

The PRIVATE functions of package AquaEnv

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Abi

Abi

Description

PRIVATE function: calculates $[A(2-)]$ of a bivalent acid

Usage

`Abi(Sum, K1, K2, H)`

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Atri

Atri

Description

PRIVATE function: calculates $[A(3-)]$ of a trivalent acid

Usage

Atri(Sum, K1, K2, K3, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Auni

Auni

Description

PRIVATE function: calculates $[A(-)]$ of an univalent acid

Usage

Auni(Sum, K, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K	the dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Cl

Cl

Description

PRIVATE function: calculates chlorinity Cl from salinity S

Usage

Cl(S)

Arguments

S salinity S in practical salinity units (i.e. no unit)

Value

chlorinity Cl in permil

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

DOE1994, Zeebe2001

ConcRelCl

ConcRelCl

Description

PUBLIC data frame: a collection of concentrations of key chemical species in seawater, relative with respect to chlorinity (DOE1994))

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

H2Abi

H2Abi

Description

PRIVATE function: calculates [H2A] of a bivalent acid

Usage

H2Abi(Sum, K1, K2, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

H2Atri

H2Atri

Description

PRIVATE function: calculates [H2A(-)] of a trivalent acid

Usage

H2Atri(Sum, K1, K2, K3, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

H3Atri	<i>H3Atri</i>
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Description

PRIVATE function: calculates [H3A] of a trivalent acid

Usage

H3Atri(Sum, K1, K2, K3, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

HAbi	<i>HAbi</i>
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Description

PRIVATE function: calculates [HA(-)] of a bivalent acid

Usage

HAbi(Sum, K1, K2, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

HAtri	<i>HAtri</i>
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Description

PRIVATE function: calculates [HA(2-)] of a trivalent acid

Usage

HAtri(Sum, K1, K2, K3, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
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H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
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Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

HAuni	<i>HAuni</i>
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Description

PRIVATE function: calculates [HA] of an univalent acid

Usage

HAuni(Sum, K, H)

Arguments

Sum	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
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K	the dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
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H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
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Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

I	<i>I</i>
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Description

PRIVATE function: calculates the ionic strength I as a function of salinity S

Usage

I(S)

Arguments

S	salinity S in practical salinity units (i.e. no unit)
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Value

ionic strength in mol/kg-H₂O (molality)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

DOE1994, Zeebe2001, Roy1993b (the carbonic acid paper)

<code>Iterms</code>	<i>Iterms</i>
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Description

PRIVATE function: returns the ionic strenght I , $I(2)$, $\text{sqrt}(I)$, and $I*\text{sqrt}(I)$

Usage

`Iterms(S)`

Arguments

`S` salinity in practical salinity units (i.e. no unit)

Value

a list containing:

<code>I</code>	the ionic strength
<code>I^2</code>	the square of the ionic strength
<code>sqrtI</code>	the square root of the ionic strength
<code>I*sqrtI</code>	the ionic strength times its square root

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

Sterms	<i>Sterms</i>
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Description

PRIVATE function: returns S, S(2), sqrt(S), and S*sqrt(S)

Usage

Sterms(S)

Arguments

S salinity in practical salinity units (i.e. no unit)

Value

a list containing:

S^2	the square of S
sqrtS	the square root of S
S*sqrtS	S times its square root

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

T	<i>T</i>
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Description

PRIVATE function: calculates the temperature in Kelvin from the temperature in degrees centigrade

Usage

T(t)

Arguments

t temperature in degrees centigrade

Value

temperature in Kelvin

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

att

att

Description

PRIVATE function: sets the attributes for calculated dissociation constants (Ks)

Usage

`att(K)`

Arguments

K the calculated dissociation constant K

Author(s)

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basicplot

basicplot

Description

PRIVATE function: basic wrapper for the R plot function for plotting objects of class aquaenv; no return value, just side-effect

Usage

```
basicplot(aquaenv, xval, type="l", mgp=c(1.8, 0.5, 0),
          mar=c(3,3,0.5,0.5), oma=c(0,0,0,0), size=c(15,13),
          mfrow=c(11,10), device="x11", filename="aquaenv",
          newdevice, setpar,...)
```

