Package 'EqSolvR'

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Title Chemical Equilibrium Solver

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Description Package for solving chemical equilibria for a given set of reactants and products. The motivation for this program was to enable the calculation, between 300°C and 400°C at 0.5 kb, of pH and speciation given a simple mix of salts. This package has been writting in such a manner that an advanced user can easily set their own reactants, products and temperature in the generic version (chemsolve_generic). chemsolve_generic is the workhorse for chemsolve.

Depends R (>= 2.12)

Imports rootSolve

BugReports https://github.com/shearwavesplitter/EqSolvR/issues

License GPL (>= 3)

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1.9000

R topics documented:

chemsolve *Mass balance and charge solver*

Description

Mass balance and charge balance solver for chemical equilibria at 0.5 kb. This is a wrapper function for chemsolve_generic and prods.

Usage

```
chemsolve(Tc = 400, Nat = 0.2, Kt = 0.2, Clt = 0.4, SO4t = 0.2,
  Cat = 0.1, Mgt = 0.1, start = c(1e-05, 1e-05, 0.15, 0.15, 0.15,
  0.104756881, 0.05, 0.05), maxitr = 100, exprod = NULL, exconstit = NULL,
  exnumz = NULL, excharges = NULL, exa = NULL, exK = NULL,
  Clbal = TRUE)
```

Arguments

Tc	Temperature (degrees C - between 300 and 400)
Nat	Sodium concentration (mol/kg); total
Kt	Potassium (mol/kg); total
Clt	Chloride (mol/kg); total
SO4t	Sulphate (mol/kg); total
Cat	Calcium (mol/kg); total
Mgt	Magnesium (mol/kg); total
start	Initial guess for the calculated equilbrium concentrations of the basis species
maxitr	Maximum number of iterations The basis species are: Na+, K+, Mg2+, Ca2+, Cl-, SO42-. The default complexes are: NaCl°, KCl°, HCl°, KOH°, NaOH°, KSO4-, NaSO4-,HSO4-,CaSO4°,MgSO4°, MgCl+,CaCl+,CaCl2°,MgOH+,CaOH+.Additional complexes based on the existing basis species are easily added. If additional complexes are required then these may be added as follows (see example below):
exprod	A vector of the names of the complex(es)
exconstit	A vector of the chemical symbol names of the the basis species that are constitute each of the the additional complexes
exnumz	A vector of the stiochiometry given by the equilibrium reaction for each of the complexes
excharges	A vector of the charge of the complex species
exa	A vector of the ion size parameters for the complexes
exK	A vector of the log K of the dissociation constants

Details

A wrapper for the chemsolve_generic function that allow easy addition of product species. Use the generic function (chemsolve_generic) if new basis species need to be added or if the log K/temperature range is extended (up or down).
Normally total moles anions = total moles cations.
The charge balance (without any speciation) is adjusted to zero
by balancing against Cl as otherwise the calculation is too sensitive to H+.
Choose reasonable starting values; for H+, OH- and equilibrium concentrations of the basis species.
If negative concentrations are calculated, choose better initial starting values.
To exclude a basis value set the basis concentration to zero and the concentrations of this and the derived species
will be vanishing small and can be ignored.
Complex dissociation constants (Log K) are from SupCrt 92 slop98.dat http://geopig.asu.edu/?q=tools
The Debye_Hückel parameters (A, B) equations are polynomial fits to data at 0.5 kb from tables in Helgeson & Kirkham (1974).
Note Bdot is not used.
Helgeson H. C. and Kirkham D. H. (1974) Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: II. Debye-Hückel parameters for activity coefficients and relative partial molar properties American Journal of Science 274, 1199-1261.

Value

A list containing the concentrations, activity coefficients, and pH at equilibrium

Examples

```
## Add H2SO4 as an additional complex given the existing list of basis species
chemsolve(exprod="H2SO4",exconstit=c("H","H","SO4"),exnumz=3,excharges=0,exa=0,exK=-6)

##Determine the equilibria at a range of temperatures
temps <- seq(300,400,10) #A vector of temperatures repeating every 10 degrees from 300 to 400
r <- lapply(temps,chemsolve,Nat=0.2,Kt=0.2,Clt=0.4,SO4t=0.2,Cat=0.1,Mgt=0.1) #Creates a list of the results
r[[1]] #Display results from first temperature
r[[10]] #Display the results of the 10th temperature
```

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chemsolve_generic *Mass balance and charge solver for general cases*

Description

Mass balance and charge balance solver for chemical equilibria. This is the workhorse for chemsolve and requires the prods function

Usage

```
chemsolve_generic(solvent = c("H", "OH"), solvcharge = c("1", "-1"),
  solva = c("9", "4"), Ksoln = -10.908, species = c("Na", "K", "Cl",
  "SO4", "Ca", "Mg"), conc = c(0.2, 0.2, 0.4, 0.2, 0.1, 0.1), a = c(4, 3,
  3.5, 4, 6, 8), charges = c(1, 1, -1, -2, 2, 2), prod, A = 1.0529,
  B = 0.385, Bdot = 0, start = c(1e-05, 1e-05, 0.15, 0.15, 0.15,
  0.104756881, 0.05, 0.05), maxitr = 100, bal = NULL)
```

Arguments

solvent	Symbols for solvent species (should not be changed for water)
solvcharge	Charges for solvent species (should not be changed for water)
solva	Ion size parameters (should not be changed for water)
Ksoln	log K of the solvent (Water at 300 degrees C - changes with temperature)
species	Chemical symbols of the basis species
conc	Total concentrations of the basis species (mol/kg)
a	Ion size parameters for the basis species
prod	Dataframe detailing the derived species (Output from prods function)
A	A value (Defaults to value for 300 degrees C and 0.5kb)
B	B value (Defaults to value for 300 degrees C and 0.5kb)
Bdot	Bdot value is zero by default
start	Initial guess for the calculated equilibrium concentration of the basis species
maxitr	Maximum number of iterations

Details

A generic function to add any basis species, product species or if the log K/temperature range need to be extended. Requires all parameters (e.g. log K at the given temperature).

Value

A list containing the concentrations, gamma values, and pH at equilibrium

Examples

```
## Add H2SO4 as an additional complex given the existing list of basis species

## Define the product species NaCl and KCl
products <- prods(names=c("NaCl","KCl"),number=c(2,2),
+ species=c("Na","Cl","K","Cl"),K=c(-6.68,0.001),a=c(0,0))
Run chemsolve with Na, K, and Cl basis species at 300 degrees
Chemsolve_generic(species=c("Na","K","Cl"), conc=c(0.2,0.2,0.4),
+ a=c(4,3,3.5),charges=c(1,1,-1),prod,start=c(0.00001,0.00001,0.15),prod=products)
```

ktable *Table of K constants*

Description

Table of K constants

Usage

```
ktable
```

Format

A data frame containing K values at given temperatures

prods *Create prod dataframe*

Description

Creates the dataframe of the derived species for use in chemsolve_generic

Usage

```
prods(names = c("NaCl", "KCl"), number = c(2, 2), species = c("Na", "Cl",
  "K", "Cl"), K = c(-6.68, 0.001), a = c(0, 0))
```

Arguments

names	A vector of names of the species which react to form the basis species
number	A vector of the number of basis consituents for each of the product species given by the equilibrium equation
species	A vector of the chemical symbols of the product species in terms of the basis species
K	A vector of log K values for the product species
a	A vector of ion size parameters for the product species

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