Package 'rxylib'

January 4, 2023

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 0.2.9

Date 2023-01-04

Author Sebastian Kreutzer [aut, trl, cre] (<https://orcid.org/0000-0002-0734-2199>), Johannes Friedrich [aut] (<https://orcid.org/0000-0002-0805-9547>), RLum Team [ctb], Marcin Wojdyr [cph] (C++ library 'xylib'), Peng Zhang [cph] (C++ library 'xylib')

Maintainer Sebastian Kreutzer <sebastian.kreutzer@uni-heidelberg.de>

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

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

License GPL-3 | LGPL-2.1

Depends R (>= 4.1), utils

Imports methods, Rcpp (>= 1.0.9)

Suggests testthat (>= 3.1.4)

LinkingTo Rcpp (>= 1.0.9), 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 7.2.3

NeedsCompilation yes

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).

From 01/2020-04/2022, Sebastian Kreutzer received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 844457 (project: CREDit).

Supported data formats:
library version: 1.6.0

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

Author(s)

Sebastian Kreutzer, Institute of Geography, Ruprecht-Karl-University of Heidelberg (Germany), 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

0.1.1

How to cite

Kreutzer, S., 2023. convert_xy2TKA(): Convert xy-data to TKA. Function version 0.1.1. In: Kreutzer, S., Friedrich, J., 2023. rxylib: Import XY-Data into R . R package version 0.2.9. https://github.com/R-LumR/rxylib

Author(s)

Sebastian Kreutzer, Institute of Geography, Universität Heidelberg, Germany

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., 2023. read_xyData(): Import xy-Data for Supported Formats into R. Function version 0.3.0. In: Kreutzer, S., Friedrich, J., 2023. rxylib: Import XY-Data into R . R package version 0.2.9. https://github.com/R-Lum/rxylib

Author(s)

Sebastian Kreutzer, Institute of Geography, Ruprecht-Karl-University of Heidelberg (Germany), 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")
```

Index