eqdata: an R function to extract data from EQ6 output files

This function extracts computational results for aqueous species at each step of reaction progress in an EQ6 output file. The results are written to a comma-separated value file that can be read by other programs.

ingredients

- R (`http://www.r-project.org`) for your operating system
- eqdata.R
- EQ6 output file(s)

setup

- Install R.
- Start up R then find your working directory by typing the following:
  `getwd()`
- Copy eqdata.R and your EQ6 output files to your working directory.

operation

- Read eqdata.R into your R session:
  `source("eqdata.R")`
- Run eqdata by typing something like:
  `eqdata("rainbow2.6o",c("h+","sio2,aq","h2,aq"))`
  - The first argument is the name of the EQ6 output file.
  - The second argument is the list of aqueous species for which you want values. The `c()` function is R's concatenation function.
  - R has tab completion of file names, so you can type the opening quotation mark and the first few letters of the file name, then TAB to complete it. This can be helpful for entering complex file names.
  - The function reads the EQ6 output file and creates a CSV (comma-separated value) file called "`rainbow2.6o.log act.csv`" in your working directory. This file lists the "`log act`" (logarithm of activity) values for the indicated species at each successful step of ξ (i.e., "`zi`" in the EQ6 output). The temperature at each step is also listed.
  - If any of the aqueous species are not present in the EQ6 file, their values are listed as NA in the CSV file.
- If you want to get values other than "`log act`" you can run something like:
  `eqdata("rainbow2.6o",c("h+","sio2,aq","h2,aq"),"moles")`
  - The output CSV file in this case is named "`rainbow2.6o.moles.csv`".
  - Valid properties are any of those in the EQ6 aqueous species blocks, i.e., "`moles`", "`grams`", "`conc`", "`log conc`", "`log g`" or "`log act`". Specifying any other property will cause an error.