$\begin{array}{c} \textbf{photobiologyInOut} \ Version \ 0.4.6.9000 \\ \textbf{User} \ Guide \end{array}$

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1 Introduction

```
# this may be needed in some geographic locations as some Windows TZ strings are
# not recognized by all versions of R
Sys.setenv(TZ = 'UTC')
library(photobiology)
library(photobiologyWavebands)
library(photobiologyInOut)
library(lubridate)
library(ggplot2)
library(ggmap)
library(ggspectra)
library(hyperSpec)
library(colorSpec)
library(pavo)
library(readr)
```

```
options(dplyr.print_max = 5)
options(dplyr.print_min = 3)
```

This package defines functions for importing spectral data from different instruments, simulation models, and for data exchange with R packages 'hyper-Spec' and 'pavo' (Table 1).

Table 1: Functions for importing measured and simulated spectral emission data.

R function	Instrument	Program	class of value
read_oo_ssirrad() read_oo_ssdata() read_oo_jazirrad() read_oo_jazdata() read_oo_pidata() read_avaspec_csv() read_macam_file() read_licor_file() read_m_licor_file()	Ocean Optics spectrom. Ocean Optics spectrom. Ocean Optics Jaz Ocean Optics Jaz Ocean Optics spectrom. Avantes spectrom. Macam LI-COR LI-1800 LI-COR LI-1800	SpectraSuite SpectraSuite instrument instrument STS DK (Raspbian) instrument instrument PC1800 (MS-DOS) PC1800 (MS-DOS)	source_spct raw_spct source_spct raw_spct source_spct source_spct source_spct source_mspct
R function	Simulation model	Version	class of value
read_tuv_usrout() read_fmi_cum() read_m_fmi_cum() read_libradtran_vesa()	TUV (S. Madronich) (A. Lindfors) (A. Lindfors) (T. & V. Kotilainen)	version 5.0 daily cumulated daily cumulated irradiance	source_spct source_mspct source_spct
R function	R package	Function	class of value
hyperSpec2mspct() mspct2hyperSpec() rspec2mspct()	'hyperSpec' 'hyperSpec' 'pavo'	import export import	source_mspct hyperSpec source_mspct

All functions attempt to decode and store as metadata as much of the information present in file headers as possible. In most cases, the unchanged header of the file is stored as is as a comment in the constructed objects.

It should be remembered, though, that this package has been developed based on the example files I had access to. Files from the same instruments with different hardware configurations, different firmware versions, or even settings may differ substantially. In many cases the output is produced by software in a host computer rather by the instrument itself, adding further uncertainties and possible differences due to for example the operating system of the host computer. A further complication is that in some cases the format of dates, times and numbers depends on the locale settings in use at the time of data acquisition, or analysis. For all those reasons, do expect to have to do some debugging, and most importantly always validate the imported data against the original file (remembering to run a new validation each time there is a software or firmware update) or update of this package as I test each version before release only with the example files I have available, which are not many.

2 Examples

2.1 Ocean Optics Jaz

2.1.1 Raw detector counts

Reading a raw data file generated by Ocean Optics' Jaz spectrometer. The light source was the Jaz PX pulsed Xenon light module.

