# Package 'lightr'

December 1, 2024

```
Title Read Spectrometric Data and Metadata
Version 1.8.0
Description Parse various reflectance/transmittance/absorbance spectra file
      formats to extract spectral data and metadata, as described in Gruson, White
      & Maia (2019) <doi:10.21105/joss.01857>. Among other formats, it can import
      files from 'Avantes' <a href="https://www.avantes.com/">https://www.avantes.com/</a>, 'CRAIC'
      <a href="https://www.microspectra.com/">https://www.microspectra.com/</a>, and 'OceanOptics'/'OceanInsight'
      <https://www.oceanoptics.com/> brands.
Depends R (>= 4.0.0)
Imports future.apply, progressr, xml2 (>= 1.0.0)
Suggests digest, future, knitr, lintr, pavo, rmarkdown, spelling,
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```

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lr\_convert\_tocsv

Convert spectral data files to csv files

# Description

Convert spectral data files to csv files

# Usage

```
lr_convert_tocsv(
  where = NULL,
  ext = "txt",
  decimal = ".",
  sep = NULL,
  subdir = FALSE,
  ignore.case = TRUE,
  overwrite = FALSE,
  metadata = TRUE
)
```

# Arguments

where	Folder in which files are located (defaults to current working directory).
ext	File extension to be searched for, without the "." (defaults to txt). You can also use a character vector to specify multiple file extensions.
decimal	Character to be used to identify decimal plates (defaults to .).
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")
subdir	Should subdirectories within the where folder be included in the search? (defaults to FALSE).
ignore.case	Should the extension search be case insensitive? (defaults to TRUE)

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overwrite	logical. Should the function overwrite existing files with the same name? (de-
	faults to FALSE).
metadata	logical (defaults to TRUE). Should metadata be exported as well? They will be

exported in csv files will the \_metadata.csv suffix.

#### **Details**

You can customise the type of parallel processing used by this function with the future::plan() function. This works on all operating systems, as well as high performance computing (HPC) environment. Similarly, you can customise the way progress is shown with the progressr::handlers() functions (progress bar, acoustic feedback, nothing, etc.)

#### Value

Convert input files to csv and invisibly return the list of created file paths

# Warning

When metadata = TRUE, if **either** the data **or** metadata export fails, nothing will be returned for this file.

lr_get_metadata	Extract metadata from spectra files	
-----------------	-------------------------------------	--

# **Description**

Finds and imports metadata from spectra files in a given location.

# Usage

```
lr_get_metadata(
  where = getwd(),
  ext = "ProcSpec",
  sep = NULL,
  subdir = FALSE,
  subdir.names = FALSE,
  ignore.case = TRUE
)
```

# Arguments

where	Folder in which files are located (defaults to current working directory).
ext	File extension to be searched for, without the "." (defaults to txt). You can also use a character vector to specify multiple file extensions.
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")

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subdir Should subdirectories within the where folder be included in the search? (de-

faults to FALSE).

subdir.names Should subdirectory path be included in the name of the spectra? (defaults to

FALSE).

ignore.case Should the extension search be case insensitive? (defaults to TRUE)

#### **Details**

You can customise the type of parallel processing used by this function with the future::plan() function. This works on all operating systems, as well as high performance computing (HPC) environment. Similarly, you can customise the way progress is shown with the progressr::handlers() functions (progress bar, acoustic feedback, nothing, etc.)

#### Value

A data.frame containing one file per row and the following columns:

- name: File name (without the extension)
- user: Name of the spectrometer operator
- datetime: Timestamp of the recording (ISO 8601 format)
- spec\_model: Model of the spectrometer
- spec\_ID: Unique ID of the spectrometer
- white\_inttime: Integration time of the white reference (in ms)
- dark\_inttime: Integration time of the dark reference (in ms)
- sample\_inttime: Integration time of the sample (in ms)
- white\_avgs: Number of averaged measurements for the white reference
- dark\_avgs: Number of averaged measurements for the dark reference
- sample\_avgs: Number of averaged measurements for the sample
- white\_boxcar: Boxcar width for the white reference
- dark\_boxcar: Boxcar width for the dark reference
- sample\_boxcar: Boxcar width for the sample reference

#### Warning

white\_inttime, dark\_inttime and sample\_inttime should be equal. The normalised data may be inaccurate otherwise.

## References

White TE, Dalrymple RL, Noble DWA, O'Hanlon JC, Zurek DB, Umbers KDL. Reproducible research in the study of biological coloration. Animal Behaviour. 2015 Aug 1;106:51-7 (doi:10.1016/j.anbehav.2015.05.007).

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# **Examples**

lr\_get\_spec

Extract spectral data from spectra files

# Description

Finds and imports reflectance/transmittance/absorbance data from spectra files in a given location.

# Usage

