Package 'seacarb'

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Title Calculates parameters of the seawater carbonate system

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Description Calculates parameters of the seawater carbonate system

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URL http://www.obs-vlfr.fr/~gattuso/seacarb.php

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R topics documented:

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

Description

First dissociation constant of carbonic acid (mol/kg)

Usage

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

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
`k1k2`	"l" for using K1 and K2 from Lueker et al. and "r" for using K1 and K2 from Roy et al. , default is "l"
`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

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

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

Author(s)

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

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

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

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

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.

See Also

K2.

Examples

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

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

Description

First dissociation constant of phosphoric acid (mol/kg)

Usage

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

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

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)

Héloïse Lavigne, Aurélien 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.

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 = "l", 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
k1k2	"l" for using K1 and K2 from Lueker et al. and "r" for using K1 and K2 from Roy and al. , default is "l"
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

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

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

Author(s)

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

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

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

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

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.

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")
```

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

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)

Héloïse Lavigne, Aurélien 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.

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")
```

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

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)

Héloïse Lavigne, Aurélien 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.

See Also

`K1p`, `K2p`.

Examples

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

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

Description

Dissociation constant of boric acid (mol/kg)

Usage

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

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

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

Value

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

Author(s)

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

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.

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.

Examples

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

`Kf` *Stability constant of hydrogen fluoride (mol/kg)*

Description

Stability constant of hydrogen fluoride (mol/kg)

Usage

```
Kf(S = 35, T = 25, P = 0, kf = "pf", 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
`kf`	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
`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)

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

`Kf`	Stability constant of hydrogen fluoride (mol/kg)

Author(s)

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

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.

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

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

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")
```

`Kh` *Henry's constant mol/(kg/atm)*

Description

Henry's constant mol/(kg/atm)

Usage

```
Kh(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

`Kh`	Henry's constant mol/(kg/atm)

Author(s)

Aurélien 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

```
Kh(35,25,0)
```

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

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 Héloïse 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")
plot(Tseq <- seq(0,30,by=0.1), Khs(T=Tseq),xlab="Temperature,dgC",ylab="Khs")
```

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

Description

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

Usage

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

Arguments

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

Details

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

Value

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

Author(s)

Karline Soetaert ⟨K.Soetaert@nioo.knaw.nl⟩ and Héloïse Lavigne

References

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

Examples

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

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

Description

Stability constant of hydrogen sulfate (mol/kg)

Usage

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

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

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

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

Author(s)

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

Ks is given by Dickson (1990) in Guide to Best Practices in Ocean CO2 Measurements 2007).

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

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.

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.

Examples

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

`Ksi` *Dissociation constant of Si(OH)4*

Description

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

Usage

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

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

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

Value

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

Author(s)

Karline Soetaert ⟨K.Soetaert@nioo.knaw.nl⟩ and Héloïse 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.

Examples

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

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

Description

Solubility product of aragonite (mol/kg)

Usage

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

Arguments

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

Details

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/kg)

Author(s)

Aurélien 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(35,25,0)
```

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

Description

Solubility product of calcite (mol/kg)

Usage

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

Arguments

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

Details

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/kg)

Author(s)

Aurélien 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(35,25,0)
```

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

Description

Ion product of water (mol2/kg2)

Usage

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

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

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

Value

Kw	Ion product of water (mol2/kg2)

Author(s)

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

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

Examples

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

amp *pH value of the AMP buffer*

Description

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

Usage

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

Arguments

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

Details

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

Value

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

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

See Also

tris, pHslope, pH.

Examples

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

`bjerrum` *Bjerrum plot*

Description

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

Usage

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

Arguments

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

Details

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

Author(s)

Karline Soetaert ⟨K.Soetaert@nioo.knaw.nl⟩

References

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

See Also

`matplot`, `par`, `speciation`.