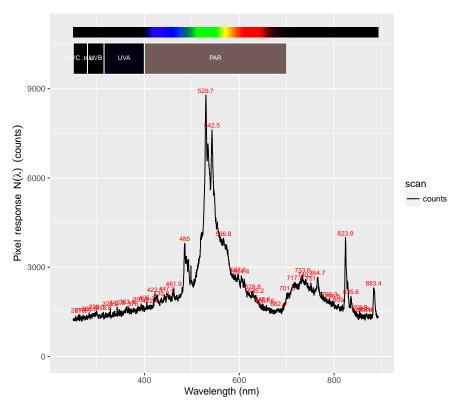
The first few lines of the file look like this, with W for wavelength, D for dark, R for reference, S for sample and P for processed (all spectral data values are raw detector counts):

```
Jaz Data File
Date: Mon Apr 25 12:49:11 2016
User: jaz
Dark Spectrum Present: Yes
Reference Spectrum Present: Yes
Processed Spectrum Present: Yes
Spectrometers: JAZA3098
Integration Time (usec): 748000 (JAZA3098)
Spectra Averaged: 1 (JAZA3098)
Boxcar Smoothing: 0 (JAZA3098)
Correct for Electrical Dark: No (JAZA3098)
Strobe/Lamp Enabled: Yes (JAZA3098)
Correct for Detector Non-linearity: No (JAZA3098)
Correct for Stray Light: No (JAZA3098)
Number of Pixels in Processed Spectrum: 2048
>>>>Begin Processed Spectral Data<>
WDRSP
190.313904 0.000000 0.000000 0.000000 0.000000
190.695511 0.000000 0.000000 0.000000 0.000000
191.077087 1138.953125 1123.134277 1102.795898 228.570541
191.458633 1184.149658 1227.086426 1059.859131 -289.473419
191.840149 1175.110352 1193.188965 1132.173584 -237.500336
```

```
jazraw.spct <- read_oo_jazdata(file = "data-vignettes/spectrum.jaz")
jazraw.spct <- trim_wl(jazraw.spct, range = c(250, 900))</pre>
```

Plotting the spectrum.

```
plot(jazraw.spct)
```



The metadata stored in attributes can be accessed with functions. It is clear, that not all settings can be recovered from the file. However, we store the record will all the fields which would have been filled if the data had been acquired directly from R using package 'ooacquire'.

```
getWhenMeasured(jazraw.spct)
## [1] "2016-04-25 12:49:11 UTC"

getInstrDesc(jazraw.spct)
## $time
## [1] "2016-04-25 12:49:11 UTC"
##
## ##
```

```
## NULL
##
## $sr.index
## [1] NA
## $ch.index
## [1] NA
##
## $spectrometer.name
## [1] "Jaz"
##
## $spectrometer.sn
## [1] "JAZA3098"
## $bench.grating
## [1] NA
## $bench.filter
## [1] NA
##
## $bench.slit
## [1] NA
##
## $min.integ.time
## [1] NA
##
## $max.integ.time
## [1] NA
## $max.counts
## [1] NA
##
## $wavelengths
## [1] NA
##
## $bad.pixs
## numeric(0)
##
## $inst.calib
## list()
```

```
getInstrSettings(jazraw.spct)

## $time
## [1] "2016-04-25 12:49:11 UTC"

##
## $w
## NULL
##
## $sr.index
## [1] NA
##
## $ch.index
## [1] NA
##
## $correct.elec.dark
```

```
## No
## 0
##
## $correct.non.lin
## No
## 0
##
## $correct.stray.light
## No
## 0
##
## $boxcar.width
## [1] "0"
##
## $integ.time
## [1] "748000"
## $num.scans
## [1] "1"
```

2.1.2 Spectral energy irradiance

Reading an "Absolute Irradiance File" (sic) generated by Ocean Optics' Jaz spectrometer results in a source_spct object. In this example, the light source measured was a 'white' fluorescent tube.

The first few lines of the file look like this:

```
Jaz Absolute Irradiance File
Date: Tue Feb 03 09:44:41 2015
User: jaz
Dark Spectrum Present: Yes
Processed Spectrum Present: Yes
Spectrometers: JAZA1065
Integration Time (usec): 193000 (JAZA1065)
Spectra Averaged: 3 (JAZA1065)
Boxcar Smoothing: 5 (JAZA1065)
Correct for Electrical Dark: Yes (JAZA1065)
Strobe/Lamp Enabled: No (JAZA1065)
Correct for Detector Non-linearity: Yes (JAZA1065)
Correct for Stray Light: No (JAZA1065)
Number of Pixels in Processed Spectrum: 2048
Fiber (micron): 3900
Collection Area: 0.119459
Int. Sphere: No
>>>>Begin Processed Spectral Data<
WDSP
188.825226 0.000000 0.000000 0.000000
189.284851 0.000000 0.000000 0.000000
189.744415 -89.659378 -90.917900 -0.000000
190.203964 -106.165916 -96.419785 0.000000
```

```
jaz.spct <- read_oo_jazirrad(file = "data-vignettes/spectrum.JazIrrad")

## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.032

jaz0.spct <- jaz.spct
jaz.spct <- trim_wl(jaz.spct, range = c(290, 800))

## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.032</pre>
```

