

# Package ‘seacarb’

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**Description** Calculates parameters of the seawater carbonate system and assists the design of ocean acidification perturbation experiments.  
Code and/or corrections were contributed by Andreas Andersson, Bernard Gentili, Andreas Hofmann, Jim Orr, Aurelien Proye and Karline Soetaert and James Rae

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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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 <a href="#">par</a> ) and any further arguments of plot, typically <a href="#">plot.default</a> , may also be supplied as arguments to this function. Hence, the high-level graphics control arguments described under <a href="#">par</a> and the arguments to <a href="#">title</a> 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 *CO<sub>2</sub> 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]~P0[4]),
expression(H[2]~P0[4]^"-"),
expression(HPO[4]^"2-"),expression(P0[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	<i>Total boron concentration (mol/kg)</i>
-----	---

---

### Description

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

### 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 "l10"

### Value

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

**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 Atlantic 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, "110")
```

---

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, P=0, Pt=0, Sit=0, k1k2="x",
kf="x", ks="d", pHscale="T", b="110")
```

**Arguments**

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

flag = 1 pH and CO<sub>2</sub> given

flag = 2 CO<sub>2</sub> and HCO<sub>3</sub> given

flag = 3 CO<sub>2</sub> and CO<sub>3</sub> given

flag = 4 CO<sub>2</sub> and ALK given

flag = 5 CO<sub>2</sub> and DIC given

flag = 6 pH and HCO<sub>3</sub> given

flag = 7 pH and CO<sub>3</sub> given

flag = 8 pH and ALK given

flag = 9 pH and DIC given

flag = 10 HCO<sub>3</sub> and CO<sub>3</sub> given

flag = 11 HCO<sub>3</sub> and ALK given

flag = 12 HCO<sub>3</sub> and DIC given



	flag = 13 CO <sub>3</sub> and ALK given
	flag = 14 CO <sub>3</sub> and DIC given
	flag = 15 ALK and DIC given
	flag = 21 pCO <sub>2</sub> and pH given
	flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given
	flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given
	flag = 24 pCO <sub>2</sub> and ALK given
	flag = 25 pCO <sub>2</sub> and DIC given
var1	enter value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu$ atm
var2	enter value of the second variable in mol/kg, except for pH
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) 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), "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 "l10"

### 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 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 CO2 ( $\mu atm$ 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 CO2 ( $\mu\text{atm}$ 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 ( $\mu\text{atm}$ 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 ( $\mu\text{atm}$ 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:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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 40°C: 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.
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- 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 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.

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, P=0, Pt=0,
Sit=0, pHscale="T", kf="pf", k1k2="1", b="110")

## 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("1", "1", "1")
pHscale <- c("T", "T", "T")
b <- c("110", "110", "110")
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	<i>Buffer capacities of the seawater carbonate system as defined by Egleston et al. (2010)</i>
---------	--

---

### 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 pCO<sub>2</sub> over that for DIC). In ESM, there are errors in the equations in Table 1 for  $S$ ,  $\Omega_{DIC}$ , and  $\Omega_{Alk}$ . 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 identical to those in the "buffer" and "carb" functions of seacarb.

### Usage

```
buffesm(flag, var1, var2, S=35, T=25, P=0, Pt=0, Sit=0, k1k2="x",
kf="x", ks="d", pHscale="T", b="110")
```

### Arguments

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO <sub>2</sub> given flag = 2 CO <sub>2</sub> and HCO <sub>3</sub> given flag = 3 CO <sub>2</sub> and CO <sub>3</sub> given flag = 4 CO <sub>2</sub> and ALK given flag = 5 CO <sub>2</sub> and DIC given flag = 6 pH and HCO <sub>3</sub> given flag = 7 pH and CO <sub>3</sub> given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO <sub>3</sub> and CO <sub>3</sub> given flag = 11 HCO <sub>3</sub> and ALK given flag = 12 HCO <sub>3</sub> and DIC given flag = 13 CO <sub>3</sub> and ALK given flag = 14 CO <sub>3</sub> and DIC given flag = 15 ALK and DIC given flag = 21 pCO <sub>2</sub> and pH given flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given flag = 24 pCO <sub>2</sub> and ALK given flag = 25 pCO <sub>2</sub> and DIC given
var1	enter value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu\text{atm}$

var2	enter value of the second variable in mol/kg, except for pH
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) 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), "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 "l10"

