

Package ‘ch’

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Type Package

Title About some Small Functions

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Description The solution to some common problems is proposed, as well as a summary of some small functions. In particular, it provides a useful function for some problems in chemistry. For example, monoa(), monob() and mono() function can be used to calculate The pH of weak acid/base. The ggpng() function can save the PNG format with transparent background. The period_table() function will show the periodic table. Also the show_ruler() function will show the ruler. The show_color() function is funny and easier to show colors. I also provide the symb() function to generate multiple symbols at once. The csv2vcf() function provides an easy method to generate a file. The sym2poly() and sym2coef() function can extract coefficients from polynomials.

Imports ggplot2, clipr, Ryacas, magrittr, utils, grDevices, MASS, crayon, polynom, pracma

Suggests scales

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ch-package	<i>ch: some small functions</i>
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Description

It's about some functions in chem and other questions.

console_cl	<i>Remove '>' and '+' from the console and add '#' to the run result.</i>
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Description

First you need to copy the console area to the clipboard, then run the console_cl() function to add a comment to the line where the output is, and to cancel the > on the original line. Finally, the result of the run is saved to the clipboard.

Usage

```
console_cl(prefix = "#>")
```

Arguments

prefix	The prefix for code. The default is '#>'. You can edit it according to your own preference, but '#' should be the first character.
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Value

the result of the run is saved to the clipboard.

Author(s)

Chai

csv2vcf

about csv2vcf

Description

A simple method to generate vcf file.

Usage

```
csv2vcf(csv_file, vcf_file, header = FALSE)
```

Arguments

csv_file	The csv file contains names and phone numbers. The style is like this: Joey 18100 Hans 12788 Tim 34689 The first column is the name, the second column is the phone number corresponding to each person. The above is an example, and it is not true personal information summary.
vcf_file	The vcf file to create.
header	For more see read.csv , the default is FALSE.

Value

NULL. t will be saved in a file with the suffix vcf.

ggpng

Create a picture with a transparent background.

Description

Use the ImageMagick command line to convert the PDF saved by ggplot2 to PNG format with a transparent background and to set the resolution.

Usage

```
ggpng(x, dpi = 600, ...)
```

```
ggPNG(x, p, dpi = 600, ...)
```

Arguments

x	A file name that does not have a suffix.
dpi	The default dpi is 600. You can enhance the dpi value to produce a higher resolution PNG file.
...	see :ggsave
p	ggplot2 object

Details

You need to install ImageMagick! Please check if the ImageMagick is added to the environment variable.

this ggplot2 object will automatically add a theme with a transparent background.

Value

You will get a PNG file with the result drawn by ggplot2.

Author(s)

Chai

ground_state	<i>Ground-State spectral term</i>
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Description

Use such a function to calculate the spectral term, and it can show the number of the spectral term.

Usage

```
ground_state(x)
```

```
state_1(l, n)
```

```
state_2(x)
```

Arguments

x	'p2', 'p3', 'd2', 'd5', 'f2', ...
l	the l:0,1,2,3,4,5,...
n	the number of electrons.

Value

It is a display of the results of the calculation of the spectral term. For more explanation, please refer to the structural chemistry. The `ground_state()` function will tell you the ground state that spectral term of equal electrons. The `state_1()` and `state_2()` will tell you the spectral term of equal electrons.

Author(s)

Chai

References

The method of `state_1()` and `state_2()` function is from: DOI:10.14159/j.cnki.0441-3776.1985.11.020

And the url is: <https://t.cnki.net/kcms/detail?v=3uoqIhG8C44YL10AiTRKqd0WnNPv0wTDjtDUwHroNz8ZoQZVLjnVK&uniplatform=NZKPT> You can get more details from this essay.

Examples

```
ground_state("p2")
ground_state("f3")
state_2("p2")
state_2("d3")
```

lat_fmt

tex format and \$\$...\$\$

Description

output to Console and clipboard. You can better check the correctness of the output.

Usage

```
lat_fmt(x)
```

```
latex_fmt(x)
```

Arguments

x symbol object, for more see [ysym](#).

Value

`lat_fmt()` will output to Console. `latex_fmt()` will output to clipboard.

Author(s)

Chai

monoa

Calculate The pH of weak acid/base

Description

Calculate the pH of weak acid or base.

Usage

```
monoa(ka, c, digits = 2)
```

```
monob(ka, c, digits = 2)
```

```
mono(ka, c, digits = 2, acid = TRUE, kw = 1e-14)
```

Arguments

ka ionization constant.

c concentration.

digits digit of the output.

acid if TRUE, it is equivalent to monoa function; if FALSE, it is equivalent to monob function.

kw the default is 1e-14

Value

monoa() will return the pH of weak acid, the monob() will return the pH of weak base. And you can also use the mono() function to replace the monoa() function and monob() function.