Arguments

aquaenv object of class aquaenv

xval x-value: the independent variable describing a change in elements of an object of class aquaenv

type standard plot parameter; default: plot lines

mgp standard plot parameter; default: axis title on line 1.8, axis labels on line 0.5, axis on line 0

mar	standard plot parameter; default: margin of 3 lines bottom and left and 0.5 lines top and right
oma	standard plot parameter; default: no outer margin
size	the size of the plot device; default: 15 (width) by 13 (height) inches
mfrow	standard plot parameter; default: 11 columns and 10 rows of plots
device	the device to plot on; default: "x11" (can also be "eps" or "pdf")
filename	filename to be used if "eps" or "pdf" is selected for device
newdevice	flag: if TRUE, new plot device is opened
setpar	flag: if TRUE parameters are set with the function par
...	further arguments will be passed

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

bjerrumplot	<i>bjerrumplot</i>
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Description

PRIVATE function: creates a bjerrumplot from the elements of an object of class aquaenv given in what; no return value, just side-effect

Usage

```
bjerrumplot(aquaenv, what, log=FALSE, palette=NULL, device="x11",
            filename="aquaenv", size=c(12,10), ylim=NULL,
            lwd=2, xlab="free scale pH",
            mgp=c(1.8, 0.5, 0), mar=c(3,3,0.5,0.5), oma=c(0,0,0,0),
            legendposition="bottomleft", legendinset=0.05, legendlwd=4,
            bg="white", newdevice, setpar,...)
```

Arguments

aquaenv	object of class aquaenv
what	vector of names of elements of aquaenv that should be plotted; if not specified: what <- c("CO2", "HCO3", "CO3", "BOH3", "BOH4", "OH", "H3PO4", "H2PO4", "HPO4", "PO4", "SiOH4", "SiOOH3", "SiO2OH2", "H2S", "HS", "S2min", "NH4", "NH3", "H2SO4", "HSO4", "SO4", "HF", "F", "HNO3", "NO3", "HNO2", "NO2")
log	should the plot be on a logarithmic y axis?
palette	a vector of colors to use in the plot (either numbers or names given in colors())
device	the device to plot on; default: "x11" (can also be "eps" or "pdf")

filename	filename to be used if "eps" or "pdf" is selected for device
size	the size of the plot device; default: 12 (width) by 10 (height) inches
ylim	standard plot parameter; if not supplied it will be calculated by range() of the elements to plot
lwd	standard plot parameter; width of the lines in the plot
xlab	x axis label
mgp	standard plot parameter; default: axis title on line 1.8, axis labels on line 0.5, axis on line 0
mar	standard plot parameter; default: margin of 3 lines bottom and left and 0.5 lines top and right
oma	standard plot parameter; default: no outer margin
legendposition	position of the legend
legendinset	standard legend parameter inset
legendlwd	standard legend parameter lwd: line width of lines in legend
bg	standard legend parameter: default background color: white
newdevice	flag: if TRUE, new plot device is opened
setpar	flag: if TRUE parameters are set with the function par
...	further arguments will be passed

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

calcH_CO2

calcH_CO2

Description

PRIVATE function: calculates [H+] from an object of class aquaenv and a given [CO2]: by analytically solving the resulting quadratic equation

Usage

```
calcH_CO2(aquaenv, CO2)
```

Arguments

aquaenv	object of class aquaenv
CO2	given [CO2] in mol/kg-solution

Value

calculated [H+] in mol/kg-solution

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`calcH_TA`

calcH_TA

Description

PRIVATE function: calculates [H+] from an object of class aquaenv and a given [TA]: first according to Follows2006, if no solution is found after Technicals\$maxiter iterations, uniroot is applied

Usage

```
calcH_TA(aquaenv, TA)
```

Arguments

aquaenv	object of class aquaenv
TA	given [TA] in mol/kg-solution

Value

calculated [H+] in mol/kg-solution

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`calcSumCO2_TA_CO2`

calcSumCO2_TA_CO2

Description

PRIVATE function: calculates [SumCO2] from an object of class aquaenv, a given [TA], and a given [CO2]: by analytically solving the resulting quadratic equation

Usage

```
calcSumCO2_TA_CO2(aquaenv, TA, CO2)
```

Arguments

aquaenv	object of class aquaenv
TA	given [TA] in mol/kg-solution
CO2	given [CO2] in mol/kg-solution

Value

calculated [SumCO2] in mol/kg-solution

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

<code>calcSumCO2_pH_CO2</code>	<i>calcSumCO2_pH_CO2</i>
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Description