Examples

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

## Plot the bjerrum plot for phosphate using the default values
bjerrum(K1p(),K2p(),K3p(),main="phosphate speciation",lwd=2)
legend("left",lty=1:4,lwd=2,legend=c(expression(H[3]~PO[4]),expression(H[2]~PO[4]^"-"),
expression(HPO[4]^"2-"),expression(PO[4]^"3-")))

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

`bor` *Total boron concentration (mol/kg)*

Description

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

Usage

```
bor(S, T, P)
```

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

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

Author(s)

Aurélien 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.

Examples

```
bor(35,25,0)
```

---

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='l', kf='pf', pHscal
```

Arguments

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

	flag = 21 pCO2 and pH given flag = 22 pCO2 and HCO3 given flag = 23 pCO2 and CO3 given flag = 24 pCO2 and ALK given flag = 25 pCO2 and DIC given
var1	enter value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	enter value of the second variable in mol/kg, except for pH
S	Salinity
T	Temperature in degrees Celsius
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) and "r" for using K1 and K2 from Roy et al. (1993), default is "l"
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
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)

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. For instance, to compute parameters from one couple of variable for a range of temperatures, a vector with temperatures required can be given in enter and other arguments can be completed be one variable this variable will be used for each temperatures.

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 (μatm per mol/kg)
PhiB	PhiB, chemical buffer factor (dpH/d[DIC]); from input/output of bicarbonate (unit pH per mol/kg)
BetaB	BetaB, homogeneous buffer factor (dln(pCO2)/dln[DIC]); input/output of bicarbonate
PiB	PiB, chemical buffer factor (dpCO2/d[DIC]); input/output of dissolved CO2 (μatm per mol/kg)
PhiC	PhiC, chemical buffer factor (dpH/d[DIC]); input/output of carbonate (unit pH per mol/kg)
BetaC	BetaC, homogeneous buffer factor (dln(pCO2)/dln[DIC]); input/output of carbonate

PiC	PiC, chemical buffer factor (dpCO2/d[DIC]); input/output of carbonate (μatm per mol/kg)
PhiH	PhiH, chemical buffer factor (dpH/d[ALK]); input/output of strong acid (unit pH per mol/kg)
PiH	PiH, chemical buffer factor (dpCO2/d[ALK]); input/output of strong acid (μatm per mol/kg)

Author(s)

HÃ©loÃ¯se Lavigne, AurÃ©lien Proye and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

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.

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 45Â°C. *Marine Chemistry* **44**, 249-267.

Examples

```
## Calcul 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"

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

## 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

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

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

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="l", kf="pf", pHscale=
```

Arguments

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO2 given flag = 2 CO2 and HCO3 given flag = 3 CO2 and CO3 given flag = 4 CO2 and ALK given flag = 5 CO2 and DIC given flag = 6 pH and HCO3 given flag = 7 pH and CO3 given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO3 and CO3 given flag = 11 HCO3 and ALK given flag = 12 HCO3 and DIC given flag = 13 CO3 and ALK given flag = 14 CO3 and DIC given flag = 15 ALK and DIC given flag = 21 pCO2 and pH given flag = 22 pCO2 and HCO3 given flag = 23 pCO2 and CO3 given flag = 24 pCO2 and ALK given flag = 25 pCO2 and DIC given
var1	enter value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	enter value of the second variable in mol/kg, except for pH
S	Salinity
T	Temperature in degrees Celsius
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. and "r" for using K1 and K2 from Roy et al. , default is "l"
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
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)

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. For instance, to compute parameters from one couple of variable for a range of temperatures, a vector with temperatures required can be given in enter and other arguments can be completed be one variable this variable will be used for each temperatures.

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

Author(s)

Héloïse Lavigne, Aurélien 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.

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.

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.

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

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

Examples

```
## With a couple of variables
carb(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Pt=0, Sit=0, pHscale="T", kf="pf",

