

Package ‘rxylib’

July 17, 2017

Type Package

Title Import XY-Data into R

Description Provides access to the 'xylib' C library for to import xy data from powder diffraction, spectroscopy and other experimental methods.

Version 0.2.0

Date 2017-XX-XX

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URL <https://github.com/R-Lum/rxylib>

BugReports <https://github.com/R-Lum/rxylib/issues>

License GPL-3 | LGPL-2.1

Depends R (>= 3.3.0), utils

Imports methods, Rcpp (>= 0.12.11)

Suggests testthat (>= 1.0.2)

LinkingTo Rcpp (>= 0.12.11), BH (>= 1.62.0-1)

Encoding UTF-8

Collate 'methods_rxylib.R' 'rxylib.R' 'RcppExports.R' 'read_xyData.R'

RoxygenNote 6.0.1

NeedsCompilation yes

R topics documented:

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rxylib-package

*Import XY-Data into R***Description**

Provides access to the 'xylib' C library for to import xy data from powder diffraction, spectroscopy and other experimental methods, like gamma-ray spectrometry.

Package: rxylib
 Type: Package
 Version: 0.2.0
 Date: 2017-XX-XX
 License: GPL-3 | LGPL-2.1 (for the C++ library 'xylib')

Details

Supported data formats library version: 1.6.0

| ID | NAME | DESCRIPTION | FILE EXTENSION | VALID_OPTIONS | DATATYPE |
|-------|--------------|----------------------------------|-------------------|---------------|----------|
| [1,] | cpi | Sietronics Sieray CPI | cpi | | ascii |
| [2,] | uxd | Bruker Diffrac-AT UXD | uxd | | ascii |
| [3,] | rigaku_dat | Rigaku DAT | dat | | ascii |
| [4,] | bruker_raw | Siemens/Bruker RAW | raw | | binary |
| [5,] | bruker_spc | Bruker ESP300-E SPC | spc | | binary |
| [6,] | vamas | VAMAS ISO-14976 | vms | | ascii |
| [7,] | philips_udf | Philips UDF | udf | | ascii |
| [8,] | spe | PI WinSpec SPE | spe | | binary |
| [9,] | pdcif | Powder Diffraction CIF | cif | | ascii |
| [10,] | philips_rd | Philips PC-APD RD/SD | rd sd | | binary |
| [11,] | xrdml | PANalytical XRDML | xrdml | | ascii |
| [12,] | canberra_mca | Canberra MCA | mca dat | | binary |
| [13,] | canberra_cnf | Canberra CNF | cnf | | binary |
| [14,] | xfit_xdd | XFIT XDD | xdd | | ascii |
| [15,] | riet7 | RIET7/LHPM/PSI_DMC | dat | | ascii |
| [16,] | dbws | DBWS data | dbw rit neu | | ascii |
| [17,] | chiplot | ChiPLOT data | chi | | ascii |
| [18,] | spectra | Spectra / VGX 900 | 1 2 3 4 5 6 7 8 9 | | ascii |
| [19,] | specsxy | SPECS SpecsLab2 xy | xy | | ascii |
| [20,] | csv | CSV or TSV | csv tsv tab | decimal-comma | ascii |
| [21,] | xsyg | Freiberg Instruments (FI) Lexsyg | xsyg | | ascii |

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France), Johannes Friedrich (University of Bayreuth, Germany), RLum Team (family support), Marcin Wojdyr (maintainer and author of the C++ library 'xylib'), Peng Zhang (author of the C++ library 'xylib')

| | |
|----------------|-----------------------|
| methods_rxylib | <i>methods_rxylib</i> |
|----------------|-----------------------|

Description

S3-methods support by the package rxylib. Listed functions can be passed directly into S3 generics (e.g., [plot](#), [print](#)) without reshaping the data.

Usage

```
## S3 method for class 'rxylib'
print(x, ...)

## S3 method for class 'rxylib'
plot(x, block = NULL, ...)
```

Arguments

| | |
|-------|---|
| x | (required) : input object |
| ... | further arguments that can be passed to the method |
| block | numeric (with default): select block for plotting, e.g. c(1:2). |

| | |
|-------------|--|
| read_xyData | <i>Import xy-Data for Supported Formats into R</i> |
|-------------|--|

Description

The function provides access to the underlying xylib to import data for supported file formats into R. In most cases, only the file path is needed with further arguments to import the data. The function automatically recognises allowed formats. See [rxylib-package](#) for supported formats.

Usage

```
read_xyData(file, options = "", verbose = TRUE, metaData = TRUE)
```

Arguments

| | |
|----------|--|
| file | character (required) : path and file to be imported. The argument accepts an URL. |
| options | character (with default): set format options (see rxylib-package) |
| verbose | logical (with default): enables/disables verbose mode |
| metaData | logical (with default): enables/disables the export of metadata |

Value

The functions returns a [list](#) of matrices.

Function version

0.2.1

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France), Johannes Friedrich,
University of Bayreuth (Germany)

Examples

```
##load example dataset
file <- system.file("extdata/ExampleSpectrum.CNF", package = "rxylib")
results <- read_xyData(file)
results

##plot xy-spectrum
plot(results,
      type = "l",
      log = "y",
      xlab = "Energy [keV]",
      ylab = "Counts",
      main = "Thorite - 1800 s")

mtext(side = 3, "Canberra Inspector 1000, 3 x 3 NaI probe")

##plot contour for TL-spectrum
##imported from an XSYG-file
spectrum <- read_xyData(system.file("extdata/TLspectrum.xsyg", package = "rxylib"))
contour(
  x = spectrum$dataset[[1]]$data_block[,1],
  y = 1:ncol(spectrum$dataset[[1]]$data_block[, -1]),
  z = spectrum$dataset[[1]]$data_block[, -1],
  xlab = "Wavelength [nm]",
  ylab = "#Channel",
  main = "TL Spectrum")
```

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