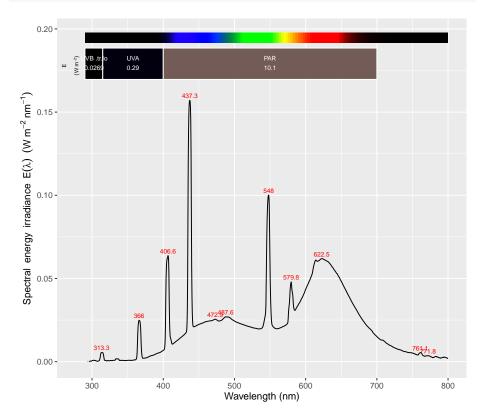
Plotting the spectrum.

```
plot(jaz.spct)

## Warning: Removed 9 rows containing non-finite values
## (stat_peaks).

## Warning: Removed 9 rows containing non-finite values
## (stat_wb_irrad).

## Warning: Removed 2 rows containing missing values (geom_path).
```

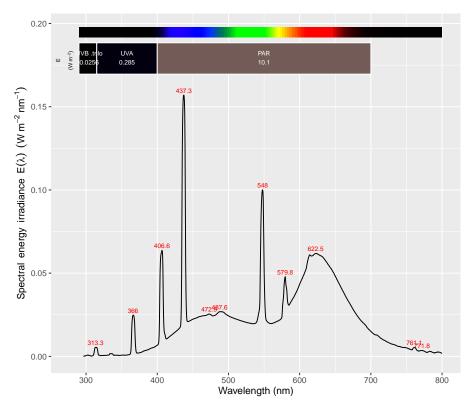


2.1.3 Cleaning spectral data

We can see that the data have problems. We get a warning because the data include negative values for spectral irradiance. We will use some methods from package 'photobiology' to correct the problem. As the data are noisy we cannot just shift the scale so that the most negative value becomes zero. Neither can we replace all negative values with zeros, as this would create bias.

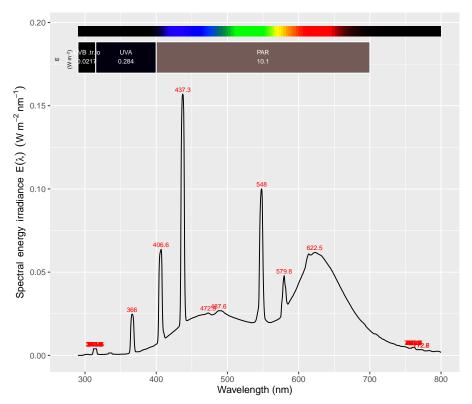
In the following code chunk we will use a region of the spectrum in which spectral irradiance is known to be equal to zero as reference to shift the scale zero. Afterwards we discard data "known" to be zero, and for which the instrument calibration is not valid, and finally we plot the spectrum.

```
jaz.spct <- fshift(jaz0.spct, range = c(255, 290), f = "mean")</pre>
## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.032
## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.00035
## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.00035
jaz.spct <- trim_wl(jaz.spct, range = c(290, 800))</pre>
## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.032
plot(jaz.spct)
## Warning: Removed 13 rows containing non-finite values
## (stat_peaks).
## Warning: Removed 13 rows containing non-finite values
## (stat_wb_irrad).
## Warning: Removed 9 rows containing missing values (geom_path).
```



We can next try to smooth the spectrum as it is very noisy outside the visible region.

```
jaz.spct <- smooth_spct(jaz.spct)
plot(jaz.spct)</pre>
```



Photon and energy irradiances.

```
e_irrad(jaz.spct, PAR()) # W m-2

## PAR
## 10.10459
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

All in one statement.

