

Package ‘powdR’

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Type Package

Title Full Pattern Summation of X-Ray Powder Diffraction Data

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Description Full pattern summation of X-ray powder diffraction data as described in Chipera and Bish (2002) <doi:10.1107/S0021889802017405>. Derives quantitative estimates of crystalline and amorphous phase concentrations in complex mixtures.

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URL <http://github.com/benmbutler/powdR>

BugReports <http://github.com/benmbutler/powdR/issues>

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R topics documented:

afps	2
afps.powdRlib	4
bkg	8
fps	9
fps.powdRlib	11
minerals	15
minerals_phases	15
minerals_xrd	16
plot.powdRafps	16
plot.powdRbkg	17
plot.powdRfps	18
plot.powdRlib	19
powdR	20
powdRlib	20
rockjock	21
rockjock_mixtures	22
run_powdR	23
soils	23
subset.powdRlib	24
summarise_mineralogy	25
Index	27

afps	<i>Automated full pattern summation</i>
------	---

Description

afps returns estimates of phase concentrations using automated full pattern summation of X-ray powder diffraction data. It is designed for high-throughput cases involving mineral quantification from large reference libraries. For more details see `?afps.powdRlib`.

Usage

```
afps(lib, ...)
```

Arguments

lib	A <code>powdRlib</code> object representing the reference library. Created using the <code>powdRlib</code> constructor function.
...	Other parameters passed to methods e.g. <code>afps.powdRlib</code>

Details

Applies automated full pattern summation to an XRPD measurement to quantify phase concentrations. Requires a `powdRlib` library of reference patterns with reference intensity ratios in order to derive mineral concentrations.

Value

a list with components:

tth	a vector of the 2theta scale of the fitted data
fitted	a vector of the fitted XRPD pattern
measured	a vector of the original XRPD measurement (aligned)
residuals	a vector of the residuals (fitted vs measured)
phases	a dataframe of the phases used to produce the fitted pattern
phases_grouped	the phases dataframe grouped by phase_name and summed
rwp	the Rwp of the fitted vs measured pattern
weighted_pure_patterns	a dataframe of reference patterns used to produce the fitted pattern. All patterns have been weighted according to the coefficients used in the fit
coefficients	a named vector of coefficients used to produce the fitted pattern
inputs	a list of input arguments used in the function call

References

Chipera, S.J., Bish, D.L., 2013. Fitting Full X-Ray Diffraction Patterns for Quantitative Analysis: A Method for Readily Quantifying Crystalline and Disordered Phases. *Adv. Mater. Phys. Chem.* 03, 47-53. doi:10.4236/amc.2013.31A007

Chipera, S.J., Bish, D.L., 2002. FULLPAT: A full-pattern quantitative analysis program for X-ray powder diffraction using measured and calculated patterns. *J. Appl. Crystallogr.* 35, 744-749. doi:10.1107/S0021889802017405

Eberl, D.D., 2003. User's guide to RockJock - A program for determining quantitative mineralogy from powder X-ray diffraction data. Boulder, CA.

Examples

```
#Load the minerals library
data(minerals)

# Load the soils data
data(soils)

## Not run:
afps_sand <- afps(lib = minerals,
                 smpl = soils$sandstone,
                 std = "QUA.2",
                 align = 0.2,
                 lod = 0.2,
                 amorphous = "ORG",
                 amorphous_lod = 1)

afps_lime <- afps(lib = minerals,
                 smpl = soils$limestone,
                 std = "QUA.2",
```

```
      align = 0.2,
      lod = 0.2,
      amorphous = "ORG",
      amorphous_lod = 1)

afps_granite <- afps(lib = minerals,
                    smpl = soils$granite,
                    std = "QUA.2",
                    align = 0.2,
                    lod = 0.2,
                    amorphous = "ORG",
                    amorphous_lod = 1)

#Alternatively run all 3 at once using lapply

afps_soils <- lapply(soils, afps,
                    lib = minerals,
                    std = "QUA.2",
                    align = 0.2,
                    lod = 0.2,
                    amorphous = "ORG",
                    amorphous_lod = 1)

#Automated quantification using the rockjock library

data(rockjock)
data(rockjock_mixtures)

#This takes a few minutes to run
rockjock_a1 <- afps(lib = rockjock,
                  smpl = rockjock_mixtures$Mix1,
                  std = "CORUNDUM",
                  align = 0.3,
                  lod = 1)

#Quantifying the same sample but defining the internal standard
#concentration (also takes a few minutes to run):
rockjock_a1s <- afps(lib = rockjock,
                   smpl = rockjock_mixtures$Mix1,
                   std = "CORUNDUM",
                   std_conc = 20,
                   align = 0.3,
                   lod = 1)

## End(Not run)
```

Description

afps.powdRlib returns estimates of phase concentrations using automated full pattern summation of X-ray powder diffraction data. It is designed for high-throughput cases involving mineral quantification from large reference libraries.