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

## Test with 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)
carb(flag=flag, var1=var1, var2=var2)

## Test using a data frame
data(seacarb_test)
tab <- seacarb_test

## 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[[7]], Pt=tab[[8]])

## 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)
```

`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)
```

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

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. & 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)
```

---

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="l", kf="pf", pHsca
```

Arguments

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO2 given flag = 2 CO2 and HCO3 given flag = 3 CO2 and CO3 given flag = 4 CO2 and ALK given flag = 5 CO2 and DIC given flag = 6 pH and HCO3 given flag = 7 pH and CO3 given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO3 and CO3 given flag = 11 HCO3 and ALK given flag = 12 HCO3 and DIC given flag = 13 CO3 and ALK given flag = 14 CO3 and DIC given flag = 15 ALK and DIC given flag = 21 pCO2 and pH given flag = 22 pCO2 and HCO3 given flag = 23 pCO2 and CO3 given flag = 24 pCO2 and ALK given flag = 25 pCO2 and DIC given
var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
Ca	Calcium concentration in mol/kg
S	Salinity
T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. and "r" for using K1 and K2 from Roy et al. , default is "l"
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
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)

Details

This function assumes that the simplified synthetic sea water recipe described by Dickson et al. (2007) was used. It is the basis of the synthetic seawater that has been used to determine a variety of equilibrium constants for use in sea water.

Note that this function does not account for the effect of the changes in the calcium concentration of the dissociation constants of carbonic acid and on the solubility product of CaCO3 (Ben-Yaakov and Goldhaber, 1973).

Value

The function returns a data frame containing the following columns:

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

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

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

Examples

```
pCa(flag=15, var1=2302e-6, var2=2050e-6, Ca=0.01028, S=35, T=20, P=0, Pt=0, Sit=0, pHscal
pCa(flag=15, var1=2302e-6, var2=2050e-6, Ca=0.01028/2, S=35, T=20, P=0, Pt=0, Sit=0, pHsc
```

---

pH *Potentiometric pH*

Description

Calculation of potentiometric pH

Usage

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

Arguments

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

Details

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

Value

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

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

See Also

tris, amp, pHslope.

Examples

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

---

pHconv *Conversion of pH*

Description

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

Usage

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

Arguments

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

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. For instance, to compute parameters from one couple of variable for a range of temperatures, a vector with temperatures required can be given in enter and other arguments can be completed be one variable this variable will be used for each temperatures.

Value

The function returns the values of pH converted

Author(s)

Héloïse Lavigne and Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

Dickson, A.G. & 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

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)

##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)

##note that pHc is a vector containing the value of the pH converted in 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 = "l", kf
```

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. and "r" for using K1 and K2 from Roy et al. , default is "l"
`kf`	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
`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)

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.

Examples

```
pHinsi(8.2,2.4e-3,25,25,35,0,0)
```

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)
```

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, k1k
```

Arguments

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO2 given flag = 2 CO2 and HCO3 given flag = 3 CO2 and CO3 given flag = 4 CO2 and ALK given flag = 5 CO2 and DIC given flag = 6 pH and HCO3 given flag = 7 pH and CO3 given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO3 and CO3 given flag = 11 HCO3 and ALK given flag = 12 HCO3 and DIC given flag = 13 CO3 and ALK given flag = 14 CO3 and DIC given flag = 15 ALK and DIC given flag = 21 pCO2 and pH given flag = 22 pCO2 and HCO3 given flag = 23 pCO2 and CO3 given flag = 24 pCO2 and ALK given flag = 25 pCO2 and DIC given
sys	0 if the manipulation is carried out in a system closed to the atmosphere or 1 if its is carried out in a system open to the atmosphere
var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
pCO2a	CO2 partial pressure in the atmosphere pCO2 in μatm. It is only used in systems open to the atmosphere (i.e. when sys=1)
co3	Amount of CO_3^{2-} added in $mol\ kg^{-1}$
hco3	Amount of HCO_3^{2-} added in $mol\ kg^{-1}$
S	Salinity
T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)

Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. and "r" for using K1 and K2 from Roy and al. , default is "l"
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
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

Value

The function returns a data frame containing the following columns:

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

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

Examples