```
plot(read_oo_jazirrad(file = "data-vignettes/spectrum.JazIrrad"))

## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.032

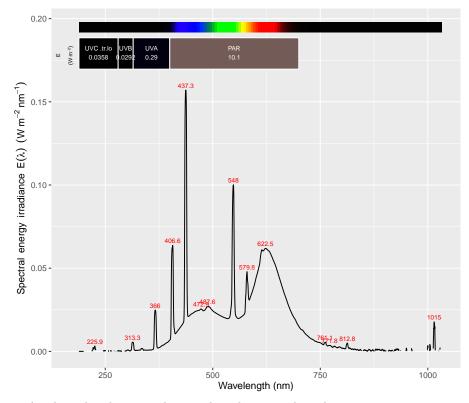
## Warning: Removed 378 rows containing non-finite values

## (stat_peaks).

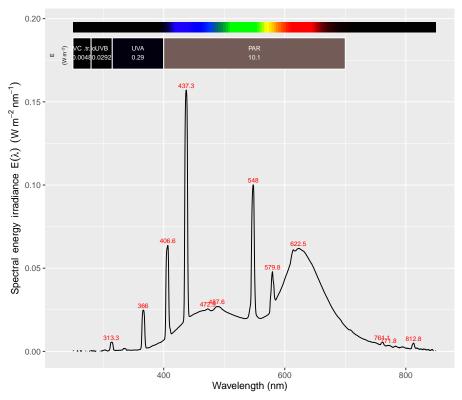
## Warning: Removed 378 rows containing non-finite values

