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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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


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.


See Also

K2.

Examples

K1p(S=35, T=25, P=0, k1k2="l", pHscale="T")

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

Description

First dissociation constant of phosphoric acid (mol/kg)

Usage

Klp(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

\[ K_1 p \]
First dissociation constant of phosphoric acid (mol/kg)

Author(s)

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

References


See Also

\[ K_2 p, K_3 p \].

Examples

\[ K_1 p(35,25,0) \]

\[ K_2 \]
Second dissociation constant of carbonic acid (mol/kg)

Description

Second dissociation constant of carbonic acid (mol/kg)

Usage

\[ K_2(S = 35, T = 25, P = 0, k1k2 = "l", pHscale = "T") \]

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 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

\[ K_2 \]
Second dissociation constant of carbonic acid (mol/kg)
K2p

Author(s)
Héloïse Lavigne, Aurélien Proux 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.

See Also
K1.

Examples
K2p(35,25,0)

<table>
<thead>
<tr>
<th>K2p</th>
<th>Second dissociation constant of phosphoric acid (mol/kg)</th>
</tr>
</thead>
</table>

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 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
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

See Also
K1p, K3p.

Examples

K2p(35, 25, 0)

### K3p

Third dissociation constant of phosphoric acid (mol/kg)

Usage

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

Arguments

<table>
<thead>
<tr>
<th>S</th>
<th>Salinity, default is 35</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius, default is 25oC</td>
</tr>
<tr>
<td>P</td>
<td>Hydrostatic pressure in bar (surface = 0), default is 0</td>
</tr>
<tr>
<td>pHscale</td>
<td>choice of pH scale: &quot;T&quot; for using the total scale, &quot;F&quot; for using the free scale and &quot;SWS&quot; for using the seawater scale, default is total scale</td>
</tr>
</tbody>
</table>

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

\( K_{3p} \) Third dissociation constant of phosphoric acid (mol/kg)

Author(s)

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso \( \langle \text{gattuso@obs-vlfr.fr} \rangle \)

References


See Also

\( K_{1p}, K_{2p} \).

Examples

\( K_{3p}(35, 25, 0) \)

<table>
<thead>
<tr>
<th>( Kb )</th>
<th>Dissociation constant of boric acid (mol/kg)</th>
</tr>
</thead>
</table>

Description

Dissociation constant of boric acid (mol/kg)

Usage

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

Arguments

| \( S \) | Salinity, default is 35 |
| \( T \) | Temperature in degrees Celsius, default is 25oC |
| \( P \) | Hydrostatic pressure in bar (surface = 0), default is 0 |
| \( \text{pHscale} \) | 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 \( \langle \text{gattuso@obs-vlfr.fr} \rangle \)
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

\[ K_f(S=35, T=25, P=0, \text{pHscale}="T") \]

**Kf**

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

**Description**

Stability constant of hydrogen fluoride (mol/kg)

**Usage**

\[ K_f(S = 35, T = 25, P = 0, \text{kf} = "pf", \text{pHscale}="T") \]

**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
- **kf**: "pf" for using \( K_f \) from Perez and Fraga (1987) and "dg" for using \( K_f \) 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**

\[ K_f \]

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

**Author(s)**

Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso (gattuso@obs-vlfr.fr)
Kh

References


Examples

\[ K_f(S=35,T=25,P=0,kf="pf","PHscale="T") \]

\[ Kh(S = 35, T = 25, P = 0) \]

Description

Henry’s constant mol/(kg/atm)

Usage

\[ Kh(S = 35, T = 25, P = 0) \]

Arguments

<table>
<thead>
<tr>
<th>S</th>
<th>Salinity, default is 35</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius, default is 25°C</td>
</tr>
<tr>
<td>P</td>
<td>Hydrostatic pressure in bar (surface = 0), default is 0</td>
</tr>
</tbody>
</table>

Value

\[ Kh \]

Henry’s constant mol/(kg/atm)

Author(s)

Aurélien Proye and Jean-Pierre Gattuso (gattuso@obs-vlfr.fr)

References


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 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

**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**


**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

\[ \text{Kn}(S=35, \ T=25, \ P=0, \ \text{pHscale}="T") \]