## 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 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	$\gamma_{DIC}$ , ocean's capacity to buffer changes in [CO <sub>2</sub> ] due to accumulation of CO <sub>2</sub> 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	$\beta_{DIC}$ , ocean's capacity to buffer changes in [H <sup>+</sup> ] due to accumulation of CO <sub>2</sub> from the atmosphere $(\partial \ln[H^+]/\partial DIC)^{-1}$ (units = mol/kg)
omegaDIC	$\Omega_{DIC}$ , ocean's capacity to buffer changes in [CO <sub>3</sub> <sup>2-</sup> ] due to accumulation of CO <sub>2</sub> 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	$\gamma_{ALK}$ , ocean's capacity to buffer changes in [CO <sub>2</sub> ] due to changes in alkalinity $(\partial \ln[CO_2]/\partial ALK)^{-1}$ (units = mol/kg)
betaALK	$\beta_{ALK}$ , ocean's capacity to buffer changes in [H <sup>+</sup> ] due to changes in alkalinity $(\partial \ln[H^+]/\partial ALK)^{-1}$ (units = mol/kg)
omegaALK	$\Omega_{ALK}$ , ocean's capacity to buffer changes in [CO <sub>3</sub> <sup>2-</sup> ] 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 <sub>2</sub> ] or pCO <sub>2</sub> over the relative change in DIC $(\partial \ln[CO_2]/\partial \ln DIC)^{-1}$ (unitless)

**Author(s)**

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

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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="1", b="110")
```

```
## 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("1", "1", "1")
pHscale <- c("T", "T", "T")
b <- c("110", "110", "110")
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, P=0, Pt=0, Sit=0,
k1k2="x", kf="x", ks="d", pHscale="T", b="110")
```

**Arguments**

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO <sub>2</sub> given flag = 2 CO <sub>2</sub> and HCO <sub>3</sub> given flag = 3 CO <sub>2</sub> and CO <sub>3</sub> given flag = 4 CO <sub>2</sub> and ALK given flag = 5 CO <sub>2</sub> and DIC given flag = 6 pH and HCO <sub>3</sub> given flag = 7 pH and CO <sub>3</sub> given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO <sub>3</sub> and CO <sub>3</sub> given flag = 11 HCO <sub>3</sub> and ALK given flag = 12 HCO <sub>3</sub> and DIC given flag = 13 CO <sub>3</sub> and ALK given flag = 14 CO <sub>3</sub> and DIC given flag = 15 ALK and DIC given flag = 21 pCO <sub>2</sub> and pH given flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given flag = 24 pCO <sub>2</sub> and ALK given flag = 25 pCO <sub>2</sub> and DIC given
var1	Value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu$ atm
var2	Value of the second variable in mol/kg, except for pH
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) 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	"110" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "110"

## 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 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
P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )
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

**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.
- Khoo H. K., Ramette R. W., Culbertson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40°C: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **22**, vol49 29-34.
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Perez F. F. and Fraga F., 1987 Association constant of fluoride and hydrogen ions in seawater. *Marine Chemistry* **21**, 161-168.

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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, Pt=0, Sit=0,
pHscale="T", kf="pf", k1k2="1", ks="d", b="110")

## 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("1", "1", "1")
pHscale <- c("T", "T", "T")
b <- c("110", "110", "110")
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

## 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)

```

---

carbex	<i>Parameters of the seawater carbonate system [EXPERIMENTAL VERSION]</i>
--------	---

---

### Description

Returns parameters of the seawater carbonate system. [THIS IS AN EXPERIMENTAL VERSION, USE carb INSTEAD]

### Usage

```
carbex(flag, var1, var2, S=35, T=25, P=0, Pt=0, Sit=0,
       k1k2="x", kf="x", ks="d", pHscale="T", b="110")
```

### Arguments

flag	select the couple of variables available. The flags which can be used are:
	flag = 1 pH and CO <sub>2</sub> given
	flag = 2 CO <sub>2</sub> and HCO <sub>3</sub> given
	flag = 3 CO <sub>2</sub> and CO <sub>3</sub> given
	flag = 4 CO <sub>2</sub> and ALK given
	flag = 5 CO <sub>2</sub> and DIC given
	flag = 6 pH and HCO <sub>3</sub> given
	flag = 7 pH and CO <sub>3</sub> given
	flag = 8 pH and ALK given
	flag = 9 pH and DIC given
	flag = 10 HCO <sub>3</sub> and CO <sub>3</sub> given
	flag = 11 HCO <sub>3</sub> and ALK given
	flag = 12 HCO <sub>3</sub> and DIC given
	flag = 13 CO <sub>3</sub> and ALK given
	flag = 14 CO <sub>3</sub> and DIC given
	flag = 15 ALK and DIC given
	flag = 21 pCO <sub>2</sub> and pH given

	flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given
	flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given
	flag = 24 pCO <sub>2</sub> and ALK given
	flag = 25 pCO <sub>2</sub> and DIC given
var1	Value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu$ atm
var2	Value of the second variable in mol/kg, except for pH
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) 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	"l10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "l10"