Usage

```
## S3 method for class 'powdRlib'
afps(lib, smpl, harmonise, solver, obj, std, force,
      std_conc, tth_align, align, manual_align, shift, shift_res, tth_fps, lod,
      amorphous, amorphous_lod, ...)
```

Arguments

lib	A powdRlib object representing the reference library. Created using the powdRlib constructor function.
smpl	A data frame. First column is 2theta, second column is counts
harmonise	logical parameter defining whether to harmonise the lib and smpl. Default = TRUE. Harmonises to the intersecting 2theta range at the coarsest resolution available.
solver	The optimisation routine to be used. One of c("BFGS", "Nelder-Mead", "CG" or "L-BFGS-B"). Default = "BFGS".
obj	The objective function to minimise. One of c("Delta", "R", "Rwp"). Default = "Rwp". See Chipera and Bish (2002) and page 247 of Bish and Post (1989) for definitions of these functions.
std	The phase ID (e.g. "QUA.1") to be used as internal standard. Must match an ID provided in the phases parameter.
force	An optional string of phase ID's specifying which phases should not be forced to remain throughout the automated full pattern summation.
std_conc	The concentration of the internal standard (if known) in weight percent. If unknown then use std_conc = NA, in which case it will be assumed that all phases sum to 100 percent (default).
tth_align	A vector defining the minimum and maximum 2theta values to be used during alignment. If not defined, then the full range is used.
align	The maximum shift that is allowed during initial 2theta alignment (degrees). Default = 0.1.
manual_align	A logical operator denoting whether to optimise the alignment within the negative/position 2theta range defined in the align argument, or to use the specified value of the align argument for alignment of the sample to the standards. Default = FALSE, i.e. alignment is optimised.
shift	The maximum shift (degrees 2theta) that is allowed during the grid search phases selected from the non-negative least squares. Default = 0.05).
shift_res	A single integer defining the increase in resolution used during grid search shifting. Higher values facilitate finer shifts at the expense of longer computation. Default = 4.

tth_fps	A vector defining the minimum and maximum 2theta values to be used during automated full pattern summation. If not defined, then the full range is used.
lod	Optional parameter used to define the limit of detection (in weight percent) of the internal standard (i.e. the phase provided in the <code>std</code> argument). The <code>lod</code> value is used to estimate the lod of other phases during the fitting process and hence remove reference patterns that are considered below detection limit. Default = 0.1. If <code>lod = 0</code> then limits of detection are not computed.
amorphous	A character string of any phase id's that should be treated as amorphous. Each must match a <code>phase_id</code> in the phases table of 'lib'.
amorphous_lod	Optional parameter used to exclude amorphous phases if they are below this specified limit (percent). Must be between 0 and 100. Default = 0.
...	other arguments

Details

Applies automated full pattern summation to an XRPD sample to quantify phase concentrations. Requires a `powdRlib` library of reference patterns with reference intensity ratios in order to derive mineral concentrations.

Value

a list with components:

tth	a vector of the 2theta scale of the fitted data
fitted	a vector of the fitted XRPD pattern
measured	a vector of the original XRPD measurement (aligned)
residuals	a vector of the residuals (fitted vs measured)
phases	a dataframe of the phases used to produce the fitted pattern
phases_grouped	the phases dataframe grouped by <code>phase_name</code> and summed
rwp	the Rwp of the fitted vs measured pattern
weighted_pure_patterns	a dataframe of reference patterns used to produce the fitted pattern. All patterns have been weighted according to the coefficients used in the fit
coefficients	a named vector of coefficients used to produce the fitted pattern
inputs	a list of input arguments used in the function call

References

- Bish, D.L., Post, J.E., 1989. Modern powder diffraction. Mineralogical Society of America.
- Chipera, S.J., Bish, D.L., 2013. Fitting Full X-Ray Diffraction Patterns for Quantitative Analysis: A Method for Readily Quantifying Crystalline and Disordered Phases. *Adv. Mater. Phys. Chem.* 03, 47-53. doi:10.4236/ampc.2013.31A007
- Chipera, S.J., Bish, D.L., 2002. FULLPAT: A full-pattern quantitative analysis program for X-ray powder diffraction using measured and calculated patterns. *J. Appl. Crystallogr.* 35, 744-749. doi:10.1107/S0021889802017405
- Eberl, D.D., 2003. User's guide to RockJock - A program for determining quantitative mineralogy from powder X-ray diffraction data. Boulder, CA.

