oC.
- Millero (2010): S ranging between 1 and 50 and T ranging between 0 and 50oC. Millero (2010) provides a K1 and K2 formulation for the seawater, total and free pH scales. Therefore, when this method is used and if P=0, K1 and K2 are computed with the formulation corresponding to the pH scale given in the flag "pHscale".

For K0:

- Perez and Fraga (1987): S ranging between 10 and 40 and T ranging between 9 and 33oC.
- Dickson and Riley (1979 in Dickson and Goyet, 1994): S ranging between 0 and 45 and T ranging between 0 and 45oC.

For Ks:

- Dickson (1990): S ranging between 5 and 45 and T ranging between 0 and 45oC.
- Khoo et al. (1977): S ranging between 20 and 45 and T ranging between 5 and 40oC.

The arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It is recommended to use either vectors with the same dimension or one vector for one argument and numbers for the other arguments.

Pressure corrections and pH scale:

- For K0, the pressure correction term of Weiss (1974) is used.
- For K1, K2, pK1, pK2, pK3, Kw, Kb, Khs and Ksi, the pressure correction was applied on the seawater scale. Hence, if needed, values were first transformed from the total scale to the seawater scale, the pressure correction applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kf, the pressure correction was applied on the free scale. The formulation of Dickson and Riley (1979 in Dickson and Goyet, 1994) provides Kf on the free scale but that of Perez and Fraga (1987) provides it on the total scale. Hence, in that case, Kf was first transformed from the total scale to the free scale. With both formulations, the pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Ks, the pressure correction was applied on the free scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).
- For Kn, The pressure correction was applied on the seawater scale. The pressure correction was applied as described by Millero (1995), and the value was transformed back to the required scale (T, F or SWS).

Value

The function returns a data frame containing the following columns:

comment	The initial or final state water
S	Salinity
T	Temperature in degrees Celsius
P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure (μatm)
fCO2	fCO2, CO2 fugacity (μatm)
HCO3	HCO3 concentration (mol/kg)
CO3	CO3 concentration (mol/kg)
DIC	DIC concentration (mol/kg)
ALK	ALK, total alkalinity (mol/kg)
OmegaAragonite	Omega aragonite, aragonite saturation state
OmegaCalcite	Omega calcite, calcite saturation state

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

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Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

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Orr J. C., Epitalon J.-M. and Gattuso J.-P., 2014. Comparison of seven packages that compute ocean carbonate chemistry. *Biogeosciences Discussions* **11**, 5327-5397.

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Waters, J., Millero, F. J., and Woosley, R. J., 2014. Corrigendum to "The free proton concentration scale for seawater pH", [MARCHE: 149 (2013) 8-22], Mar. Chem. 165, 66-67.

Weiss, R. F., 1974. Carbon dioxide in water and seawater: the solubility of a non-ideal gas, *Mar. Chem.*, **2**, 203-215.

Examples

```
pTA(flag=24, sys=0, var1=384, var2=2302e-6, pCO2a=384, co3=260e-6,
hco3=1000e-6, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="l", ks="d", b="u74")

pTA(flag=24, sys=1, var1=384, var2=2302e-6, pCO2a=384, co3=260e-6,
hco3=1000e-6, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="l", ks="d", b="u74")
```

---

rho   *Density of seawater (kg/m3)*

Description

Calculates the density of seawater ($kg\ m^{-3}$)

Usage

```
rho(S = 35, T = 25, P = 0)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0), default is 0

Value

rho   Density of seawater (kg/m3)

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References

Millero F. J. and Poisson A., 1981 International one-atmosphere equation of state of seawater. *Deep-Sea Research* **28A**, 625-629.

Examples

rho(35,25,0)

---

seacarb_test_P0   *Test data file (at P=0) to test the use of the carb function*

Description

The variables are:

- Flag indicating which couple of variables is used
- Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
- Value of the second variable in mol/kg, except for pH
- Salinity
- Temperature in degrees Celsius
- Hydrostatic pressure in bar (surface = 0)
- Value of the concentration of total phosphate in mol/kg
- Value of the total silicate in mol/kg

Usage

seacarb_test_P0

Format

A data frame with 20 rows and 8 variables

Source

None, these data were invented for this purpose. The input variables were chosen in order to check that the carbonate chemistry is identical for all flags.

---

seacarb_test_P300   *Test data file (at P=300) to test the use of the carb function*

Description

The variables are:

- Flag indicating which couple of variables is used
- Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
- Value of the second variable in mol/kg, except for pH
- Salinity
- Temperature in degrees Celsius
- Hydrostatic pressure in bar (P=300)
- Value of the concentration of total phosphate in mol/kg
- Value of the total silicate in mol/kg

Usage