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
- **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

\[ \text{Kn} \]

Dissociation constant of ammonium (mol/kg)

Author(s)

Karline Soetaert (K.Soetaert@nioo.knaw.nl) and Héloïse Lavigne

References


Examples

\[ \text{Kn}(S=35, \ T=25, \ P=0, \ \text{pHscale}="T") \]
$K_s$  

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

**Description**

Stability constant of hydrogen sulfate (mol/kg)

**Usage**

$$K_s(S = 35, \ T = 25, \ P = 0)$$

**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

**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**

$$K_s$$  
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**


Dickson, A. G. 1990 Standard potential of the reaction: $\text{AgCl}(s) + \frac{1}{2}\text{H}_2(g) = \text{Ag}(s) + \text{HCl(aq)}$, 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.


**Examples**

$$K_s(S=35,T=25,P=0)$$
**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 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

**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**


**Examples**

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

Solubility product of aragonite (mol/kg)

### Usage

\[ \text{Kspa}(S = 35, \ T = 25, \ P = 0) \]

### 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

### 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

\[ \text{Kspa} \quad \text{Solubility product of aragonite (mol/kg)} \]

### Author(s)

Aurélien Proye and Jean-Pierre Gattuso (gattuso@obs-vlfr.fr)

### References


### See Also

Kspc.

### Examples

Kspa(35, 25, 0)
Description

Solubility product of calcite (mol/kg)

Usage

\[ \text{Kspc}(S = 35, T = 25, P = 0) \]

Arguments

\begin{itemize}
  \item \textbf{S} \hspace{1cm} \text{Salinity, default is 35}
  \item \textbf{T} \hspace{1cm} \text{Temperature in degrees Celsius, default is 25oC}
  \item \textbf{P} \hspace{1cm} \text{Hydrostatic pressure in bar (surface = 0), default is 0}
\end{itemize}

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

\[ \text{Kspc} \quad \text{Solubility product of calcite (mol/kg)} \]

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. \textit{American Journal of Science} \textbf{283}: 780-799.

See Also

\text{Kspa}.

Examples

\[ \text{Kspc}(35, 25, 0) \]
**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 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

**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**


**Examples**

\[ Kw(S=35,T=25,P=0,pHscale="T") \]
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 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

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

Author(s)

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

References


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

See Also
matplot, par, speciation.
Examples

```r
## 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")

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

## Plot the bjerrum plot for the carbonate system using the values other than the default values, 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"))

## Plot the bjerrum plot for the carbonate system using the values other than the default values, showing the effect of salinity
bjerrum(K1(T=25, S=35), K2(T=25, S=5), 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"))

## Plot the bjerrum plot for the carbonate system using the values other than the default values, 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")
```

### bor

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

**Description**

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

**Usage**

`bor(S, T, P)`

**Arguments**

- `S` Salinity, default is 35
buffer

$T$  Temperature in degrees Celsius, default is 25°C
$P$  Hydrostatic pressure in bar (surface = 0), default is 0

Value

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

Author(s)

Aurélien Proye and Jean-Pierre Gattuso (gattuso@obs-vlfr.fr)

References


Examples

$\text{bor}(35,25,0)$

Buffer parameters of the seawater carbonate system

Description

Returns buffer parameters of the seawater carbonate system.

Usage

$\text{buffer}(\text{flag, var1, var2, S=35, T=25, P=0, Pt=0, Sit=0, k1k2='l', kf='pf', pHscale="T")}$

Arguments

$\text{flag}$  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
klk2 "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)
Héloïse Lavigne, Aurélien Proye and Jean-Pierre Gattuso (gattuso@obs-vlfr.fr)