Examples

```
#Load the minerals library
data(minerals)

# Load the soils data
data(soils)

## Not run:
afps_sand <- afps(lib = minerals,
                 smpl = soils$sandstone,
                 std = "QUA.2",
                 align = 0.2,
                 lod = 0.2,
                 amorphous = "ORG",
                 amorphous_lod = 1)

afps_lime <- afps(lib = minerals,
                 smpl = soils$limestone,
                 std = "QUA.2",
                 align = 0.2,
                 lod = 0.2,
                 amorphous = "ORG",
                 amorphous_lod = 1)

afps_granite <- afps(lib = minerals,
                    smpl = soils$granite,
                    std = "QUA.2",
                    align = 0.2,
                    lod = 0.2,
                    amorphous = "ORG",
                    amorphous_lod = 1)

#Alternatively run all 3 at once using lapply

afps_soils <- lapply(soils, afps,
                    lib = minerals,
                    std = "QUA.2",
                    align = 0.2,
                    lod = 0.2,
                    amorphous = "ORG",
                    amorphous_lod = 1)

#Automated quantification using the rockjock library

data(rockjock)
data(rockjock_mixtures)

#This takes a few minutes to run
rockjock_a1 <- afps(lib = rockjock,
                  smpl = rockjock_mixtures$Mix1,
                  std = "CORUNDUM",
                  align = 0.3,
```

```

lod = 1)

#Quantifying the same sample but defining the internal standard
#concentration (also takes a few minutes to run):
rockjock_a1s <- afps(lib = rockjock,
                    smpl = rockjock_mixtures$Mix1,
                    std = "CORUNDUM",
                    std_conc = 20,
                    align = 0.3,
                    lod = 1)

## End(Not run)

```

bkg

Fit a background to XRPD data

Description

bkg fits a background to X-Ray Powder Diffraction data

Usage

```
bkg(xrd, lambda, hwi, it, int)
```

Arguments

xrd	an xy data frame of the data to fit a background to. First column is the 2theta scale, second column is count intensities
lambda	second derivative penalty for primary smoothing. Default = 0.5.
hwi	Half width of local windows. Default = 25.
it	Number of iterations in suppression loop. Default = 50.
int	Number of buckets to divide the data into. Default = round(nrow(xrd)/4).

Details

A wrapper for the `baseline.fillPeaks` in the `baseline` package.

Value

a list of 3 vectors

tth	The 2theta axis of the measurement
counts	The count intensities of the measurement
background	The fitted background

Examples

```
data(soils)
fit_bkg <- bkg(soils$granite)
```

 fps

Full pattern summation

Description

fps returns estimates of phase concentrations using full pattern summation of X-ray powder diffraction data. For more details see `?fps.powdRlib`.

Usage

```
fps(lib, ...)
```

Arguments

lib	A powdRlib object representing the reference library. Created using the powdRlib constructor function.
...	Other parameters passed to methods e.g. fps.powdRlib

Details

Applies full pattern summation (Chipera & Bish, 2002, 2013; Eberl, 2003) to an XRPD measurement to quantify phase concentrations. Requires a powdRlib library of reference patterns with reference intensity ratios in order to derive mineral concentrations.

Value

a list with components:

tth	a vector of the 2theta scale of the fitted data
fitted	a vector of the fitted XRPD pattern
measured	a vector of the original XRPD measurement (aligned)
residuals	a vector of the residuals (fitted vs measured)
phases	a dataframe of the phases used to produce the fitted pattern
phases_grouped	the phases dataframe grouped by phase_name and summed
rwp	the Rwp of the fitted vs measured pattern
weighted_pure_patterns	a dataframe of reference patterns used to produce the fitted pattern. All patterns have been weighted according to the coefficients used in the fit
coefficients	a named vector of coefficients used to produce the fitted pattern
inputs	a list of input arguments used in the function call

References

Chipera, S.J., Bish, D.L., 2013. Fitting Full X-Ray Diffraction Patterns for Quantitative Analysis: A Method for Readily Quantifying Crystalline and Disordered Phases. *Adv. Mater. Phys. Chem.* 03, 47-53. doi:10.4236/ampc.2013.31A007

Chipera, S.J., Bish, D.L., 2002. FULLPAT: A full-pattern quantitative analysis program for X-ray powder diffraction using measured and calculated patterns. *J. Appl. Crystallogr.* 35, 744-749. doi:10.1107/S0021889802017405

Eberl, D.D., 2003. User's guide to RockJock - A program for determining quantitative mineralogy from powder X-ray diffraction data. Boulder, CA.