```
seacarb_test_P300
```

Format

A data frame with 20 rows and 8 variables

Source

None, these data were invented for this purpose. The input variables were chosen in order to check that the carbonate chemistry is identical for all flags.

---

speciation   *ionic forms as a function of pH*

Description

Estimates the concentration of the various ionic forms of a molecule as a function of pH

Usage

```
speciation(K1=K1(), K2=NULL, K3=NULL, pH, conc=1)
```

Arguments

K1	First dissociation constant
K2	Second dissociation constant, default is NULL
K3	Third dissociation constant, default is NULL
pH	pH value, default is 8
conc	concentration of molecule in mol/kg, default is 1 mol/kg

Value

The function returns a data frame containing the following concentrations (in mol/kg if conc is given in mol/kg):

C1	ionic form 1, univalent, bivalent and trivalent molecules
C2	ionic form 2, univalent, bivalent and trivalent molecules
C3	ionic form 3, bivalent and trivalent molecules
C4	ionic form 4, trivalent molecules

Author(s)

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References

Zeebe R. E. and Wolf-Gladrow D. A., 2001 *CO2 in seawater: equilibrium, kinetics, isotopes.* Amsterdam: Elsevier, 346 pp.

See Also

bjerrum.

Examples

```
## Speciation of divalent species; example to estimate the various ionic forms
## of dissolved inorganic carbon  (DIC = 0.0021 mol/kg) at a salinity of 35,
## a temperature of 25oC and an hydrostatic pressure of 0:
spec <- speciation (K1(35, 25, 0), K2(35, 25, 0), pH=8, conc=0.0021)
## where (spec$C1=[CO2], spec$C2=[HCO3-], spec$C3=[CO3--])

## Speciation of trivalent species (e.g.,  H3PO4, H2PO4-, HPO4--, PO4---)
speciation(K1p(), K2p(), K3p(), conc=0.001)

## Effect of temperature on pCO2 - Figure 1.4.18 of Zeebe and Wolf-Gladrow (2001)
Tseq <- seq(0, 30, by=0.5)
pHseq <- carb(flag=15, var1=2300e-6, var2=1900e-6, S=35, T=Tseq, P=0)$pH
CO2  <- speciation(K1(T=Tseq), K2(T=Tseq), conc=1900, pH=pHseq)$C1
pCO2 <- CO2/K0(T=Tseq)
plot(Tseq, pCO2, xlab="Temperature (oC)", ylab="pCO2 (uatm)", type="l",
main="effect of temperature on pCO2")
legend("topleft", c(expression(sum(CO[2])==1900~umol~kg^"-1"),
expression(TA==2300~umol~kg^"-1")))
```

theta   *Potential temperature of seawater*

Description

Computes theta, the potential temperature of seawater given original temperature, salinity, pressure, and reference pressure

Usage

```
theta(S=35, T=25, P=0, Pref=0)
```

Arguments

S	Salinity on the practical salinity scale, default is 35
T	Temperature in degrees Celsius, default is 25oC
P	Hydrostatic pressure in bar (surface = 0; 1000 db = 100 bar), default is 0
Pref	Reference hydrostatic pressure in bar, default is 0

Details

Computes the potential temperature of seawater relative to a chosen reference pressure following Fofonoff and Millard (1983). The potential temperature θ is the temperature that a water parcel would have if were moved adiabatically to another pressure level Pref. Typically, the potential temperature is referenced to the surface ($Pref = 0$). The potential teperature depends on the original salinity S, *in-situ* temperature T and pressure P.

This routine is essentially a wrapper for the [swTheta](#) routine of the 'oce' package. Unlike the latter, pressure units here are given in bars and method="unesco" is prescribed.

Value

theta	potential temperature of seawater (C)

Author(s)

James Orr <james.orr@lsce.ipsl.fr>

References

Fofonoff, P. and R. C. Millard Jr, 1983. Algorithms for computation of fundamental properties of seawater. *Unesco Technical Papers in Marine Science*, **44**, 53 pp.

See Also

[swTheta](#).

Examples

```
#Calculate the potential temperature for a sample at 1000 db referenced to the surface
theta <- theta(S=35, T=25, P=100, Pref=0)
```

---

tris	*pH value of the TRIS buffer*

Description

pH value of the TRIS buffer (on the total scale in mol/kg)

Usage