```
pTA(flag=24, sys=0, var1=384, var2=2302e-6, pCO2a=384, co3=260e-6, hco3=1000e-6, S=34.3,

pTA(flag=24, sys=1, var1=384, var2=2302e-6, pCO2a=384, co3=260e-6, hco3=1000e-6, S=34.3,
```

pgas *pgas*

Description

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

Usage

```
pgas(flag, var1, var2, pCO2g, S=35, T=20, P=0, Pt=0, Sit=0, k1k2="l", kf="pf", p
```

Arguments

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO2 given flag = 2 CO2 and HCO3 given flag = 3 CO2 and CO3 given flag = 4 CO2 and ALK given flag = 5 CO2 and DIC given flag = 6 pH and HCO3 given flag = 7 pH and CO3 given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO3 and CO3 given flag = 11 HCO3 and ALK given flag = 12 HCO3 and DIC given flag = 13 CO3 and ALK given flag = 14 CO3 and DIC given flag = 15 ALK and DIC given flag = 21 pCO2 and pH given flag = 22 pCO2 and HCO3 given flag = 23 pCO2 and CO3 given flag = 24 pCO2 and ALK given flag = 25 pCO2 and DIC given
var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
pCO2g	CO2 partial pressure of the gas used for bubbling in μatm
S	Salinity
T	Temperature in degrees Celsius
P	Hydrostatic pressure in bar (surface = 0)
Pt	Concentration of total phosphate in mol/kg
Sit	Concentration of total silicate in mol/kg
k1k2	"l" for using K1 and K2 from Lueker et al. and "r" for using K1 and K2 from Roy and al. , default is "l"
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
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

Value

The function returns a data frame containing the following columns:

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

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

Examples

```
pgas(flag=15, var1=2302e-6, var2=2050e-6, pCO2g=750, S=35, T=20, P=0, Pt=0, Sit=0, pHscal
```

---

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="l", kf="pf
```

Arguments

flag	select the couple of variables available. The flags which can be used are: flag = 1 pH and CO2 given flag = 2 CO2 and HCO3 given flag = 3 CO2 and CO3 given flag = 4 CO2 and ALK given flag = 5 CO2 and DIC given flag = 6 pH and HCO3 given flag = 7 pH and CO3 given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO3 and CO3 given flag = 11 HCO3 and ALK given flag = 12 HCO3 and DIC given flag = 13 CO3 and ALK given flag = 14 CO3 and DIC given flag = 15 ALK and DIC given flag = 21 pCO2 and pH given flag = 22 pCO2 and HCO3 given flag = 23 pCO2 and CO3 given flag = 24 pCO2 and ALK given flag = 25 pCO2 and DIC given
var1	Value of the first variable in mol/kg except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg except for pH
pCO2s	Partial pressure of the high CO2 component in μatm
wf	Weight fraction of the high CO2 seawater vs normal 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. and "r" for using K1 and K2 from Roy and al. , default is "l"
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
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

Value

The function returns a data frame containing the following columns:

comment	The initial or final state water
S	Salinity
T	Temperature in degrees Celsius

P	Pressure in bar
pH	pH
CO2	CO2 concentration (mol/kg)
pCO2	pCO2, CO2 partial pressure (μatm)
fCO2	fCO2, CO2 fugacity (μatm)
HCO3	HCO3 concentration (mol/kg)
CO3	CO3 concentration (mol/kg)
DIC	DIC concentration (mol/kg)
ALK	ALK, total alkalinity (mol/kg)
OmegaAragonite	Omega aragonite, aragonite saturation state
OmegaCalcite	Omega calcite, calcite saturation state