## (stat_wb_irrad).

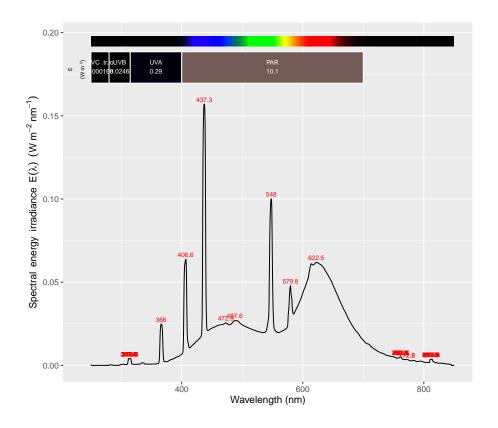
## Warning: Removed 1 rows containing missing values (geom_path).
```



As above but limiting the wavelength range plotted.



Adding our custom "adaptive" smoothing.



2.2 Other modular spectrometers from Ocean Optics

Now a file from an Ocean Optics' Q6500 spectrometer, with data processed with the Spectra Suite software.

Format of the header is similar, but not identical. The first few lines of the file look like this:

SpectraSuite Data File

Date: Mon May 06 15:13:40 CEST 2013

User: User

Dark Spectrum Present: Yes Reference Spectrum Present: No

Number of Sampled Component Spectra: 1

Spectrometers: QEB1523

Integration Time (usec): 100000 (QEB1523)

Spectra Averaged: 1 (QEB1523) Boxcar Smoothing: 0 (QEB1523)

Correct for Electrical Dark: No (QEB1523)

Strobe/Lamp Enabled: No (QEB1523)

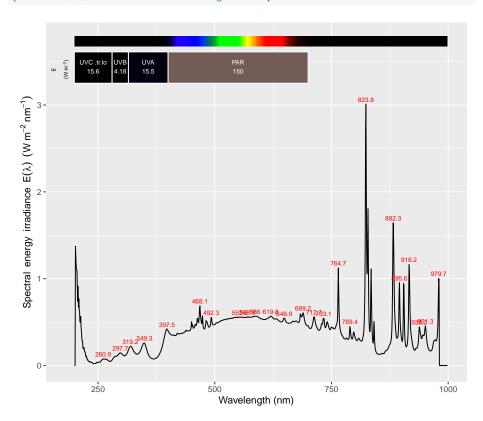
Correct for Detector Non-linearity: No (QEB1523)

Correct for Stray Light: Yes (QEB1523)
Number of Pixels in Processed Spectrum: 1044
>>>>Begin Processed Spectral Data<

199.08 0.0000E00

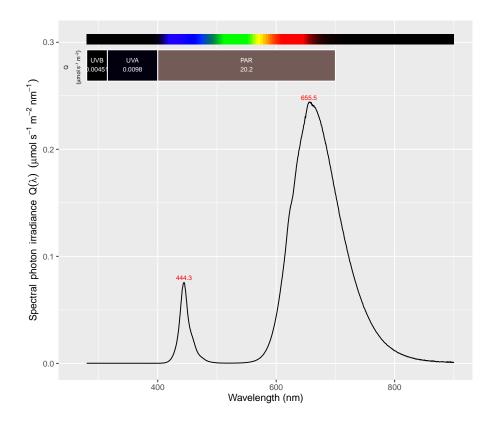
```
199.89 0.0000E00
200.70 0.0000E00
```

plot(read_oo_ssirrad(file = "data-vignettes/spectrum.SSIrrad"))



2.3 Modular spectrometers from Avantes

Avantes' two column .csv files can also be imported.

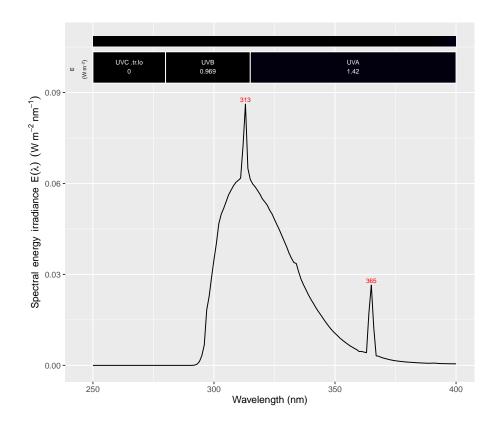


Scanning spectrometer from Macam 2.4

Macam's single column DTA files can also be imported. The first few lines of the file look like this with all data in a single column with alternate rows for wavelengths (in nm) and irradiances, and a very terse header:

```
@19/5/1997
@17:44:58
#No Title
2.5000000000E+02
0.000000000E+00
 2.5100000000E+02
0.000000000E+00
 2.5200000000E+02
0.000000000E+00
```

plot(read_macam_dta(file = "data-vignettes/spectrum.DTA"))



2.5 LI-1800 scanning spectrometer from LI-COR

And a file generated by LI-COR's PC1800 program for the LI-1800 spectroradiometer.

The output has a relatively detailed header, but it lacks year information. Files can contain either energy or photon based spectral irradiances, and this is signalled in the header. In this example photon (= quantum) spectral irradiance is returned. The first few lines of the file look like this:

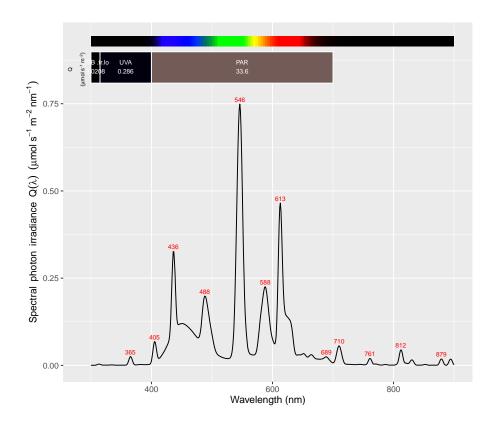
```
"FILE:FL2"
"REM: TLD 36W/865 (QNTM)"
"LIMS: 300- 900NM"
"INT: 1NM"
"DATE:08/23 16:32"
"MIN: 300NM 1.518E-04"
"MAX: 546NM 7.491E-01"
300 1.518E-04
301 3.355E-04
302 2.197E-04
303 3.240E-04
```

Function read_licor_prn will automatically detect whether the data is energy or photon based.