Examples

```
#Load the minerals library
data(minerals)

# Load the soils data
data(soils)

#Since the reference library is relatively small,
#the whole library can be used at once to get an
#estimate of the phases within each sample.
## Not run:
fps_sand <- fps(lib = minerals,
               smpl = soils$sandstone,
               refs = minerals$phases$phase_id,
               std = "QUA.1",
               align = 0.2)

fps_lime <- fps(lib = minerals,
               smpl = soils$limestone,
               refs = minerals$phases$phase_id,
               std = "QUA.1",
               align = 0.2)

fps_granite <- fps(lib = minerals,
                  smpl = soils$granite,
                  refs = minerals$phases$phase_id,
                  std = "QUA.1",
                  align = 0.2)

#Alternatively run all 3 at once using lapply

fps_soils <- lapply(soils, fps,
                   lib = minerals,
                   std = "QUA.2",
                   refs = minerals$phases$phase_id,
                   align = 0.2)

#Using the rockjock library:

data(rockjock)
```

```

data(rockjock_mixtures)

rockjock_1 <- fps(lib = rockjock,
  smpl = rockjock_mixtures$Mix1,
  refs = c("ORDERED_MICROCLINE",
    "LABRADORITE",
    "KAOLINITE_DRY_BRANCH",
    "MONTMORILLONITE_WYO",
    "ILLITE_1M_RM30",
    "CORUNDUM"),
  std = "CORUNDUM",
  align = 0.3)

#Alternatively you can specify the internal standard
#concentration if known:
rockjock_1s <- fps(lib = rockjock,
  smpl = rockjock_mixtures$Mix1,
  refs = c("ORDERED_MICROCLINE",
    "LABRADORITE",
    "KAOLINITE_DRY_BRANCH",
    "MONTMORILLONITE_WYO",
    "ILLITE_1M_RM30",
    "CORUNDUM"),
  std = "CORUNDUM",
  std_conc = 20,
  align = 0.3)

## End(Not run)

```

 fps.powdRlib

Full pattern summation

Description

fps.powdRlib returns estimates of phase concentrations using full pattern summation of X-ray powder diffraction data.

Usage

```

## S3 method for class 'powdRlib'
fps(lib, smpl, harmonise, solver, obj, refs, std,
  std_conc, tth_align, align, manual_align, tth_fps, shift, shift_res,
  remove_trace, ...)

```

Arguments

lib A powdRlib object representing the reference library. Created using the powdRlib constructor function.

smp1	A data frame. First column is 2theta, second column is counts
harmonise	logical parameter defining whether to harmonise the lib and smp1. Default = TRUE. Harmonises to the intersecting 2theta range at the coarsest resolution available.
solver	The optimisation routine to be used. One of c("BFGS", "Nelder-Mead", "CG", "L-BFGS-B", or "NNLS"). Default = "BFGS".
obj	The objective function to minimise when "BFGS", "Nelder-Mead", "CG" or "L-BFGS-B" are used as the 'solver' argument. One of c("Delta", "R", "Rwp"). Default = "Rwp". See Chipera and Bish (2002) and page 247 of Bish and Post (1989) for definitions of these functions.
refs	A character string of reference pattern ID's from the specified library. The ID's must match ID's in the lib\$phases\$phase_id column.
std	The phase ID (e.g. "QUA.1") to be used as internal standard. Must match an ID provided in the phases parameter.
std_conc	The concentration of the internal standard (if known) in weight percent. If unknown then use std_conc = NA, in which case it will be assumed that all phases sum to 100 percent (default).
tth_align	A vector defining the minimum and maximum 2theta values to be used during alignment. If not defined, then the full range is used.
align	The maximum shift that is allowed during initial 2theta alignment (degrees). Default = 0.1.
manual_align	A logical operator denoting whether to optimise the alignment within the negative/position 2theta range defined in the align argument, or to use the specified value of the align argument for alignment of the sample to the standards. Default = FALSE, i.e. alignment is optimised.
tth_fps	A vector defining the minimum and maximum 2theta values to be used during full pattern summation. If not defined, then the full range is used.
shift	The maximum shift (degrees 2theta) that is allowed during the grid search phases selected from the non-negative least squares. Default = 0.05).
shift_res	A single integer defining the increase in resolution used during grid search shifting. Higher values facilitate finer shifts at the expense of longer computation. Default = 4.
remove_trace	A single numeric value representing the limit for the concentration of trace phases to be retained, i.e. any mineral with an estimated concentration below 'remove_trace' will be omitted. Default = 0.
...	other arguments

Details

Applies full pattern summation (Chipera & Bish, 2002, 2013; Eberl, 2003) to an XRPD sample to quantify phase concentrations. Requires a powdRlib library of reference patterns with reference intensity ratios in order to derive mineral concentrations.