PRIVATE function: calculates [SumCO2] from an object of class aquaenv, a given pH, and a given [CO2]: by analytically solving the resulting equation

Usage

```
calcSumCO2_pH_CO2(aquaenv, pH, CO2)
```

Arguments

<code>aquaenv</code>	object of class aquaenv
<code>pH</code>	given pH on the free proton scale
<code>CO2</code>	given [CO2] in mol/kg-solution

Value

calculated [SumCO2] in mol/kg-solution

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

<code>calcSumCO2_pH_TA</code>	<i>calcSumCO2_pH_TA</i>
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Description

PRIVATE function: calculates [SumCO2] from an object of class aquaenv, a given pH, and a given [TA]: by analytically solving the resulting quadratic equation

Usage

```
calcSumCO2_pH_TA(aquaenv, pH, TA)
```

Arguments

aquaenv	object of class aquaenv
pH	given pH on the free proton scale
TA	given [TA] in mol/kg-solution

Value

calculated [SumCO2] in mol/kg-solution

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

calcTA

calcTA

Description

PRIVATE function: calculates [TA] from an object of class aquaenv and a given [H+]

Usage

calcTA(aquaenv, H)

Arguments

aquaenv	object of class aquaenv
H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)given [H+] in mol/kg-solution

Value

the calculated [TA]

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`calcTAMinor`*calcTAMinor*

Description

PRIVATE function: calculates minor contributions to [TA] from an object of class aquaenv and a given [H+]

Usage

```
calcTAMinor(aquaenv, H)
```

Arguments

<code>aquaenv</code>	object of class aquaenv
<code>H</code>	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution) given [H+] in mol/kg-solution

Value

calculated minor contributions to [TA]

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`cloneaquaenv`*cloneaquaenv*

Description

PRIVATE function: clones an object of class aquaenv: it is possible to supply a new value for either TA or pH; the switches speciation, skeleton, revelle, and dsa are obtained from the object to be cloned

Usage

```
cloneaquaenv(aquaenv, TA=NULL, pH=NULL, k_co2=NULL, k1k2="roy", khf="dickson")
```


Arguments

<code>aquaenv</code>	object of class <code>aquaenv</code>
<code>TA</code>	optional new value for TA
<code>pH</code>	optional new value for pH
<code>k_co2</code>	used for TA fitting: give a <code>K_CO2</code> and NOT calculate it from T and S: i.e. <code>K_CO2</code> can be fitted in the routine as well
<code>k1k2</code>	either "roy" (default, Roy1993a) or "lueker" (Lueker2000, calculated with seacarb) for <code>K_CO2</code> and <code>K_HCO3</code> .
<code>khf</code>	either "dickson" (default, Dickson1979a) or "perez" (Perez1987a, calculated with seacarb) for <code>K_HF</code>

Value

cloned object of class `aquaenv`

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

<code>convert.standard</code>	<i>convert.standard</i>
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Description

PRIVATE function: converts either the pH scale of a pH value, the pH scale of a dissociation constant (K^*), or the unit of a concentration value

Usage

```
convert.standard(x, vartype, what, S, t, p=0, SumH2SO4=NULL,
                SumHF=NULL, khf="dickson")
```

Arguments

<code>x</code>	the object to be converted (pH value, K^* value, or concentration value)
<code>vartype</code>	the type of x, either "pHscale", "KHscale", or "conc"
<code>what</code>	the type of conversion to be done, for pH scales one of "free2tot", "free2sws", "free2nbs", ... (any combination of "free", "tot", "sws", and "nbs"); for concentrations one of "molar2molal", "molar2molin", ... (any combination of "molar" (mol/l), "molal" (mol/kg-H ₂ O), and "molin" (mol/kg-solution))
<code>S</code>	salinity (in practical salinity units: no unit)
<code>t</code>	temperature in degrees centigrade
<code>p</code>	gauge pressure (total pressure minus atmospheric pressure) in bars

SumH2SO4	total sulfate concentration in mol/kg-solution; if not supplied this is calculated from S
SumHF	total fluoride concentration in mol/kg-solution; if not supplied this is calculated from S
khf	either "dickson" (default, Dickson1979a) or "perez" (using seacarb, Perez1987a) for K_HF

Value

converted pH, K*, or concentration value, attributed with the new unit/pH scale

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

cumulativeplot	<i>cumulativeplot</i>
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Description

PRIVATE function: creates a cumulative plot from the elements of an object of class aquaenv given in what; no return value, just side-effect