## 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 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
P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )
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



**Author(s)**

Heloise Lavigne 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., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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  $\text{CO}_2$  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 40°C: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **22**, vol49 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 Atlantic oceans. *Geochimica et Cosmochimica Acta* **74** 1801-1811.
- Lueker T. J., Dickson A. G. and Keeling C. D., 2000 Ocean  $\text{pCO}_2$  calculated from dissolved inorganic carbon, alkalinity, and equations for  $K_1$  and  $K_2$ : validation based on laboratory measurements of  $\text{CO}_2$  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., 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 45°C. *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.
- Zeebe R. E. and Wolf-Gladrow D. A., 2001 *CO<sub>2</sub> in seawater: equilibrium, kinetics, isotopes*. Amsterdam: Elsevier, 346 pp.

**Examples**

```
## With a couple of variables
carbex(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Pt=0, Sit=0,
pHscale="T", kf="pf", k1k2="1", ks="d", b="110")
```

```

## 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("1", "1", "1")
pHscale <- c("T", "T", "T")
b <- c("110", "110", "110")
carbex(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)
carbex(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

## method 1 using the column numbers
carbex(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
carbex(flag=tab$flag, var1=tab$var1, var2=tab$var2, S=tab$S, T=tab$T, P=tab$P,
Sit=tab$Sit, Pt=tab$Pt)

```

---

carbm

*Parameters of the seawater carbonate system, in case of artificial addition of boron*

---

## Description

Returns parameters of the seawater carbonate system, in case of artificial addition of boron in seawater.

**Usage**

```
carbm(flag, var1, var2, badd=0, S=35, T=25, P=0, Pt=0, Sit=0,
k1k2="x", kf="x", ks="d", pHscale="T", b="110")
```

**Arguments**

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO <sub>2</sub> given flag = 2 CO <sub>2</sub> and HCO <sub>3</sub> given flag = 3 CO <sub>2</sub> and CO <sub>3</sub> given flag = 4 CO <sub>2</sub> and ALK given flag = 5 CO <sub>2</sub> and DIC given flag = 6 pH and HCO <sub>3</sub> given flag = 7 pH and CO <sub>3</sub> given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO <sub>3</sub> and CO <sub>3</sub> given flag = 11 HCO <sub>3</sub> and ALK given flag = 12 HCO <sub>3</sub> and DIC given flag = 13 CO <sub>3</sub> and ALK given flag = 14 CO <sub>3</sub> and DIC given flag = 15 ALK and DIC given flag = 21 pCO <sub>2</sub> and pH given flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given flag = 24 pCO <sub>2</sub> and ALK given flag = 25 pCO <sub>2</sub> and DIC given
var1	Value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu$ atm
var2	Value of the second variable in mol/kg, except for pH
badd	Quantity of boron added in seawater in mol/kg, default is 0
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) 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 35°C 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	"I10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "I10"

### 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 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
P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )
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

### Author(s)

Heloise Lavigne 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., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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 40°C: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **22**, vol49 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 Atlantic oceans. *Geochimica et Cosmochimica Acta* **74** 1801-1811.

Lueker T. J., Dickson A. G. and Keeling C. D., 2000 Ocean pCO<sub>2</sub> calculated from dissolved inorganic carbon, alkalinity, and equations for K<sub>1</sub> and K<sub>2</sub>: validation based on laboratory measurements of CO<sub>2</sub> 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., 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 45°C. *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.

Zeebe R. E. and Wolf-Gladrow D. A., 2001 *CO<sub>2</sub> in seawater: equilibrium, kinetics, isotopes*. Amsterdam: Elsevier, 346 pp.