Value

a list with components:

tth	a vector of the 2theta scale of the fitted data
fitted	a vector of the fitted XRPD pattern
measured	a vector of the original XRPD measurement (aligned)
residuals	a vector of the residuals (fitted vs measured)
phases	a dataframe of the phases used to produce the fitted pattern
phases_grouped	the phases dataframe grouped by phase_name and summed
rwp	the Rwp of the fitted vs measured pattern
weighted_pure_patterns	a dataframe of reference patterns used to produce the fitted pattern. All patterns have been weighted according to the coefficients used in the fit
coefficients	a named vector of coefficients used to produce the fitted pattern
inputs	a list of input arguments used in the function call

References

- Bish, D.L., Post, J.E., 1989. Modern powder diffraction. Mineralogical Society of America.
- Chipera, S.J., Bish, D.L., 2013. Fitting Full X-Ray Diffraction Patterns for Quantitative Analysis: A Method for Readily Quantifying Crystalline and Disordered Phases. *Adv. Mater. Phys. Chem.* 03, 47-53. doi:10.4236/ampc.2013.31A007
- Chipera, S.J., Bish, D.L., 2002. FULLPAT: A full-pattern quantitative analysis program for X-ray powder diffraction using measured and calculated patterns. *J. Appl. Crystallogr.* 35, 744-749. doi:10.1107/S0021889802017405
- Eberl, D.D., 2003. User's guide to RockJock - A program for determining quantitative mineralogy from powder X-ray diffraction data. Boulder, CA.

Examples

```
#Load the minerals library
data(minerals)

# Load the soils data
data(soils)

#Since the reference library is relatively small,
#the whole library can be used at once to get an
#estimate of the phases within each sample.
## Not run:
fps_sand <- fps(lib = minerals,
               smpl = soils$sandstone,
               refs = minerals$phases$phase_id,
               std = "QUA.1",
               align = 0.2)
```

```
fps_lime <- fps(lib = minerals,
               smpl = soils$limestone,
               refs = minerals$phases$phase_id,
               std = "QUA.1",
               align = 0.2)

fps_granite <- fps(lib = minerals,
                  smpl = soils$granite,
                  refs = minerals$phases$phase_id,
                  std = "QUA.1",
                  align = 0.2)

#Alternatively run all 3 at once using lapply

fps_soils <- lapply(soils, fps,
                   lib = minerals,
                   std = "QUA.2",
                   refs = minerals$phases$phase_id,
                   align = 0.2)

#Using the rockjock library:

data(rockjock)
data(rockjock_mixtures)

rockjock_1 <- fps(lib = rockjock,
                 smpl = rockjock_mixtures$Mix1,
                 refs = c("ORDERED_MICROCLINE",
                          "LABRADORITE",
                          "KAOLINITE_DRY_BRANCH",
                          "MONTMORILLONITE_WYO",
                          "ILLITE_1M_RM30",
                          "CORUNDUM"),
                 std = "CORUNDUM",
                 align = 0.3)

#Alternatively you can specify the internal standard
#concentration if known:
rockjock_1s <- fps(lib = rockjock,
                  smpl = rockjock_mixtures$Mix1,
                  refs = c("ORDERED_MICROCLINE",
                           "LABRADORITE",
                           "KAOLINITE_DRY_BRANCH",
                           "MONTMORILLONITE_WYO",
                           "ILLITE_1M_RM30",
                           "CORUNDUM"),
                  std = "CORUNDUM",
                  std_conc = 20,
                  align = 0.3)

## End(Not run)
```

minerals	<i>An example powdRlib reference library</i>
----------	--

Description

This `powdRlib` object, built using the `powdRlib` constructor function, contains a range of measured XRPD data (Cu K-alpha radiation) along with their reference intensity ratios. The library can be used with the `soils` example data for full pattern summation.

Usage

```
minerals
```

Format

A list of 3

xrd A dataframe of all xrd data (counts only). Column names denote the reference sample

tth A vector of 2theta intervals of all measurements in the library

phases A dataframe the phase ID's, names and reference intensity ratios (RIR)

minerals_phases	<i>A table of associated data for the minerals_xrd table, which can be combined with a xrd data table to create a powdRlib object when using the powdRlib constructor function. Use the same layout to create custom reference libraries.</i>
-----------------	---

Description

A table of associated data for the `minerals_xrd` table, which can be combined with a xrd data table to create a `powdRlib` object when using the `powdRlib` constructor function. Use the same layout to create custom reference libraries.

Usage

```
minerals_phases
```

Format

A 3 column dataframe

The first column is a character string defining the unique mineral ID's that should match those defined as column names of the `minerals` table (e.g. `minerals_xrd`).

The second column is a character string defining the mineral group that each reference pattern belongs to.

