Package 'EqSolvR'

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Title Chemical Equilibrium Solver

Version 1.1.0

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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, 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.

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.

Usage

```
chemsolve(Tc = 300, 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)
```

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 equalibrium concentration of the basis species
maxitr	Maximum number of iteration 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 complexe(s)
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 stiochiometery 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 paramters 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).
Charge balance is fixed on H+.
Normally total initial moles anions = total moles cations but excess anions will be balanced by more H+ and vice versa. It is important to choose good initial starting values; for H+, OH- and equilibrium concentrations of the basis species.
Complex dissociation constants (Log K) are from SupCrt 92 slop98.dat http://geopig.asu.edu/?q=tools
The Debye_Hückel parameters (A, B & Bdot) equations are polynomial fits to data from tables in Helgeson (1969) Helgeson & Kirkham (1974) by Nellie Olsen (Note Bdot not used at temperatures

greater than 300°C).
Helgeson H. C. (1969) Thermodynamics of hydrothermal systems at elevated temperatures and pressures. American Journal of Science 267, 729-804.
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

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, Tc = 300,
  start = c(1e-05, 1e-05, 0.15, 0.15, 0.15, 0.104756881, 0.05, 0.05),
  maxitr = 100)
```

Arguments

solvent	Symbols for solvent species (should not be changed)
solvcharge	Charges for solvent species (should not be changed)
solva	Ion size parameters (should not be changed)
Ksoln	log K of the solvent (should not be changed)
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
Tc	Temperature (degrees centigrade)
start	Initial guess for the calculated equalibrium 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,Tc=300,start=c(0.00001,0.00001,0.15),prod=products)
```

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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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