## Examples

```
## With a couple of variables
carbm(flag=8, var1=8.7, var2=0.002571, S=38, T=21, P=0, Pt=0, Sit=0, pHscale="T",
      kf="pf", k1k2="1", ks="d", badd=0.003)
```

---

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, fCO2)
```

**Arguments**

T                    Temperature in degrees Celsius, default is 25oC  
 fCO2                Fugacity of CO2 in  $\mu\text{atm}$

**Value**

pCO2                Partial pressure of CO2 in  $\mu\text{atm}$ .

**Author(s)**

Heloise Lavigne 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 CO<sub>2</sub> measurements. *PICES Special Publication 3*, 1-191.

**See Also**

[p2fCO2](#).

**Examples**

f2pCO2(T=25, fCO2=380)

---

K0	<i>Henry's constant mol/(kg/atm)</i>
----	--------------------------------------

---

**Description**

Henry's constant mol/(kg/atm)

**Usage**

K0(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 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 and 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

$K_0(S=35, T=25, P=0)$

---

K1	<i>First dissociation constant of carbonic acid (mol/kg)</i>
----	--

---

## Description

First dissociation constant of carbonic acid (mol/kg)

## Usage

$K1(S = 35, T = 25, P = 0, k1k2="x", pHscale="T", kSWS2scale=0, ktotalsWS_P0=0)$

## 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) 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" and the hydrostatic pressure is 0. If it is required and not given, it is computed, which slows down computations.
ktotalsWS_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 CO<sub>2</sub> 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".

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 CO<sub>2</sub> 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 pCO<sub>2</sub> calculated from dissolved inorganic carbon, alkalinity, and equations for K1 and K2: validation based on laboratory measurements of CO<sub>2</sub> 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.

### See Also

[K2](#).

### Examples

```
K1(S=35,T=25,P=0,k1k2="1",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 CO<sub>2</sub> 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, ktotalsWS\_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) 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" 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 CO<sub>2</sub> 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".

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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 pCO<sub>2</sub> calculated from dissolved inorganic carbon, alkalinity, and equations for K<sub>1</sub> and K<sub>2</sub>: validation based on laboratory measurements of CO<sub>2</sub> 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.

### 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 CO<sub>2</sub> 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)





## 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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 CO<sub>2</sub> 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")
```







## References

Dickson A. G., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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  $\text{CO}_2$  measurements. *PICES Special Publication* **3**, 1-191.

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

## Examples

$\text{Ks}(\text{S}=35, \text{T}=25, \text{P}=0, \text{ks}=\text{"d"})$

---

Ksi *Dissociation constant of Si(OH)<sub>4</sub>*

---

## Description

Dissociation constant of  $\text{Si(OH)}_4$  on total scale (mol/kg)

## Usage

$\text{Ksi}(\text{S}=35, \text{T}=25, \text{P}=0, \text{pHscale}=\text{"T"}, \text{kSWS2scale}=0)$

## Arguments

S	Salinity, default is 35
T	Temperature in degrees Celsius, default is 25°C
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 45°C.

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)<sub>4</sub> (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	<i>Solubility product of aragonite (mol/kg)</i>
------	---

---

**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 (mol<sup>2</sup>/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	<i>Solubility product of calcite (mol/kg)</i>
------	---

---

**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 (mol<sup>2</sup>/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	<i>Ion product of water (mol<sup>2</sup>/kg<sup>2</sup>)</i>
----	--

---

**Description**

Ion product of water (mol<sup>2</sup>/kg<sup>2</sup>)

**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 (mol<sup>2</sup>/kg<sup>2</sup>)

**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 CO<sub>2</sub> 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="110")
```

