

Package ‘rxylib’

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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 0.2.1

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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'
'convert_xy2TKA.R'

RoxygenNote 6.0.1

NeedsCompilation yes

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rxylib-package	<i>Import XY-Data into R</i>
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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: 0.2.1
Date: 2017-12-20
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	B
[1,]	cpi	Sietronics Sieray CPI	cpi		ascii	si
[2,]	uxd	Bruker Diffrac-AT UXD	uxd		ascii	m
[3,]	rigaku_dat	Rigaku DAT	dat		ascii	m
[4,]	bruker_raw	Siemens/Bruker RAW	raw		binary	m
[5,]	bruker_spc	Bruker ESP300-E SPC	spc		binary	si
[6,]	vamas	VAMAS ISO-14976	vms		ascii	m
[7,]	philips_udf	Philips UDF	udf		ascii	si
[8,]	spe	PI WinSpec SPE	spe		binary	m
[9,]	pdcif	Powder Diffraction CIF	cif		ascii	m
[10,]	philips_rd	Philips PC-APD RD/SD	rd sd		binary	si
[11,]	xrdml	PANalytical XRDML	xrdml		ascii	m
[12,]	canberra_mca	Canberra MCA	mca dat		binary	si
[13,]	canberra_cnf	Canberra CNF	cnf		binary	si
[14,]	xfit_xdd	XFIT XDD	xdd		ascii	si
[15,]	riet7	RIET7/LHPM/PSI_DMC	dat		ascii	si
[16,]	dbws	DBWS data	dbw rit neu		ascii	si
[17,]	chiplot	ChiPLOT data	chi		ascii	si

[18,]	spectra	Spectra / VGX 900	1 2 3 4 5 6 7 8 9	ascii	m
[19,]	specsxy	SPECS SpecsLab2 xy	xy	ascii	m
[20,]	csv	CSV or TSV	csv tsv tab	decimal-comma	si
[21,]	xsyg	Freiberg Instruments (FI) Lexsyg	xsyg	ascii	m

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')

convert_xy2TKA	<i>Convert xy-data to TKA</i>
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Description

Convert data to the Toolkit file format (TKA) as exported by, e.g., by the software Canberra Genie 2000.

Usage

```
convert_xy2TKA(object, file = NULL, overwrite = FALSE)
```

Arguments

object	rxylib (required) : xy data as imported by the function read_xyData . Optional a file supported by the rxylib-package can be provided as input. Arguments can be provided as list .
file	character (optional) : optional file path or file name for the output to be written. If only a path is provided the output file name is derived from the input file name. Argument can be provided as list .
overwrite	logical (with default) : force overwriting of existing files if TRUE.

Details**Supported formats**

- Canberra CNF
- further formats on request ...

Value

Returns a [list](#) of [matrix](#) objects or an output TKA-file.

Function version

0.1.0

Author(s)

Sebastian Kreuzer, IRAMAT-CRP2A, Université Bordeaux Montaigne (France)

Examples

```
##convert CNF data
convert_xy2TKA(
  object = system.file("extdata/ExampleSpectrum.CNF", package = "rxylib"))

## Not run:
##export as file
convert_xy2TKA(
  object = system.file("extdata/ExampleSpectrum.CNF", package = "rxylib"),
  file = "~/Desktop/")

## End(Not run)
```

methods_rxylib

methods_rxylib

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`*Import xy-Data for Supported Formats into R*

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

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

Value

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

Function version

0.3.0

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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