```
lr_get_spec(
  where = getwd(),
  ext = "txt",
  lim = c(300, 700),
  decimal = ".",
  sep = NULL,
  subdir = FALSE,
  subdir.names = FALSE,
  ignore.case = TRUE,
  interpolate = TRUE
)
```

# Arguments

where	Folder in which files are located (defaults to current working directory).
ext	File extension to be searched for, without the "." (defaults to txt). You can also use a character vector to specify multiple file extensions.
lim	A vector with two numbers determining the wavelength limits to be considered (defaults to $c(300, 700)$ ).
decimal	Character to be used to identify decimal plates (defaults to .).
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")
subdir	Should subdirectories within the where folder be included in the search? (defaults to FALSE).
subdir.names	Should subdirectory path be included in the name of the spectra? (defaults to FALSE).
ignore.case	Should the extension search be case insensitive? (defaults to TRUE)
interpolate	Boolean indicated whether spectral data should be interpolated and pruned at every nanometre. Note that this option can only work if all input data samples the same wavelengths. Defaults to TRUE.

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#### **Details**

You can customise the type of parallel processing used by this function with the future::plan() function. This works on all operating systems, as well as high performance computing (HPC) environment. Similarly, you can customise the way progress is shown with the progressr::handlers() functions (progress bar, acoustic feedback, nothing, etc.)

# Value

A data.frame, containing the wavelengths in the first column and individual imported spectral files in the subsequent columns.

#### See Also

```
pavo::getspec()
```

# Examples

```
spcs <- lr_get_spec(system.file("testdata", package = "lightr"), ext = "jdx")
head(spcs)</pre>
```

lr\_parse\_generic

Generic function to parse spectra files that don't have a specific parser

# Description

Generic function to parse spectra files that don't have a specific parser

# Usage

```
lr_parse_generic(filename, decimal = ".", sep = NULL)
```

## Arguments

filename	Path of the file to parse
decimal	Character to be used to identify decimal plates (defaults to .).
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")

#### **Details**

'processed' column computed by official software and provided as is.

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#### Value

A named list of two elements:

• data: a dataframe with columns "wl", "dark", "white", "scope" and "processed", in this order.

- metadata: a character vector with metadata including:
  - user: Name of the spectrometer operator
  - datetime: Timestamp of the recording in format '%Y-%m-%d %H:%M:%S' and UTC timezone. If timezone is missing in source file, UTC time will be assumed (for reproducibility purposes across computers with different localtimes).
  - spec\_model: Model of the spectrometer
  - spec\_ID: Unique ID of the spectrometer
  - white\_inttime: Integration time of the white reference (in ms)
  - dark\_inttime: Integration time of the dark reference (in ms)
  - sample\_inttime: Integration time of the sample (in ms)
  - white\_avgs: Number of averaged measurements for the white reference
  - dark\_avgs: Number of averaged measurements for the dark reference
  - sample\_avgs: Number of averaged measurements for the sample
  - white\_boxcar: Boxcar width for the white reference
  - dark\_boxcar: Boxcar width for the dark reference
  - sample\_boxcar: Boxcar width for the sample reference

#### **Examples**

```
res_csv <- lr_parse_generic(
   system.file("testdata", "spec.csv", package = "lightr"),
   sep = ","
)
head(res_csv$data)
# No metadata is extracted with this parser
res_csv$metadata

res_craic <- lr_parse_generic(
   system.file("testdata", "CRAIC_export.txt", package = "lightr")
)
head(res_craic$data)
# No metadata is extracted with this parser
res_craic$metadata</pre>
```

lr\_parse\_jaz

Parse OceanOptics converted file

# Description

Parse OceanOptics/OceanInsight converted file. https://www.oceanoptics.com/

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#### Usage

```
lr_parse_jaz(filename)
lr_parse_jazirrad(filename)
```

#### **Arguments**

filename

Path of the file to parse

#### **Details**

'processed' column computed by official software and provided as is.

#### Value

A named list of two elements:

- data: a dataframe with columns "wl", "dark", "white", "scope" and "processed", in this order.
- metadata: a character vector with metadata including:
  - user: Name of the spectrometer operator
  - datetime: Timestamp of the recording in format '%Y-%m-%d %H:%M:%S' and UTC timezone. If timezone is missing in source file, UTC time will be assumed (for reproducibility purposes across computers with different localtimes).
  - spec\_model: Model of the spectrometer
  - spec\_ID: Unique ID of the spectrometer
  - white\_inttime: Integration time of the white reference (in ms)
  - dark\_inttime: Integration time of the dark reference (in ms)
  - sample\_inttime: Integration time of the sample (in ms)
  - white\_avgs: Number of averaged measurements for the white reference
  - dark\_avgs: Number of averaged measurements for the dark reference
  - sample\_avgs: Number of averaged measurements for the sample
  - white\_boxcar: Boxcar width for the white reference
  - dark\_boxcar: Boxcar width for the dark reference
  - sample\_boxcar: Boxcar width for the sample reference

# **Examples**

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lr\_parse\_jdx

Parse OceanOptics JCAMP-DX (.jdx) file

#### **Description**

Parse OceanOptics/OceanInsight JCAMP-DX (.jdx) file. https://www.oceanoptics.com/

# Usage