**Arguments**

flag	<p>select the couple of variables available to describe the initial seawater. The flags which can be used are:</p> <p>flag = 1 pH and CO<sub>2</sub> given</p> <p>flag = 2 CO<sub>2</sub> and HCO<sub>3</sub> given</p> <p>flag = 3 CO<sub>2</sub> and CO<sub>3</sub> given</p> <p>flag = 4 CO<sub>2</sub> and ALK given</p> <p>flag = 5 CO<sub>2</sub> and DIC given</p> <p>flag = 6 pH and HCO<sub>3</sub> given</p> <p>flag = 7 pH and CO<sub>3</sub> given</p> <p>flag = 8 pH and ALK given</p> <p>flag = 9 pH and DIC given</p> <p>flag = 10 HCO<sub>3</sub> and CO<sub>3</sub> given</p> <p>flag = 11 HCO<sub>3</sub> and ALK given</p> <p>flag = 12 HCO<sub>3</sub> and DIC given</p> <p>flag = 13 CO<sub>3</sub> and ALK given</p> <p>flag = 14 CO<sub>3</sub> and DIC given</p> <p>flag = 15 ALK and DIC given</p> <p>flag = 21 pCO<sub>2</sub> and pH given</p> <p>flag = 22 pCO<sub>2</sub> and HCO<sub>3</sub> given</p> <p>flag = 23 pCO<sub>2</sub> and CO<sub>3</sub> given</p> <p>flag = 24 pCO<sub>2</sub> and ALK given</p> <p>flag = 25 pCO<sub>2</sub> and DIC given</p>
var1	Value of the first variable available to describe the initial seawater, in mol/kg except for pH and for pCO <sub>2</sub> in uatm
var2	Value of the second variable available to describe the initial seawater, in mol/kg except for pH
pCO2f	pCO <sub>2</sub> target value, in uatm
pCO2s	pCO <sub>2s</sub> is the pCO <sub>2</sub> , in uatm, of the "high-CO <sub>2</sub> " seawater that will be mixed with "normal seawater". The default value is 10 <sup>6</sup> uatm, that is seawater bubbled with pure CO <sub>2</sub> gas and saturated with CO <sub>2</sub> .
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) 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 35°C 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), "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 pCO <sub>2</sub> isoclines are drawn in the back. Default is false.
b	"I10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "I10"

### 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 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 pCO <sub>2</sub> . Note that if a vector is given in argument only the first value is used.
perturbation	Table providing key parameters for the following methods: <i>CO<sub>2</sub> bubbling</i> : high-CO <sub>2</sub> air is bubbled in seawater. The first parameter is the value of the pCO <sub>2</sub> in the air required to bubble the seawater (in uatm). <i>SW mixing</i> : mixing of “normal” and “high-CO <sub>2</sub> ” seawater. The first parameter, “Weight fraction high-CO <sub>2</sub> SW” or wf, is the weight fraction of the high-CO <sub>2</sub> seawater per kg seawater. <i>Addition of acid</i> : 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 <sup>+</sup> (mol/kg), is the amount of H <sup>+</sup> that must be added (mol/kg). The acid must be fortified with NaCl in order to have the same salinity than seawater. <i>Addition of HCO<sub>3</sub> and acid</i> : bicarbonate (HCO <sub>3</sub> ) and a strong acid are added. The first parameter, HCO <sub>3</sub> , is the amount of HCO <sub>3</sub> that must be added (mol/kg). The second parameter, H <sup>+</sup> , is the quantity of H <sup>+</sup> that must be added (mol/kg). The acid must be fortified with NaCl in order to have the same salinity than seawater. <i>Addition of CO<sub>3</sub> and acid</i> : carbonate, CO <sub>3</sub> , and a strong acid are added. The first parameter, HCO <sub>3</sub> , is the quantity of CO <sub>3</sub> that must be added (mol/kg). The second parameter, H <sup>+</sup> , is the quantity of H <sup>+</sup> that must be added (mol/kg).
summary	Table summarizing the carbonate chemistry before and after applying each perturbation: pCO <sub>2</sub> bubbling, mixing with high-CO <sub>2</sub> 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:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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  $\text{CO}_2$  measurements. *PICES Special Publication* **3**, 1-191.
- Khoo H. K., Ramette R. W., Culbertson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40°C: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **49**, 29-34.
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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 45°C. *Marine Chemistry* **44**, 249-267.
- Schulz K. G., Barcelos e Ramos J., Zeebe R. E. and Riebesell U., 2009  $\text{CO}_2$  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.
- Zeebe R. E. and Wolf-Gladrow D. A., 2001  *$\text{CO}_2$  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="1", ks="d", plot=TRUE, b="110")
```

---

 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="110")
```

**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 CO <sub>2</sub> given flag = 2 CO <sub>2</sub> and HCO <sub>3</sub> given flag = 3 CO <sub>2</sub> and CO <sub>3</sub> given flag = 4 CO <sub>2</sub> and ALK given flag = 5 CO <sub>2</sub> and DIC given flag = 6 pH and HCO <sub>3</sub> given flag = 7 pH and CO <sub>3</sub> given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO <sub>3</sub> and CO <sub>3</sub> given flag = 11 HCO <sub>3</sub> and ALK given flag = 12 HCO <sub>3</sub> and DIC given flag = 13 CO <sub>3</sub> and ALK given flag = 14 CO <sub>3</sub> and DIC given flag = 15 ALK and DIC given flag = 21 pCO <sub>2</sub> and pH given flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given flag = 24 pCO <sub>2</sub> and ALK given flag = 25 pCO <sub>2</sub> and DIC given

var1	Value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu\text{atm}$
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) 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 35°C 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 33°C 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	"l10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "l10"