The third column is a numeric vector defining the reference intensity ratios of each reference pattern.

minerals_xrd	<i>A table of 14 reference patterns and their corresponding two theta scale that can be combined with the minerals_phases table to create a powdRlib object when using the powdRlib constructor function. Use the same layout to create custom reference libraries.</i>
--------------	---

Description

A table of 14 reference patterns and their corresponding two theta scale that can be combined with the minerals_phases table to create a powdRlib object when using the powdRlib constructor function. Use the same layout to create custom reference libraries.

Usage

```
minerals_xrd
```

Format

A dataframe

The first column defines the two theta scale, and remaining columns are individual reference patterns of pure minerals or amorphous phases. Each column title should be a unique mineral ID

plot.powdRafps	<i>Plotting elements of a powdRafps object</i>
----------------	--

Description

plot.powdRafps is designed to provide easy, adaptable plots of full pattern summation outputs produced from [afps](#).

Usage

```
## S3 method for class 'powdRafps'
plot(x, wavelength, interactive, ...)
```

Arguments

x	a powdRfaps object
wavelength	One of "Cu", "Co" or a custom numeric value defining the wavelength (in Angstroms). Used to compute d-spacings. When "Cu" or "Co" are supplied, wavelengths of 1.54056 or 1.78897 are used, respectively.
interactive	logical. If TRUE then the output will be an interactive ggplotly object. If FALSE then the output will be a ggplot object.
...	other arguments

Details

The only mandatory argument is `x`, which must be a `powdRlib` object. When seeking to inspect the results from full pattern summation, interactive plots are particularly useful and can be specified with the `interactive` argument.

Examples

```
#Load the minerals library
data(minerals)

# Load the soils data
data(soils)

## Not run:
afps_sand <- afps(lib = minerals,
                 smpl = soils$sandstone,
                 std = "QUA.1",
                 amorphous = "ORG",
                 align = 0.2,
                 lod = 0.1)

plot(afps_sand, wavelength = "Cu")
plot(afps_sand, wavelength = "Cu", interactive = TRUE)

## End(Not run)
```

plot.powdRbkg

Plotting a powdRbkg object

Description

`plot.powdRbkg` is designed to provide quick plots to inspect the fitted backgrounds obtained from `bkg`.

Usage

```
## S3 method for class 'powdRbkg'
plot(x, interactive, ...)
```

Arguments

<code>x</code>	a <code>powdRlib</code> object
<code>interactive</code>	Logical. If <code>TRUE</code> then the output will be an interactive <code>ggplotly</code> object. If <code>FALSE</code> then the output will be a <code>ggplot</code> object.
<code>...</code>	other arguments

Details

The only mandatory argument is `x`, which must be a `powdRbkg` object. Plots can be made interactive using the logical `interactive` argument.

Examples

```
# Load the minerals library
data(minerals)

## Not run:
plot(minerals, interactive = TRUE)

## End(Not run)
```

plot.powdRfps

Plotting elements of a powdRfps object

Description

`plot.powdRfps` is designed to provide easy, adaptable plots of full pattern summation outputs produced from [fps](#).

Usage

```
## S3 method for class 'powdRfps'
plot(x, wavelength, interactive, ...)
```

Arguments

<code>x</code>	a <code>powdRfps</code> object
<code>wavelength</code>	One of "Cu", "Co" or a custom numeric value defining the wavelength (in Angstroms). Used to compute d-spacings. When "Cu" or "Co" are supplied, wavelengths of 1.54056 or 1.78897 are used, respectively.
<code>interactive</code>	logical. If TRUE then the output will be an interactive ggplotly object. If FALSE then the output will be a ggplot object.
<code>...</code>	other arguments

Details

The only mandatory argument is `x`, which must be a `powdRlib` object. When seeking to inspect the results from full pattern summation, interactive plots are particularly useful and can be specified with the `interactive` argument.

Examples

```
#Load the minerals library
data(minerals)

# Load the soils data
data(soils)

## Not run:
fps_sand <- fps(lib = minerals,
               smpl = soils$sandstone,
               refs = minerals$phases$phase_id,
               std = "QUA.1",
               align = 0.2)

plot(fps_sand, wavelength = "Cu")
plot(fps_sand, wavelength = "Cu", interactive = TRUE)

## End(Not run)
```

plot.powdRlib

Plotting elements of a powdRlib object

Description

plot.powdRlib is designed to provide easy, adaptable plots of an XRPD reference library built using the powdRlib constructor function.