```
lr_parse_jdx(filename)
```

#### **Arguments**

filename

Path of the file to parse

## **Details**

'processed' column computed by **lightr** with the function lr\_compute\_processed().

# Value

A named list of two elements:

- data: a dataframe with columns "wl", "dark", "white", "scope" and "processed", in this order.
- metadata: a character vector with metadata including:
  - user: Name of the spectrometer operator
  - datetime: Timestamp of the recording in format '%Y-%m-%d %H:%M:%S' and UTC timezone. If timezone is missing in source file, UTC time will be assumed (for reproducibility purposes across computers with different localtimes).
  - spec\_model: Model of the spectrometer
  - spec\_ID: Unique ID of the spectrometer
  - white\_inttime: Integration time of the white reference (in ms)
  - dark\_inttime: Integration time of the dark reference (in ms)
  - sample\_inttime: Integration time of the sample (in ms)
  - white\_avgs: Number of averaged measurements for the white reference

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- dark\_avgs: Number of averaged measurements for the dark reference
- sample\_avgs: Number of averaged measurements for the sample
- white\_boxcar: Boxcar width for the white reference
- dark\_boxcar: Boxcar width for the dark reference
- sample\_boxcar: Boxcar width for the sample reference

#### References

McDonald RS, Wilks PA. JCAMP-DX: A Standard Form for Exchange of Infrared Spectra in Computer Readable Form. Applied Spectroscopy. 1988;42(1):151-62.

## **Examples**

lr\_parse\_procspec

Parse OceanOptics ProcSpec file

#### **Description**

Parse OceanOptics/OceanInsight ProcSpec file. https://www.oceanoptics.com/

# Usage

```
lr_parse_procspec(filename)
```

#### **Arguments**

filename

Path of the file to parse

# **Details**

'processed' column computed by official software and provided as is.

#### Value

A named list of two elements:

- data: a dataframe with columns "wl", "dark", "white", "scope" and "processed", in this order.
- metadata: a character vector with metadata including:
  - user: Name of the spectrometer operator
  - datetime: Timestamp of the recording in format '%Y-%m-%d %H:%M:%S' and UTC timezone. If timezone is missing in source file, UTC time will be assumed (for reproducibility purposes across computers with different localtimes).

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- spec\_model: Model of the spectrometer
- spec\_ID: Unique ID of the spectrometer
- white\_inttime: Integration time of the white reference (in ms)
- dark\_inttime: Integration time of the dark reference (in ms)
- sample\_inttime: Integration time of the sample (in ms)
- white\_avgs: Number of averaged measurements for the white reference
- dark\_avgs: Number of averaged measurements for the dark reference
- sample\_avgs: Number of averaged measurements for the sample
- white\_boxcar: Boxcar width for the white reference
- dark\_boxcar: Boxcar width for the dark reference
- sample\_boxcar: Boxcar width for the sample reference

#### References

```
https://www.oceanoptics.com/software/
```

# **Examples**

lr\_parse\_spc

Parse SPC binary file

# **Description**

```
Parse SPC binary file. (Used by CRAIC https://www.microspectra.com/ and OceanOptics https://www.oceanoptics.com/)
```

# Usage

```
lr_parse_spc(filename)
```

## **Arguments**

filename

Path of the file to parse

#### **Details**

'processed' column computed by official software and provided as is.

lr\_parse\_trm

#### Value

A named list of two elements:

• data: a dataframe with columns "wl", "dark", "white", "scope" and "processed", in this order.

- metadata: a character vector with metadata including:
  - user: Name of the spectrometer operator
  - datetime: Timestamp of the recording in format '%Y-%m-%d %H:%M:%S' and UTC timezone. If timezone is missing in source file, UTC time will be assumed (for reproducibility purposes across computers with different localtimes).
  - spec\_model: Model of the spectrometer
  - spec\_ID: Unique ID of the spectrometer
  - white\_inttime: Integration time of the white reference (in ms)
  - dark\_inttime: Integration time of the dark reference (in ms)
  - sample\_inttime: Integration time of the sample (in ms)
  - white\_avgs: Number of averaged measurements for the white reference
  - dark\_avgs: Number of averaged measurements for the dark reference
  - sample\_avgs: Number of averaged measurements for the sample
  - white boxcar: Boxcar width for the white reference
  - dark\_boxcar: Boxcar width for the dark reference
  - sample\_boxcar: Boxcar width for the sample reference

# In development

Metadata parsing has not yet been implemented for this file format.

## **Examples**

lr\_parse\_trm

Parse Avantes binary file

#### **Description**

Parse Avantes binary file (TRM, ABS, ROH, DRK, REF, RAW8, RFL8 file extensions). https://www.avantes.com/products/spectrometers/

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#### Usage