References

Examples

```r
## 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", k1k2="l")

## 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, pHscale=pHscale)

## 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, 0.002888382, 0.002391252, 0.001981340, 0.001685024,
buffer(flag=flag, var1=var1, var2=var2)
```
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="T")
```

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:

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>Salinity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature in degrees Celsius</td>
</tr>
<tr>
<td>P</td>
<td>Pressure in bar</td>
</tr>
<tr>
<td>pH</td>
<td>pH</td>
</tr>
<tr>
<td>CO2</td>
<td>CO2 concentration (mol/kg)</td>
</tr>
<tr>
<td>pCO2</td>
<td>pCO2, CO2 partial pressure (µatm)</td>
</tr>
<tr>
<td>fCO2</td>
<td>fCO2, CO2 fugacity (µatm)</td>
</tr>
<tr>
<td>HCO3</td>
<td>HCO3 concentration (mol/kg)</td>
</tr>
<tr>
<td>CO3</td>
<td>CO3 concentration (mol/kg)</td>
</tr>
<tr>
<td>DIC</td>
<td>DIC concentration (mol/kg)</td>
</tr>
<tr>
<td>ALK</td>
<td>ALK, total alkalinity (mol/kg)</td>
</tr>
<tr>
<td>OmegaAragonite</td>
<td>Omega aragonite, aragonite saturation state</td>
</tr>
<tr>
<td>OmegaCalcite</td>
<td>Omega calcite, calcite saturation state</td>
</tr>
</tbody>
</table>

Author(s)

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

References


## Examples

### With a couple of variables

```r
carb(flag=8, var1=8.2, var2=0.00234, S=35, T=25, P=0, Pt=0, Sit=0, pHscale="T", kf="pf", k1k2="l")
```

### Using vectors as arguments

```r
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")
carb(flag=flag, var1=var1, var2=var2, S=S, T=T, P=P, Pt=Pt, Sit=Sit, kf=kf, k1k2=k1k2, pHscale=pHscale)
```

### Test with all flags

```r
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, 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, 0.002888382, 0.002391252, 0.0002888382, 0.0002888382, 0.002391252, 0.0002888382, 0.0002888382, 0.0002888382, 0.0002888382, 0.001981340, 0.001981340, 0.001981340, 0.001981340, 0.001981340, 0.001981340, 0.001981340, 0.001981340, 0.001981340)
carb(flag=flag, var1=var1, var2=var2)
```

### Test using a data frame

```r
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

```r
kconv(S=35, T=25, P=0)
```
Arguments

S  Salinity, default is 35
T  Temperature in degrees Celsius, default is 25\(^{\circ}\)C
P  Hydrostatic pressure in bar (surface = 0), default is 0

Value

The function returns a list with 3 conversion factors:

\texttt{ktotal2SWS}  to convert from the total scale to seawater scale
\texttt{ktotal2free}  to convert from the total scale to the free scale
\texttt{kfree2SWS}  to convert from the free scale to the seawater scale

Author(s)

Karline Soetaert \(\langle\text{K.Soetaert@nioo.knaw.nl}\rangle\)

References


See Also

\texttt{pHconv}.

Examples

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

Description

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

Usage

```r
pCa(flag, var1, var2, Ca, S=35, T=20, P=0, Pt=0,Sit=0, k1k2="l", kf="pf", pHscale="T")
```
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 CO2 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
klk2 "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).
The function returns a data frame containing the following columns:

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

**Author(s)**

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

**References**


**Examples**

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

**Description**

Calculation of potentiometric pH

**Usage**

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

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


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 25°C

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


See Also

kconv.

Examples

```r
# To convert pH=8.10 from the seawater scale to the total scale
# at salinity=35, temperature=25°C 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 = "pf", pHscale = "T")
```

**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**


**Examples**

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

Author(s)
Jean-Pierre Gattuso ⟨gattuso@obs-vlfr.fr⟩

References

See Also
tris, amp, pH.

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

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

Usage

\[
pTA\{\text{flag, sys=0, var1, var2, pCO2a, co3, hco3, S=35, T=20, P=0, Pt=0, Sit=0, k1k2="l", kf="pf", pHscale="T"} \}
\]

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 pCO2 in $\mu$atm

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

- **pCO2a**: CO2 partial pressure in the atmosphere pCO2 in $\mu$atm. 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 $HCO_3^-$ added in mol kg$^{-1}$