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

Examples

```
pmix(flag=24, var1=384, var2=2302e-6, pCO2s=1e6, wf=0.003, S=34.3, T=16, P=0, pHscale="T"
```

---

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=
```

Arguments

flag	Select the couple of variables available. The flags which can be used are: flag = 1 pH and CO2 given flag = 2 CO2 and HCO3 given flag = 3 CO2 and CO3 given flag = 4 CO2 and ALK given flag = 5 CO2 and DIC given flag = 6 pH and HCO3 given flag = 7 pH and CO3 given flag = 8 pH and ALK given flag = 9 pH and DIC given flag = 10 HCO3 and CO3 given flag = 11 HCO3 and ALK given flag = 12 HCO3 and DIC given

	flag = 13 CO3 and ALK given flag = 14 CO3 and DIC given flag = 15 ALK and DIC given flag = 21 pCO2 and pH given flag = 22 pCO2 and HCO3 given flag = 23 pCO2 and CO3 given flag = 24 pCO2 and ALK given flag = 25 pCO2 and DIC given
sys	0 if the manipulation is carried out in a system closed to the atmosphere or 1 if its is carried out in a system open to the atmosphere
var1	Value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	Value of the second variable in mol/kg, except for pH
pCO2a	CO2 partial pressure in the atmosphere pCO2 in μatm. It is only used in systems open to the atmosphere (i.e. when sys=1)
vol	Volume of acid or base added in liter. By convention, it is given a negative sign for acid additions and a positive sign for base additions
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
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
k1k2	"l" for using K1 and K2 from Lueker et al. and "r" for using K1 and K2 from Roy and al. , default is "l"
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"

Value

The function returns a data frame containing the following columns:

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

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

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,

ppH(flag=24, sys=1, var1=384, var2=2302e-6, pCO2a=384, vol=-12e-3, N=0.01, S=34.3, T=16,
```

---

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="pf", k1k2="
```

Arguments

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

var1	enter value of the first variable in mol/kg, except for pH and for pCO2 in μatm
var2	enter value of the second variable in mol/kg, except for pH
S	Salinity
T	Temperature in degrees Celsius
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)
kf	"pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
k1k2	"l" for using K1 and K2 from Lueker et al. and "r" for using K1 and K2 from Roy et al. , default is "l"

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. For instance, to compute parameters from one couple of variable for a range of temperatures, a vector with temperatures required can be given in enter and other arguments can be completed be one variable this variable will be used for each temperatures.

Value

The function returns a data frame containing the following columns:

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

Author(s)

Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

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

Frankignoulle, M., Canon, C. & Gattuso, J.-P., 1994. Marine calcification as a source of carbon dioxide- Positive feedback of increasing atmospheric CO2. *Limnology and Oceanography* **2**, 458-462.

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",
```

rho *Density of seawater (kg/m3)*

Description

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

Usage

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

Arguments

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

Value

rho	Density of seawater (kg/m3)

Author(s)

Aurélien 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 *Test data file to test the use of the carb function*

Description

The variables are:

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

Usage

```
seacarb_test
```

Format

A data frame with 20 rows and 8 variables

Source

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

---

speciation *ionic forms as a function of pH*

Description

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

Usage

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

Arguments

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

Value

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

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

Author(s)

Karline Soetaert ⟨K.Soetaert@nioo.knaw.nl⟩

References

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

See Also

bjerrum.

Examples

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

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

## Effect of temperature on pCO2 - Figure 1.4.18 of Zeebe and Wolf-Gladrow (2001)
Tseq <- seq(0, 30, by=0.5)
pHseq <- carb(flag=15, var1=2300e-6, var2=1900e-6, S=35, T=Tseq, P=0)$pH
CO2  <- speciation(K1(T=Tseq), K2(T=Tseq), conc=1900, pH=pHseq)$C1
pCO2 <- CO2/Kh(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 CO2 measurements. *PICES Special Publication* **3**, 1-191.

See Also

amp, pHslope, pH.

Examples

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

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