### 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,  $\gamma_T$ , which has been determined experimentally or from theory (e.g. Millero & Pierrot 1998): {a}= $\gamma_T$ [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 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 pCO<sub>2</sub> 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="110")
```

---

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, pCO2)
```

**Arguments**

T	Temperature in degrees Celsius, default is 25oC
pCO2	Partial pressure in CO2, the unit given here define the unit of fugacity in output

**Value**

fCO2	Fugacity of CO2, given in the same unit than pCO2, entered in argument.
------	---

**Author(s)**

Heloise Lavigne 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.

**See Also**

[f2pCO2](#).

**Examples**

```
p2fCO2(T=25, pCO2=380)
```

---

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="110")
```

**Arguments**

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO <sub>2</sub> given flag = 2 CO <sub>2</sub> and HCO <sub>3</sub> given flag = 3 CO <sub>2</sub> and CO <sub>3</sub> given flag = 4 CO <sub>2</sub> and ALK given flag = 5 CO <sub>2</sub> and DIC given flag = 6 pH and HCO <sub>3</sub> given flag = 7 pH and CO <sub>3</sub> given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO <sub>3</sub> and CO <sub>3</sub> given flag = 11 HCO <sub>3</sub> and ALK given flag = 12 HCO <sub>3</sub> and DIC given flag = 13 CO <sub>3</sub> and ALK given flag = 14 CO <sub>3</sub> and DIC given flag = 15 ALK and DIC given flag = 21 pCO <sub>2</sub> and pH given flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given flag = 24 pCO <sub>2</sub> and ALK given flag = 25 pCO <sub>2</sub> and DIC given
var1	Value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu\text{atm}$
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) 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), "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 "l10"

## 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 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 ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )
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

**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:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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  $\text{CO}_2$  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., Culbertson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40°C: 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 Atlantic 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.
- 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

```
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="1", ks="d", b="110") # 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="1", ks="d", b="110") # with 0.5 * Ca concentration
```

---

Pcoeffs

*Coefficients used for pressure-correcting the equilibrium constants*

---

## Description

Pressure corrections are based on the following equations:

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

with

$$\Delta V_i = a_0 + a_1T + a_2T^2$$

and

$$\Delta K_i = b_0 + b_1T + b_2T^2$$

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 Cosmochimica 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, <ul style="list-style-type: none"> <li>• K1 First dissociation constant of carbonic acid (mol/kg)</li> <li>• K2 Second dissociation constant of carbonic acid (mol/kg)</li> <li>• Kb Dissociation constant of boric acid (mol/kg)</li> <li>• Kw Ion product of water (mol<sup>2</sup>/kg<sup>2</sup>)</li> <li>• Ks Stability constant of hydrogen sulfate (mol/kg)</li> <li>• Kf Stability constant of hydrogen fluoride (mol/kg)</li> <li>• Kspc Solubility product of calcite (mol/kg)</li> <li>• Kspa Solubility product of aragonite (mol/kg)</li> <li>• K1p First dissociation constant of phosphoric acid (mol/kg)</li> <li>• K2p Second dissociation constant of phosphoric acid (mol/kg)</li> <li>• K3p Third dissociation constant of phosphoric acid (mol/kg)</li> <li>• Khs Dissociation constant of hydrogen sulfide (mol/kg)</li> <li>• Kn Dissociation constant of ammonium (mol/kg)</li> <li>• Ksi Dissociation constant of Si(OH)<sub>4</sub> (mol/kg)</li> </ul>
T	Temperature in degrees Celsius, default is 25°C
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 K<sub>1</sub>, K<sub>2</sub>, K<sub>1p</sub>, K<sub>2p</sub>, K<sub>3p</sub>, K<sub>b</sub>, K<sub>hs</sub>, K<sub>n</sub>, K<sub>si</sub> and K<sub>w</sub>. 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 K<sub>f</sub>.
- There is no issue of pH scale for K<sub>s</sub>, K<sub>spa</sub> and K<sub>spc</sub>.

**Value**

The equilibrium constant given in argument but after pressure correction

**Author(s)**

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

**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")
```

