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 *ch: some small functions*

Description

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

console_cl *Remove '>' and '+' from the console and add '#' to the run result.*

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.

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` *Ground-State spectral term*

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=3uoqIhG8C44YLTlOAiTRKqd0WnNPv0wTDjtDUwHroNz8ZoQZVLjnVKa` `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 *Draw the Periodic table*

Description

use ggplot2 to draw the periodic table.

Usage

```
period_table()
```

Value

A ggplot2 object.

Author(s)

Chai

plot_table *Use ggplot2 to plot a table*

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` *Read the text to data.frame*

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` *Round of Numbers that is improved.*

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

colors	string about colors
ncol	the number f col
byrow	logical
label	logical
number	logical, the default is
size	the size of label, the default is 1.
border	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

sym2ploy 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, ’3x^2 + 6x^6 + 2 + 25*x’.

`var,` The var from polynomials, for examples, the var of ’3x^2 + x^6 + x8 + x*5^2’ 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(), quite = FALSE)
```

Arguments

`...`	The multiple vectors.
`envir`	The environment.
`quite`	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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