Usage

```
cumulativeplot(aquaenv, xval, what, total=TRUE, palette=NULL,
               device="x11", filename="aquaenv", size=c(12,10),
               ylim=NULL, lwd=2, mgp=c(1.8, 0.5, 0),
               mar=c(3,3,0.5,0.5), oma=c(0,0,0,0),
               legendposition="bottomleft", legendinset=0.05,
               legendlwd=4, bg="white",
               y.intersp=1.2, newdevice, setpar,...)
```

Arguments

aquaenv	object of class aquaenv
xval	x-value: the independent variable describing a change in elements of an object of class aquaenv
what	vector of names of elements of aquaenv that should be plotted
total	should the sum of all elements specified in what be plotted as well?
palette	a vector of colors to use in the plot (either numbers or names given in colors())
device	the device to plot on; default: "x11" (can also be "eps" or "pdf")
filename	filename to be used if "eps" or "pdf" is selected for device
size	the size of the plot device; default: 12 (width) by 10 (height) inches

<code>ylim</code>	standard plot parameter; if not supplied it will be calculated by an adaptation of <code>range()</code> of the elements to plot
<code>lwd</code>	standard plot parameter; width of the lines in the plot
<code>mgp</code>	standard plot parameter; default: axis title on line 1.8, axis labels on line 0.5, axis on line 0
<code>mar</code>	standard plot parameter; default: margin of 3 lines bottom and left and 0.5 lines top and right
<code>oma</code>	standard plot parameter; default: no outer margin
<code>legendposition</code>	position of the legend
<code>legendinset</code>	standard legend parameter inset
<code>legendlwd</code>	standard legend parameter lwd: line width of lines in legend
<code>bg</code>	standard legend parameter: default background color: white
<code>y.intersp</code>	standard legend parameter; default: 1.2 lines space between the lines in the legend
<code>newdevice</code>	flag: if TRUE, new plot device is opened
<code>setpar</code>	flag: if TRUE parameters are set with the function <code>par</code>
<code>...</code>	further arguments will be passed

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`dAdH_bi`

dAdH_bi

Description

PRIVATE function: calculates the derivative of $[A(2-)]$ of a bivalent acid with respect to $[H+]$

Usage

```
dAdH_bi(H, SumA, K1, K2)
```

Arguments

<code>H</code>	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
<code>SumA</code>	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
<code>K1</code>	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
<code>K2</code>	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dAdH_tri

dAdH_tri

Description

PRIVATE function: calculates the derivative of $[A(3-)]$ of a trivalent acid with respect to $[H+]$

Usage

dAdH_tri(H, SumA, K1, K2, K3)

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dAdH_uni

dAdH_uni

Description

PRIVATE function: calculates the derivative of $[A(-)]$ of a univalent acid with respect to $[H+]$

Usage

dAdH_uni(H, SumA, K)

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K	the dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dH2AdH_bi

dH2AdH_bi

Description

PRIVATE function: calculates the derivative of [H2A] of a bivalent acid with respect to [H+]

Usage

dH2AdH_bi(H, SumA, K1, K2)

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dH2AdH_tri

dH2AdH_tri

Description

PRIVATE function: calculates the derivative of [H2A(-)] of a trivalent acid with respect to [H+]

Usage

dH2AdH_tri(H, SumA, K1, K2, K3)

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dH3AdH_tri

dH3AdH_tri

Description

PRIVATE function: calculates the derivative of [H3A] of a trivalent acid with respect to [H+]

Usage

dH3AdH_tri(H, SumA, K1, K2, K3)

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dHAdH_bi

dHAdH_bi

Description

PRIVATE function: calculates the derivative of [HA(-)] of a bivalent acid with respect to [H+]

Usage

dHAdH_bi(H, SumA, K1, K2)

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`dHAdH_tri`

dHAdH_tri

Description

PRIVATE function: calculates the derivative of [HA(2-)] of a trivalent acid with respect to [H+]

Usage

`dHAdH_tri(H, SumA, K1, K2, K3)`

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K1	the first dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K2	the second dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K3	the third dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`dHAdH_uni`

dHAdH_uni

Description

PRIVATE function: calculates the derivative of [HA] of a univalent acid with respect to [H+]