Usage

```
## S3 method for class 'powdRlib'
plot(x, wavelength, refs, interactive, ...)
```

Arguments

x	a powdRlib object
wavelength	One of "Cu", "Co" or a custom numeric value defining the wavelength (in Angstroms). Used to compute d-spacings. When "Cu" or "Co" are supplied, wavelengths of 1.54056 or 1.78897 are used, respectively.
refs	a character string of reference pattern id's to be plotted
interactive	Logical. If TRUE then the output will be an interactive ggplotly object. If FALSE then the output will be a ggplot object.
...	other arguments

Details

The only mandatory argument is x, which must be a powdRlib object. Plots can be made interactive using the logical interactive argument.

Examples

```
# Load the minerals library
data(minerals)
## Not run:
plot(minerals, wavelength = "Cu", refs = "ALB")
plot(minerals, wavelength = "Cu", refs = "ALB", interactive = TRUE)

## End(Not run)
```

powdR

powdR: Full Pattern Summation of X-Ray Powder Diffraction Data

Description

An implementation of the full pattern summation approach to quantitative mineralogy from X-ray powder diffraction data (Chipera & Bish, 2002, 2013; Eberl, 2003).

Author(s)

Benjamin Butler, The James Hutton Institute, Aberdeen, UK

References

Chipera, S.J., Bish, D.L., 2013. Fitting Full X-Ray Diffraction Patterns for Quantitative Analysis: A Method for Readily Quantifying Crystalline and Disordered Phases. *Adv. Mater. Phys. Chem.* 03, 47-53. doi:10.4236/ampc.2013.31A007

Chipera, S.J., Bish, D.L., 2002. FULLPAT: A full-pattern quantitative analysis program for X-ray powder diffraction using measured and calculated patterns. *J. Appl. Crystallogr.* 35, 744-749. doi:10.1107/S0021889802017405

Eberl, D.D., 2003. User's guide to ROCKJOCK - A program for determining quantitative mineralogy from powder X-ray diffraction data. Boulder, CA.

powdRlib

Create an XRD reference library

Description

A constructor function for creating a powdRlib object from two tables of data. The resulting reference library object is required when using [fps](#).

Usage

```
powdRlib(xrd_table, phases_table)
```

Arguments

<code>xrd_table</code>	A data frame of the count intensities of the xrd reference patterns, all scaled to same maximum intensity, with their 2theta axis as the first column. Must all be on the same 2theta scale.
<code>phases_table</code>	A data frame of the required data (phase ID, phase name, and reference intensity ratio) for each reference pattern.

Value

a list with components:

<code>xrd</code>	a data frame of reference patterns
<code>tth</code>	a vector of the 2theta measurement intervals
<code>phases</code>	a data frame of the id, name and reference intensity ratio of each reference pattern

Examples

```
#load an example xrd_table
data(minerals_xrd)
#load an example phases_table
data(minerals_phases)

#Create a reference library object
xrd_lib <- powdRlib(xrd_table = minerals_xrd,
                  phases_table = minerals_phases)
```

rockjock

RockJock reference library

Description

A `powdRlib` object of 168 pure reference patterns from the RockJock library (Cu K-alpha radiation) along with reference intensity ratios. Can be used with the `fps()` and `afps()` functions for quantitative analysis. Example mixtures for testing the rockjock library with known concentrations are available in the `rockjock_mixtures` data. See `?rockjock_mixtures`.

Usage

```
rockjock
```

Format

A list of 3 components

xrd A dataframe of all xrd data (counts only). Column names denote the reference sample

tth A vector of 2theta intervals of all measurements in the library

phases A dataframe the phase ID's, names and reference intensity ratios (RIR)

Author(s)

Dennis Eberl

References

<https://pubs.er.usgs.gov/publication/ofr200378>

rockjock_mixtures	<i>RockJock synthetic mixtures</i>
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Description

A list containing 8 XRPD measurements (Cu K-alpha radiation) of synthetic mixtures that can be used to assess accuracy of quantitative analysis from the `fps()` and `afps()` functions. The mixtures contain various amounts of quartz (QUARTZ standard in of the rockjock library), K-feldspar (ORDERED_MICROCLINE), plagioclase (LABRADORITE), kaolinite (KAOLINITE_DRY_BRANCH), dioctahedral smectite (MONTMORILLIONITE_WYO), illite (ILLITE_1M_RM30) and corundum (CORUNDUM).

Usage

```
rockjock_mixtures
```

Format

A list of 8 components, each comprised of two columns. Column `t |` specifies the 2θ axis and `counts` specifies the count intensities

Mix1 Contains: 4 % K-feldspar, 20 % plagioclase, 12 % kaolinite, 36 % dioctahedral smectite, 8 % illite and 20 % corundum.

Mix2 Contains: 4 % quartz, 8 % K-feldspar, 36 % plagioclase, 20 % kaolinite, 12 % illite and 20 % corundum.