---

p<sub>gas</sub>

p<sub>gas</sub>

---

**Description**

Calculates the carbonate chemistry after changes in pCO<sub>2</sub> 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="110")
```

**Arguments**

flag	<p>select the couple of variables available. The flags which can be used are:</p> <p>flag = 1 pH and CO<sub>2</sub> given</p> <p>flag = 2 CO<sub>2</sub> and HCO<sub>3</sub> given</p> <p>flag = 3 CO<sub>2</sub> and CO<sub>3</sub> given</p> <p>flag = 4 CO<sub>2</sub> and ALK given</p> <p>flag = 5 CO<sub>2</sub> and DIC given</p> <p>flag = 6 pH and HCO<sub>3</sub> given</p> <p>flag = 7 pH and CO<sub>3</sub> given</p> <p>flag = 8 pH and ALK given</p> <p>flag = 9 pH and DIC given</p> <p>flag = 10 HCO<sub>3</sub> and CO<sub>3</sub> given</p> <p>flag = 11 HCO<sub>3</sub> and ALK given</p> <p>flag = 12 HCO<sub>3</sub> and DIC given</p> <p>flag = 13 CO<sub>3</sub> and ALK given</p> <p>flag = 14 CO<sub>3</sub> and DIC given</p> <p>flag = 15 ALK and DIC given</p> <p>flag = 21 pCO<sub>2</sub> and pH given</p> <p>flag = 22 pCO<sub>2</sub> and HCO<sub>3</sub> given</p> <p>flag = 23 pCO<sub>2</sub> and CO<sub>3</sub> given</p> <p>flag = 24 pCO<sub>2</sub> and ALK given</p> <p>flag = 25 pCO<sub>2</sub> and DIC given</p>
var1	Value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu$ atm
var2	Value of the second variable in mol/kg, except for pH
pCO2g	CO <sub>2</sub> partial pressure of the gas used for bubbling in $\mu$ atm
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) 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 35°C 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 33°C 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), "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	"I10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "I10"

## 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 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 ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )
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

## Author(s)

Jean-Pierre Gattuso and Heloise Lavigne <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., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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 40°C: 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 Atlantic 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.

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

```
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="1", ks="d", b="110")
```

---

pH	<i>Potentiometric pH</i>
----	--------------------------

---

### 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 25°C

### 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 CO<sub>2</sub> 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 CO<sub>2</sub> 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)

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

## 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:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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 CO<sub>2</sub> 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="110")
```

### 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) 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	"110" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "110"

## 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 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)**

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

**References**

Hunter K. A., 1998. The temperature dependence of pH in surface seawater. *Deep-Sea Research (Part I, Oceanographic Research Papers)* **45**(11):1919-1930.

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.

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**

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="110")
```

**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 HCO <sub>3</sub> given
	flag = 7 pH and CO <sub>3</sub> given
	flag = 8 pH and ALK given
	flag = 9 pH and DIC given
	flag = 10 HCO <sub>3</sub> and CO <sub>3</sub> given
	flag = 11 HCO <sub>3</sub> and ALK given
	flag = 12 HCO <sub>3</sub> and DIC given
	flag = 13 CO <sub>3</sub> and ALK given
	flag = 14 CO <sub>3</sub> and DIC given
	flag = 15 ALK and DIC given
	flag = 21 pCO <sub>2</sub> and pH given
	flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given
	flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given
	flag = 24 pCO <sub>2</sub> and ALK given
	flag = 25 pCO <sub>2</sub> and DIC given
var1	Value of the first variable in mol/kg except for pH and for pCO <sub>2</sub> in $\mu\text{atm}$
var2	Value of the second variable in mol/kg except for pH
pCO <sub>2s</sub>	Partial pressure of the high CO <sub>2</sub> component in $\mu\text{atm}$
wf	Weight fraction of the high CO <sub>2</sub> 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) 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	"l10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "l10"



## 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 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 ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )
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

**Author(s)**

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**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., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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., Culbertson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40°C: 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 Atlantic 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.

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