- **S**: Salinity

- **T**: Temperature in degrees Celsius

- **P**: Hydrostatic pressure in bar (surface = 0)


\begin{itemize}
\item \textbf{Pt}  Concentration of total phosphate in mol/kg
\item \textbf{Sit}  Concentration of total silicate in mol/kg
\item \textbf{k1k2}  "l" for using $K_1$ and $K_2$ from Lueker et al. and "r" for using $K_1$ and $K_2$ from Roy and al., default is "l"
\item \textbf{kf}  "pf" for using $K_f$ from Perez and Fraga (1987) and "dg" for using $K_f$ from Dickson and Goyet (1979), default is "pf"
\item \textbf{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
\end{itemize}

\textbf{Value}

The function returns a data frame containing the following columns:

\begin{itemize}
\item \textbf{comment}  The initial or final state water
\item \textbf{S}  Salinity
\item \textbf{T}  Temperature in degrees Celsius
\item \textbf{P}  Pressure in bar
\item \textbf{pH}  pH
\item \textbf{CO2}  CO2 concentration (mol/kg)
\item \textbf{pCO2}  pCO2, CO2 partial pressure ($\mu$atm)
\item \textbf{fCO2}  fCO2, CO2 fugacity ($\mu$atm)
\item \textbf{HCO3}  HCO3 concentration (mol/kg)
\item \textbf{CO3}  CO3 concentration (mol/kg)
\item \textbf{DIC}  DIC concentration (mol/kg)
\item \textbf{ALK}  ALK, total alkalinity (mol/kg)
\item \textbf{OmegaAragonite}  Omega aragonite, aragonite saturation state
\item \textbf{OmegaCalcite}  Omega calcite, calcite saturation state
\end{itemize}

\textbf{Author(s)}

Jean-Pierre Gattuso (gattuso@obs-vlfr.fr)

\textbf{Examples}

\begin{verbatim}
pTA(flag=24, sys=0, var1=384, var2=2302e-6, pCO2a=384, co3=260e-6, hco3=1000e-6, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="l")
pTA(flag=24, sys=1, var1=384, var2=2302e-6, pCO2a=384, co3=260e-6, hco3=1000e-6, S=34.3, T=16, P=0, pHscale="T", kf="pf", k1k2="l")
\end{verbatim}
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", pHscale="T")
```

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 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 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

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

Description

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

Usage

```r
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")

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")

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
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

\[ \text{psi}(\text{flag}, \text{var1}, \text{var2}, S=35, T=20, P=0, Pt=0, Stit=0, \text{pHscale}="T", k\text{f}="pf", k1k2="l") \]

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
psi

```r
var1 <- enter value of the first variable in mol/kg, except for pH and for pCO2 in µatm
des
```

```r
var2 <- enter value of the second variable in mol/kg, except for pH
des
```

```r
S <- Salinity
des
```

```r
T <- Temperature in degrees Celsius
des
```

```r
P <- Hydrostatic pressure in bar (surface = 0)
des
```

```r
Pt <- Concentration of total phosphate in mol/kg
des
```

```r
Sit <- Concentration of total silicate in mol/kg
des
```

```r
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)
des
```

```r
kf <- "pf" for using Kf from Perez and Fraga (1987) and "dg" for using Kf from Dickson and Goyet (1979), default is "pf"
des
```

```r
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"
des
```

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:

```r
psi <- ratio of CO2 released vs CaCO3 precipitated (mol/mol)
des
```

Author(s)

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

References


See Also

speciation.

Examples

```r
## Calculation using the numerical example given in Frankignoulle et al. (1994)
psi(flag=24, var1=350, var2=2400e-6, S=35, T=25, P=0, Pt=0, Sit=0, pHscale="T", kf="pf", k1k2="l")
```
### Density of seawater (kg/m^3)

**Description**

Calculates the density of seawater (kg m^−3).

**Usage**

\[
\text{rho}(S = 35, \; T = 25, \; P = 0)
\]

**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

**Value**

\[
\text{rho} \quad \text{Density of seawater (kg/m3)}
\]

**Author(s)**

Aurélien Proye and Jean-Pierre Gattuso \(\langle\text{gattuso@obs-vlfr.fr}\rangle\)

**References**


**Examples**

\[
\text{rho}(35, 25, 0)
\]

---

**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
speciation

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

See Also

bjerrum.

Examples

```r
## 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

```r
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⟩
tris

References


See Also

amp, pHslope, pH.

Examples

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