Mix3 Contains: 8 % quartz, 12 % K-feldspar, 36 % kaolinite, 4 % dioctahedral smectite, 20 % illite and 20 % corundum.

Mix4 Contains: 12 % quartz, 20 % K-feldspar, 4 % plagioclase, 8 % dioctahedral smectite, 36 % illite and 20 % corundum.

Mix5 Contains: 20 % quartz, 36 % K-feldspar, 8 % plagioclase, 4 % kaolinite, 12 % dioctahedral smectite and 20 % corundum.

Mix6 Contains: 36 % quartz, 12 % plagioclase, 8 % kaolinite, 20 % dioctahedral smectite, 4 % illite and 20 % corundum.

Mix7 Contains: 8 % K-feldspar, 40 % plagioclase, 4 % kaolinite, 12 % dioctahedral smectite, 16 % illite and 20 % corundum.

Mix8 Contains: 8 % quartz, 4 % K-feldspar, 4 % plagioclase, 24 % dioctahedral smectite, 40 % illite and 20 % corundum.

Author(s)

Dennis Eberl

References<https://pubs.er.usgs.gov/publication/ofr200378>

`run_powdR`*Run the powdR shiny app*

DescriptionA wrapper for `runApp` to start the Shiny app for powdR.**Usage**`run_powdR(...)`**Arguments**`...` further arguments to pass to `runApp`**Examples**

```
## Not run:  
run_powdR()  
  
## End(Not run)
```

`soils`*Example soil XRPD data*

Description

3 soil samples from different parent materials measured by XRPD (Cu K-alpha radiation)

Usage`soils`

Format

A list of 3 dataframes (named according to rock type), with each dataframe containing two columns of:

tth The 2theta measurement intervals

counts The count intensities

subset.powdRlib	<i>Subset a powdRlib object</i>
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Description

subset.powdRlib is designed to provide an easy way of subsetting a powdRlib object by defining the phase ID's that the user wishes to either keep or remove.

Usage

```
## S3 method for class 'powdRlib'
subset(x, refs, mode, ...)
```

Arguments

x	a powdRlib object.
refs	a string of the phase ID's of reference patterns to be subset
mode	denotes whether the phase ID's defined in the refs argument are retained ("keep") or removed ("remove").
...	other arguments

Value

a powdRlib object.

Examples

```
#Load the minerals library
data(minerals)

minerals_keep <- subset(minerals,
                        refs = c("QUA.1", "QUA.2"),
                        mode = "keep")

minerals_remove <- subset(minerals,
                          refs = c("QUA.1", "QUA.2"),
                          mode = "remove")
```

summarise_mineralogy *Summarise the mineralogy from multiple powdRfyps and powdRafyps outputs*

Description

summarise_mineralogy creates a summary table of quantified mineral concentrations across a given dataset using list of multiple powdRfyps or powdRafyps derived from fps() and afps(), respectively.

Usage

```
summarise_mineralogy(x, type, order)
```

Arguments

x a list of powdRfyps or powdRafyps objects.

type a string specifying whether the table uses all phase ID's, or summarises them according to the phase name. One of "all" or "grouped".

order a logical operator denoting whether the columns of the resulting summary table are ordered in descending order according to the summed abundance of each phase across the dataset.

Value

a dataframe

Examples

```
data(minerals)
data(soils)

## Not run:
multiple_afps <- lapply(soils, afps,
  lib = minerals,
  std = "QUA.1",
  align = 0.2,
  lod = 0.1,
  amorphous = "ORG",
  amorphous_lod = 1)

sm1 <- summarise_mineralogy(multiple_afps,
  type = "all",
  order = TRUE)

sm2 <- summarise_mineralogy(multiple_afps,
  type = "grouped",
  order = TRUE)
```

End(Not run)

Index

*Topic **datasets**

- minerals, [15](#)
- minerals_phases, [15](#)
- minerals_xrd, [16](#)
- rockjock, [21](#)
- rockjock_mixtures, [22](#)
- soils, [23](#)

afps, [2](#), [16](#)
afps.powdRlib, [4](#)

bkg, [8](#)

fps, [9](#), [18](#), [20](#)
fps.powdRlib, [11](#)

minerals, [15](#)
minerals_phases, [15](#)
minerals_xrd, [16](#)

plot.powdRafps, [16](#)
plot.powdRbkg, [17](#)
plot.powdRfps, [18](#)
plot.powdRlib, [19](#)
powdR, [20](#)
powdR-package (powdR), [20](#)
powdRlib, [20](#)

rockjock, [21](#)
rockjock_mixtures, [22](#)
run_powdR, [23](#)
runApp, [23](#)

soils, [23](#)
subset.powdRlib, [24](#)
summarise_mineralogy, [25](#)