Package 'rxylib'

February 20, 2022

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 0.2.7

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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 (>= 4.0), utils

Imports methods, Rcpp (>= 1.0.8)

Suggests testthat (>= 3.1.0)

LinkingTo Rcpp (>= 1.0.8), BH (>= 1.78.0)

Encoding UTF-8

Language en-GB

Collate 'methods_rxylib.R' 'rxylib.R' 'RcppExports.R' 'read_xyData.R' 'convert_xy2TKA.R'

RoxygenNote 7.1.2

NeedsCompilation yes

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R topics documented:

`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.

License: GPL-3 | LGPL-2.1 (for the C++ library 'xylib')

Details

Funding

Between 2017-2019, the work of Sebastian Kreutzer as maintainer of the package was supported by LabEx LaScArBx (ANR - n. ANR-10-LABX-52).

Supported data formats:
library version: 1.6.0

ID	NAME	DESCRIPTION	FILE EXTENSION	VALID_OPTIONS	DATATYPE	BLOC
[1,]	cpi	Sietronics Sieray CPI	cpi		ascii	single
[2,]	uxd	Bruker Diffrac-AT UXD	uxd		ascii	multipl
[3,]	rigaku_dat	Rigaku DAT	dat		ascii	multipl
[4,]	bruker_raw	Siemens/Bruker RAW	raw		binary	multipl
[5,]	bruker_spc	Bruker ESP300-E SPC	spc		binary	single
[6,]	vamas	VAMAS ISO-14976	vms		ascii	multipl
[7,]	philips_udf	Philips UDF	udf		ascii	single
[8,]	spe	PI WinSpec SPE	spe		binary	multipl
[9,]	pdcif	Powder Diffraction CIF	cif		ascii	multipl
[10,]	philips_rd	Philips PC-APD RD/SD	rd sd		binary	single
[11,]	xrdml	PANalytical XRDML	xrdml		ascii	multipl
[12,]	canberra_mca	Canberra MCA	mca dat		binary	single
[13,]	canberra_cnf	Canberra CNF	cnf		binary	single
[14,]	xfit_xdd	XFIT XDD	xdd		ascii	single
[15,]	riet7	RIET7/LHPM/PSI_DMC	dat		ascii	single
[16,]	dbws	DBWS data	dbw rit neu		ascii	single
[17,]	chiplot	ChiPLOT data	chi		ascii	single

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

Author(s)

Sebastian Kreutzer, Geography & Earth Sciences, Aberystwyth University (United Kingdom), 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` *Convert xy-data to TKA*

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

How to cite

Kreutzer, S., 2022. convert_xy2TKA(): Convert xy-data to TKA. Function version 0.1.0. In: Kreutzer, S., Friedrich, J., 2022. rxylib: Import XY-Data into R . R package version 0.2.7. https://github.com/R-Lum/rxylib

Author(s)

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

Examples

```
##convert CNF data (no export to file system)
convert_xy2TKA(
 object = system.file("extdata/ExampleSpectrum.CNF", package = "rxylib"))

## Not run:
##export as file

##create temporary filepath
##(for usage replace by own path)
temp_file <- tempfile(pattern = "output", fileext = ".TKA")

##convert and write to file system
convert_xy2TKA(
 object = system.file("extdata/ExampleSpectrum.CNF", package = "rxylib"),
 file = temp_file)


## 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

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

0.3.0

How to cite

Kreutzer, S., Friedrich, J., 2022. read_xyData(): Import xy-Data for Supported Formats into R. Function version 0.3.0. In: Kreutzer, S., Friedrich, J., 2022. rxylib: Import XY-Data into R . R package version 0.2.7. https://github.com/R-Lum/rxylib

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université 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",
 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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