Usage

`dHAdH_uni(H, SumA, K)`

Arguments

H	the proton concentration in a unit consistent with all other input variables (e.g. mol/kg-solution)
SumA	the total concentration of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)
K	the dissociation constant of the acid in question in a unit consistent with all other input variables (e.g. mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dTAdH	$dTAdH$
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Description

PRIVATE function: calculates the derivative of [TA] with respect to [H+]: the buffer factor

Usage

dTAdH(ae)

Arguments

ae object of class aquaenv

Value

derivative of [TA] with respect to [H+]: the buffer factor

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dTAdKdKdS

dTAdKdKdS

Description

PRIVATE function: calculates the derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to salinity S

Usage

dTAdKdKdS(ae)

Arguments

ae object of class aquaenv

Value

derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to salinity S

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dTAdKdKdSumH2SO4

dTAdKdKdSumH2SO4

Description

PRIVATE function: calculates the derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to the total sulfate concentration (influence via scale conversion)

Usage

dTAdKdKdSumH2SO4(ae)

Arguments

ae object of class aquaenv

Value

derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to the total sulfate concentration (influence via scale conversion)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dTAdKdKdSumHF

dTAdKdKdSumHF

Description

PRIVATE function: calculates the derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to the total fluoride concentration (influence via scale conversion)

Usage

dTAdKdKdSumHF(ae)

Arguments

ae object of class aquaenv

Value

derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to the total fluoride concentration (influence via scale conversion)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dTAdKdKdT

dTAdKdKdT

Description

PRIVATE function: calculates the derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to temperature T

Usage

dTAdKdKdT(ae)

Arguments

ae object of class aquaenv

Value

derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to temperature T

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

dTAdKdKdp

dTAdKdKdp

Description

PRIVATE function: calculates the derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to gauge pressure p

Usage

dTAdKdKdp(ae)

Arguments

ae object of class aquaenv

Value

derivative of [TA] with respect to changes in the dissociation constants (Ks) times the derivative of the dissociation constants with respect to gauge pressure p

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

deltaPlnK

deltaPlnK

Description

PRIVATE function: the generic function for the pressure correction for dissociation constants and solubility products according to Millero1995

Usage

deltaPlnK(T, d, coeff)

Arguments

<code>T</code>	temperature in Kelvin
<code>d</code>	the depth in meters
<code>coeff</code>	a vector containing the coefficients <code>a0</code> , <code>a1</code> , <code>a2</code> , <code>b0</code> , <code>b1</code> , <code>b2</code> for the respective dissociation constant or solubility product

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1995, corrected by Lewis1998

<code>from.data.frame</code>	<i>from.data.frame</i>
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Description

PRIVATE function: creates an object of class `aquaenv` from a data frame (e.g. as supplied from the numerical solver of a dynamic model)

Usage

```
from.data.frame(df)
```

Arguments

<code>df</code>	data frame
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Value

object of class `aquaenv`

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

<code>lnK</code>	<i>lnK</i>
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Description

PRIVATE function: generic formula (see publication associated with AquaEnv) for K calculations that use the natural logarithm (ln)

Usage

`lnK(A, B, C, D, E, T)`

Arguments

A	coefficient A
B	coefficient B
C	coefficient C
D	coefficient D
E	coefficient E
T	temperature in Kelvin

Value

the ln of the K associated with the coefficients

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

<code>logK</code>	<i>logK</i>
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Description

PRIVATE function: generic formula (see publication associated with AquaEnv) for K calculations that use the decadal logarithm (log)

Usage

`logK(A, B, C, D, E, T)`

Arguments

A	coefficient A
B	coefficient B
C	coefficient C
D	coefficient D
E	coefficient E
T	temperature in Kelvin

Value

the log of the K associated with the coefficients

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`molal2molin`

molal2molin

Description

PRIVATE function: calculates the conversion factor converting from molality (mol/kg-H₂O) to molinity (mol/kg-solution) from salinity S

Usage

`molal2molin(S)`

Arguments

S	salinity S in practical salinity units (i.e. no unit)
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Value

the conversion factor from molality (mol/kg-H₂O) to molinity (mol/kg-solution)

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Roy1993b (the carbonic acid paper), DOE1994

<code>opendevice</code>	<i>opendevice</i>
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Description

PRIVATE function: opens a device for plotting; no return value, just side-effect

Usage

```
opendevice(device, size, filename)
```

Arguments

<code>device</code>	either "x11", "eps", or "pdf"
<code>size</code>	size of the plot device in the form c(width, height)
<code>filename</code>	filename to use if "eps" or "pdf" is used