```
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="1", ks="d", b="110")
```

---

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 CO<sub>2</sub> given  
flag = 2 CO<sub>2</sub> and HCO<sub>3</sub> given  
flag = 3 CO<sub>2</sub> and CO<sub>3</sub> given  
flag = 4 CO<sub>2</sub> and ALK given  
flag = 5 CO<sub>2</sub> and DIC given  
flag = 6 pH and HCO<sub>3</sub> given  
flag = 7 pH and CO<sub>3</sub> given  
flag = 8 pH and ALK given  
flag = 9 pH and DIC given  
flag = 10 HCO<sub>3</sub> and CO<sub>3</sub> given  
flag = 11 HCO<sub>3</sub> and ALK given  
flag = 12 HCO<sub>3</sub> and DIC given  
flag = 13 CO<sub>3</sub> and ALK given  
flag = 14 CO<sub>3</sub> and DIC given  
flag = 15 ALK and DIC given  
flag = 21 pCO<sub>2</sub> and pH given

	flag = 22 pCO <sub>2</sub> and HCO <sub>3</sub> given
	flag = 23 pCO <sub>2</sub> and CO <sub>3</sub> given
	flag = 24 pCO <sub>2</sub> and ALK given
	flag = 25 pCO <sub>2</sub> 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 pCO <sub>2</sub> in $\mu$ atm
var2	Value of the second variable in mol/kg, except for pH
pCO <sub>2a</sub>	CO <sub>2</sub> partial pressure in the atmosphere pCO <sub>2</sub> in $\mu$ atm. 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) 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 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 ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )
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

### Author(s)

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### References

- Dickson A. G., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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., Culbertson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40°C: Standard Potentials at Salinities from 20 to 45. *Analytical Chemistry* **49**, 29-34.
- Gattuso J.-P. and Lavigne H., 2009 Perturbation experiments to investigate the impact of ocean acidification: approaches and software tools. *Biogeosciences* **6**, 4413-4439.
- 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.

### 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="1", 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="1", 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, 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 $\mu\text{atm}$
var2	enter value of the second variable in mol/kg, except for pH
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
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) 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), "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 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 CO<sub>2</sub> released vs CaCO<sub>3</sub> precipitated (mol/mol)

### Author(s)

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

### References

- Dickson A. G., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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 CO<sub>2</sub> measurements. *PICES Special Publication* **3**, 1-191.
- Khoo H. K., Ramette R. W., Culbertson C. H. and Bates R. G., 1977 Determination of Hydrogen Ion Concentration in Seawater from 5 to 40°C: 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 CO<sub>2</sub> system in seawater. *Journal of Marine Systems* **5**, 111-118.
- Frankignoulle M., Canon C. and Gattuso J.P., 1994 Marine calcification as a source of carbon dioxide- Positive feedback of increasing atmospheric CO<sub>2</sub>. *Limnology and Oceanography* **2**, 458-462.
- 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.

**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="1", 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="110")
```

**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 it is carried out in a system open to the atmosphere
var1	Value of the first variable in mol/kg, except for pH and for pCO <sub>2</sub> in $\mu\text{atm}$
var2	Value of the second variable in mol/kg, except for pH
pCO <sub>2a</sub>	CO <sub>2</sub> partial pressure in the atmosphere pCO <sub>2</sub> in $\mu\text{atm}$ . It is only used in systems open to the atmosphere (i.e. when sys=1)
co3	Amount of $\text{CO}_3^{2-}$ added in $\text{mol kg}^{-1}$
hco3	Amount of $\text{HCO}_3^{-}$ added in $\text{mol kg}^{-1}$
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) 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), "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	"l10" for computing boron total from the Lee et al. (2010) formulation or "u74" for using the Uppstrom (1974) formulation, default is "l10"

### 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 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 ( $\mu\text{atm}$ )
fCO2	fCO2, CO2 fugacity ( $\mu\text{atm}$ )

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

### Author(s)

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., 1990 Standard potential of the reaction:  $\text{AgCl(s)} + 1/2\text{H}_2(\text{g}) = \text{Ag(s)} + \text{HCl(aq)}$ , and the standard acidity constant of the ion  $\text{HSO}_4$  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.
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- 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 Atlantic 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.
- 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

```
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="1", ks="d", b="110")
```

```
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="1", ks="d", b="110")
```

---

rho	<i>Density of seawater (kg/m<sup>3</sup>)</i>
-----	---

---

**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/m <sup>3</sup> )
-----	--

**Author(s)**

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

**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	<i>Test data file (at P=0) to test the use of the carb function</i>
-----------------	---

---

**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 pCO<sub>2</sub> in  $\mu\text{atm}$
- 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 pCO<sub>2</sub> in  $\mu\text{atm}$
- 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	<i>ionic forms as a function of pH</i>
------------	--

---

**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)**

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

**References**

Zeebe R. E. and Wolf-Gladrow D. A., 2001 *CO<sub>2</sub> 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-, HP04--, P04---)
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")))
```

---

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 CO<sub>2</sub> measurements. *PICES Special Publication* **3**, 1-191.

**See Also**

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

**Examples**

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

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