```
lr_parse_trm(filename)
lr_parse_abs(filename)
lr_parse_roh(filename)
lr_parse_rfl8(filename, specnum = 1L)
lr_parse_raw8(filename, specnum = 1L)
lr_parse_irr8(filename, specnum = 1L)
```

#### **Arguments**

filename Path of the file to parse

specnum Integer representing the position of the spectrum to read in the file. This option

only makes sense for AvaSoft8 files and is ignored in the other cases.

#### **Details**

'processed' column computed by **lightr** with the function lr\_compute\_processed().

#### Value

A named list of two elements:

- data: a dataframe with columns "wl", "dark", "white", "scope" and "processed", in this order.
- metadata: a character vector with metadata including:
  - user: Name of the spectrometer operator
  - datetime: Timestamp of the recording in format '%Y-%m-%d %H:%M:%S' and UTC timezone. If timezone is missing in source file, UTC time will be assumed (for reproducibility purposes across computers with different localtimes).
  - spec\_model: Model of the spectrometer
  - spec\_ID: Unique ID of the spectrometer
  - white\_inttime: Integration time of the white reference (in ms)
  - dark\_inttime: Integration time of the dark reference (in ms)
  - sample\_inttime: Integration time of the sample (in ms)
  - white\_avgs: Number of averaged measurements for the white reference
  - dark\_avgs: Number of averaged measurements for the dark reference
  - sample\_avgs: Number of averaged measurements for the sample
  - white\_boxcar: Boxcar width for the white reference
  - dark\_boxcar: Boxcar width for the dark reference
  - sample\_boxcar: Boxcar width for the sample reference

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#### **Examples**

```
res_trm <- lr_parse_trm(</pre>
  system.file("testdata", "avantes_trans.TRM", package = "lightr")
head(res_trm$data)
res_trm$metadata
res_roh <- lr_parse_roh(</pre>
  system.file("testdata", "avantes_reflect.ROH", package = "lightr")
head(res_roh$data)
res_roh$metadata
# This parser has a unique `specnum` argument
res_rfl8_1 <- lr_parse_rfl8(</pre>
  system.file("testdata", "compare", "Avantes", "feather.RFL8", package = "lightr"),
  specnum = 1
)
head(res_rfl8_1$data)
res_rfl8_1$metadata
res_rfl8_2 <- lr_parse_rfl8(</pre>
  system.file("testdata", "compare", "Avantes", "feather.RFL8", package = "lightr"),
  specnum = 2
head(res_rf18_2$data)
res_rfl8_2$metadata
```

lr\_parse\_ttt

Parse Avantes converted file

#### **Description**

Parse Avantes converted file. https://www.avantes.com/products/spectrometers/

# Usage

```
lr_parse_ttt(filename)
lr_parse_trt(filename)
```

# Arguments

filename

Path of the file to parse

## **Details**

'processed' column computed by official software and provided as is.

lr\_parse\_ttt

#### Value

A named list of two elements:

- data: a dataframe with columns "wl", "dark", "white", "scope" and "processed", in this order.
- metadata: a character vector with metadata including:
  - user: Name of the spectrometer operator
  - datetime: Timestamp of the recording in format '%Y-%m-%d %H:%M:%S' and UTC timezone. If timezone is missing in source file, UTC time will be assumed (for reproducibility purposes across computers with different localtimes).
  - spec\_model: Model of the spectrometer
  - spec\_ID: Unique ID of the spectrometer
  - white\_inttime: Integration time of the white reference (in ms)
  - dark\_inttime: Integration time of the dark reference (in ms)
  - sample\_inttime: Integration time of the sample (in ms)
  - white\_avgs: Number of averaged measurements for the white reference
  - dark\_avgs: Number of averaged measurements for the dark reference
  - sample\_avgs: Number of averaged measurements for the sample
  - white\_boxcar: Boxcar width for the white reference
  - dark\_boxcar: Boxcar width for the dark reference
  - sample\_boxcar: Boxcar width for the sample reference

#### **Examples**

```
res_ttt <- lr_parse_ttt(
    system.file("testdata", "avantes_export.ttt", package = "lightr")
)
head(res_ttt$data)
res_ttt$metadata

res_trt <- lr_parse_trt(
    system.file("testdata", "avantes_export2.trt", package = "lightr")
)
head(res_trt$data)
res_trt$metadata</pre>
```

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