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

<code>plotall</code>	<i>plotall</i>
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Description

PRIVATE function: plots all elements of an object of class aquaenv; no return value, just side-effect

Usage

```
plotall(aquaenv, xval, ...)
```

Arguments

<code>aquaenv</code>	object of class aquaenv
<code>xval</code>	x-value: the independent variable describing a change in elements of an object of class aquaenv
<code>...</code>	further arguments will be passed

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

revelle

revelle

Description

PRIVATE function: calculates the revelle factor

Usage

```
revelle(ae)
```

Arguments

ae object of class aquaenv

Value

the revelle factor

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Sundquist1979, Zeebe2001, Emerson2008

scaleconvert

scaleconvert

Description

PRIVATE function: provides pH scale conversion factors (caution: the activity coefficient for H⁺ (needed for NBS scale conversions) is calculated with the Davies equation (Zeebe2001) which is only accurate up to ionic strengthes of $I = 0.5$)

Usage

```
scaleconvert(S, t, p=0, SumH2SO4=NULL, SumHF=NULL, khf="dickson")
```

Arguments

S	salinity S in practical salinity units (i.e. no unit)
t	temperature in degrees centigrade
p	gauge pressure (total pressure minus atmospheric pressure) in bars
SumH2SO4	total sulfate concentration in mol/kg-solution; if not supplied this is calculated from S
SumHF	total fluoride concentration in mol/kg-solution; if not supplied this is calculated from S
khf	either "dickson" (default, Dickson1979a) or "perez" (using seacarb, Perez1987a) for K_HF

Value

a list of conversion factors "free2tot", "free2sws", etc.

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Dickson1984, DOE1994, Zeebe2001

seaconc	<i>seaconc</i>
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Description

PRIVATE function: calculates concentrations of constituents of natural seawater from a given salinity S

Usage

`seaconc(spec, S)`

Arguments

spec	constituent of seawater (chemical species) of which the concentration should be calculated. can be any name of the vectors ConcRelCl and MeanMolecularWeight: "Cl", "SO4", "Br", "F", "Na", "Mg", "Ca", "K", "Sr", "B", "S"
S	salinity S in practical salinity units (i.e. no unit)

Value

concentration of the constituent of seawater specified in spec in mol/kg-solution (molality): this is determined by the data in ConcRelCl and MeanMolecularWeight

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

DOE1994

`seadensity`

seadensity

Description

PRIVATE function: calculates seawater density (in kg/m³) from temperature (in degrees centigrade) and salinity

Usage

`seadensity(S, t)`

Arguments

<code>S</code>	salinity S in practical salinity units (i.e. no unit)
<code>t</code>	temperature in degrees centigrade

Value

seawater density in kg/m³

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

References

Millero1981, DOE1994

<code>selectplot</code>	<i>selectplot</i>
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Description

PRIVATE function: plots just the elements of an object of class `aquaenv` given in `what`; no return value, just side-effect

Usage

```
selectplot(aquaenv, xval, what, mfrow=c(1,1), size=c(7,7), ...)
```

Arguments

<code>aquaenv</code>	object of class <code>aquaenv</code>
<code>xval</code>	x-value: the independent variable describing a change in elements of an object of class <code>aquaenv</code>
<code>what</code>	vector of names of elements of <code>aquaenv</code> that should be plotted
<code>mfrow</code>	standard plot parameter; default: just one plot
<code>size</code>	the size of the plot device; default: 7 (width) by 7 (height) inches
<code>...</code>	further arguments will be passed

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

<code>splitS_K_CO2</code>	<i>splitS_K_CO2</i>
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Description

PRIVATE function: returns the intersection of the formulae for `K_CO2` for $S < 5$ and $S \geq 5$

Usage

```
splitS_K_CO2(T)
```

Arguments

<code>T</code>	temperature in Kelvin
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Value

the value for `S` where the two formulae intersect at temperature `T`

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)

`splitS_K_HCO3`

splitS_K_HCO3

Description

PRIVATE function: returns the intersection of the formulae for K_HCO3 for $S < 5$ and $S \geq 5$

Usage

`splitS_K_HCO3(T)`

Arguments

T temperature in Kelvin

Value

the value for S where the two formulae intersect at temperature T

Author(s)

Andreas F. Hofmann (a.hofmann@nioo.knaw.nl)