```
tris(S=35,T=25)
```

Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25oC

Details

Note that the arguments can be given as a unique number or as vectors. If the lengths of the vectors are different, the longer vector is retained and only the first value of the other vectors is used. It can therefore be critical to use vectors of the same length.

Value

tris	pH value of the TRIS buffer (on the total scale in mol/kg)

Author(s)

Jean-Pierre Gattuso <gattuso@obs-vlfr.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

See Also

[amp](), [pHslope](), [pH]().

Examples

```
##Example from Dickson et al. (2007)
tris(S=35,T=25)
```

---

vapress   *Computes vapor pressure of seawater*

Description

Computes vapor pressure of seawater (atm) from temperature and salinity

Usage

```
vapress(S=35, T=25, form="d2007")
```

Arguments

S	Salinity on the practical salinity scale, default is 35
T	Temperature in degrees Celsius, default is 25oC
form	choose either "d2007" for the best-practices formulation to compute vapor pressure of seawater from Dickson et al. (2007) or "wp1980" for the formulation from weiss and Price (1980).

Details

Computes the vapor pressure of seawater pH20 following best practices (Dickson et al., 2007). That computed pH20 is identical, when rounded to the 4th decimal place, with that computed by the equation from Weiss and Price (1980).

Value

vapress	Vapor pressure of seawater in atm

Author(s)

James Orr <james.orr@lsce.ipsl.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R. (2007) Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Weiss, R. F. (1974) Carbon dioxide in water and seawater: the solubility of a non-ideal gas, Mar. Chem., **2**, 203-215.

Weiss, R. F. and Price, B. A. (1980) Nitrous oxide solubility in water and seawater, Mar. Chem., **8**, 347-359.

See Also

x2pCO2, and p2xCO2.

Examples

```
pH20 <- vapress(S=35, T=25, form="d2007")
```

---

x2pCO2   *Converts mole fraction to partial pressure of CO2*

Description

Converts xCO2 (mole fraction of CO2) into pCO2 (partial pressure of CO2)

Usage

```
x2pCO2(S=35, T=25, Patm=1.0, xCO2=400)
```

Arguments

S	Salinity on the practical salinity scale, default is 35
T	Temperature in degrees Celsius, default is 25oC
Patm	Atmospheric pressure in atmospheres, default is 1.0
xCO2	Mole fraction of CO2 in ppm, default is 400

Details

The mole fraction xCO2 (ppm) is computed from pCO2 (μatm) using the following equation: $pCO2 = xCO2(Patm - pH2O)$, where pH20 is the vapor pressure of seawater computed following best practices (Dickson et al., 2007). That computed pH20 is identical, when rounded to the 4th decimal place, with that computed by the equation from Weiss and Price (1980).

Value

pCO2	Partial pressure of CO2 in μatm.

Note

Warning: pCO2 estimates below 100 m are subject to considerable uncertainty. See Weiss (1974) and Orr et al. (2014)

Author(s)

James Orr <james.orr@lsce.ipsl.fr>

References

Dickson A. G., Sabine C. L. and Christian J. R., 2007 Guide to best practices for ocean CO2 measurements. *PICES Special Publication* **3**, 1-191.

Orr J. C., Epitalon J.-M. and Gattuso J.-P., 2014. Comparison of seven packages that compute ocean carbonate chemistry. *Biogeosciences Discussions* **11**, 5327-5397.

Weiss, R. F. (1974) Carbon dioxide in water and seawater: the solubility of a non-ideal gas, Mar. Chem., **2**, 203-215.

Weiss, R. F. and Price, B. A. (1980) Nitrous oxide solubility in water and seawater, Mar. Chem., **8**, 347-359.

See Also

p2xCO2 and vapress

Examples

```
## Atmospheric pressure is rarely equal to 1 atm exactly
## Over the Southern Ocean Patm=0.97 is more realistic
   pCO2_socn <- x2pCO2(S=35, T=0, Patm=0.97, xCO2=400.0)
   print(pCO2_socn)
## The result (385.6322 uatm) is 12 uatm less than if it was wrongly assumed that Patm=1.0

## Show effect of temperature on pCO2 computed from xCO2, and on resulting variables from "carb"
S <- 35
ALK <- 2300e-6
T <- seq(0,30,5)
xCO2 <- 400
pCO2 <- x2pCO2(S=35, T=T, Patm=1, xCO2=400)
results <- carb(flag=24, var1=pCO2, var2=ALK, S=S, T=T, P=0, Pt=0, Sit=0,
  pHscale="T", kf="pf", k1k2="l", ks="d", b="u74")
print(results)
```

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