Examples

```
monoa(1.4 - 6, 2.35e-2)
```

```
monoa(2.78e-8, 0.01)
```

```
monob(1.35e-5, 0.01)
```

```
monob(2.4 - 6, 1e-4)
```

period_table	<i>Draw the Periodic table</i>
--------------	--------------------------------

Description

use ggplot2 to draw the periodic table.

Usage

```
period_table()
```

Value

A ggplot2 object.

Author(s)

Chai

plot_table	<i>Use ggplot2 to plot a table</i>
------------	------------------------------------

Description

You can use plot_table to draw table in ggplot2, but it only applies to expressions(see [expression](#)). For more information , you can see [plotmath](#). But it's a ggplot2 object!

Usage

```
plot_table(Str, ncol, byrow = TRUE)
```

Arguments

Str	some expressions
ncol	the number f col
byrow	logical, the default is

Value

It will output a ggplot object that contains a table.

Author(s)

Chai

Examples

```
a1 <- c(
  "x %*% y", "x %/% y", "alpha", "sigma", "beta",
  "x == y", "frac(x,y)", "x %up% y", "hat(x)",
  "symbol(a)", "underline(x)"
)
plot_table(a1, 2)
plot_table(a1, 3)
```

read.txt	<i>Read the text to data.frame</i>
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Description

Read the strings and transform to the data.frame.

Usage

```
read.txt(text, header = TRUE, ...)
```

Arguments

text	strings
header	logical value
...	for more see read.table

Value

A data.frame

Author(s)

Chai

Round	<i>Round of Numbers that is improved.</i>
-------	---

Description

Round : rounding off to five in double. round_1 and Round2: to achieve the standard sense of rounding.

Usage

```
Round(x, n = 0)
```

```
round_1(x, n)
```

```
Round2(x, n)
```

Arguments

x vector or matrix

n digits

Value

It rounds the values and output to console.

Author(s)

Chai

scan.str *Read string into a vector*

Description

Read data into a vector from a string.

Usage

```
scan.str(string)
```

Arguments

string a string that number is separated by ' '.

Value

A vector that contains numbers.

Author(s)

Chai

Examples

```
m <- "12 23 45 78 90 89 97"  
scan.str(m)
```

`show_color`*An easy way to show colors in ggplot2*

Description

the same function can see [show_col](#), but it is a ggplot2 object. You can use it like the `show_col()` function in scales package, but it can save by `ggsave()` function.

Usage

```
show_color(  
  colors,  
  ncol,  
  byrow = TRUE,  
  label = FALSE,  
  number = FALSE,  
  size = 1,  
  border = "black"  
)
```

Arguments

<code>colors</code>	string about colors
<code>ncol</code>	the number of col
<code>byrow</code>	logical
<code>label</code>	logical
<code>number</code>	logical, the default is
<code>size</code>	the size of label, the default is 1.
<code>border</code>	The color of border

Author(s)

Chai

`show_ruler`*Use ggplot to draw ruler*

Description

You can draw a ruler that uses ggplot2. Also It's funny and you can get a lot of methods from this function.

Usage

```
show_ruler(len = 5)
```

Arguments

len the length of ruler

Value

A ggplot2 object.

Author(s)

Chai

sym2poly *Extracting coefficients from polynomials*

Description

sym2poly can extract coefficients from polynomials and gives the roots of polynomials. The roots is calculated from [polyroot](#) and the [polyroots](#) function.

Usage

```
sym2poly(x, var = "x")
```

```
sym2coef(x, var = "x")
```

Arguments

x The polynomials, for examples, '3x² + 6x⁶ + 2 + 25*x'.

var, The var from polynomials, for examples, the var of '3x² + x⁶ + x⁸ + x⁵²' is 'x'.

Value

sym2poly() returns Coefficients and the roots. sym2coef() only returns coefficients.

Author(s)

Chai

Examples

```
sym2poly("3*x^2 + x^5 + x*8")
```

`symb`*Generating multiple symbols at once*

Description

It may be faster than using `ysym`.

Usage

```
symb(..., envir = parent.frame(), quiet = FALSE)
```

Arguments

<code>...</code>	The multiple vectors.
<code>envir</code>	The environment.
<code>quiet</code>	If FALSE, it will show the message in the end.

Value

The multiple symbols.

Author(s)

Chai

Examples

```
library(Ryacas)
symb(x, y, z)
str(x)
```

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