Package 'EqSolvR'

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Version 1.1.0

Title Chemical Equilibrium Solver

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Description Package for solving chemical equilibria for a given set of reactants and products

Depends R (>= 2.12)

Imports rootSolve

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

License GPL (>= 3)

Encoding UTF-8

LazyData true

RoxygenNote 6.0.1.9000

R topics documented:

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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)
Nat	Sodium concentration (mol/kg)
Kt	Potassium (mol/kg)
Clt	Chlorine (mol/kg)
SO4t	Sulphate (mol/kg)
Cat	Calcium (mol/kg)
Mgt	Magnesium (mol/kg)
start	Initial guess for the calculated equalibrium concentration of the basis species
maxitr	Maximum number of iteration
exprod	A vector of the names of the additional product species which react to form the basis species
exconstit	A vector of the chemical symbols of the additional product species in terms of the basis species
exnumz	A vector of the number of basis consituents for each of the additional product species given by the equilibrium equation
excharges	A vector of the total charage of the additional product species
exa	A vector of the ion size paramters for the additional species
exK	A vector of the log K values of the additional product species

Details

A wrapper for the chemsolve_generic function that allow easy addition of product species. If you want to add additional reactant species (i.e. basis species) then the chemsolve_generic function must be used

Value

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

Examples

```
## Add H2SO4 as an extra product species

chemsolve(exprod="H2SO4",exconstit="H","H","SO4",exnumz=3,excharges=0,exa=0,exa=-6)
```

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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

Value

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

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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

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prods   *Create prod dataframe*

Description

Creates the dataframe of the derived species for use in chemsolve

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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