```
licor.spct <- read_licor_prn(file = "data-vignettes/spectrum.PRN")</pre>
```

In all cases as much information as possible is decoded, and the data file headers are preserved as comments in the source.spct objects.

```
licor.spct
## Object: source_spct [601 x 2]
## Wavelength range 300 to 900 nm, step 1 nm
## Label: File: data-vignettes/spectrum.PRN
## Measured on 0000-08-23 16:32:00 UTC
## Time unit 1s
##
## # A tibble: 601 x 2
## w.length s.q.irrad
##
      <dbl> <dbl>
## 1
         300 1.518e-10
        301 3.355e-10
## 2
## 3
        302 2.197e-10
## # ... with 598 more rows
cat(comment(licor.spct))
## LICOR LI-1800 file 'data-vignettes/spectrum.PRN' imported on 2016-07-16 20:29:37 UTC
## "FILE:FL2"
## "REM: TLD 36W/865
                          (QNTM)"
## "LIMS: 300- 900NM"
## "INT: 1NM"
## "DATE:08/23 16:32"
## "MIN: 300NM 1.518E-04"
## "MAX: 546NM 7.491E-01"
plot(licor.spct, unit.out = "photon")
```



3 Output from simulation models

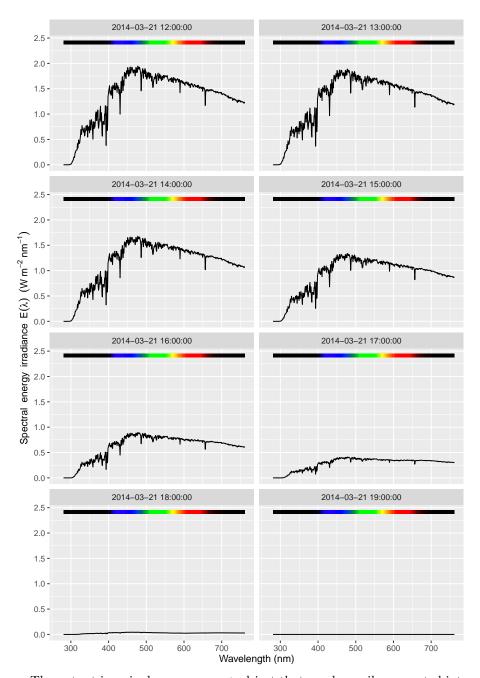
3.1 TUV

The output from the TUV model can be imported either by editing it before import, or by making a simple edit to the output routine of TUV. This function is known to work with TUV version 5.0 output. The output from TUV can contain a variable number of spectra in "parallel" columns, which are *melted* into a single column, with a factor with letter as levels, a numeric variable with the zenith angle and a POSIXct column with times. A date needs to be always supplied as the output file from TUV has only time of day information.

```
## Min. :280.5 A :482 Min. :0.000
## 1st Qu.:400.8 B : 0
## Median :521.0 C : 0
## Mean :521.0 D : 0
                                 1st Qu.:1.216
                                 Median :1.483
                                 Mean :1.322
## 3rd Qu.:641.2 E : 0 3rd Qu.:1.680
## Max. :761.5 F : 0 Max. :1.947
                  (Other): 0
##
##
       angle
                       date
## Min. :1.829 Min. :2014-03-21 12:00:00
  1st Qu.:1.829 1st Qu.:2014-03-21 12:00:00
##
## Median :1.829 Median :2014-03-21 12:00:00
## Mean :1.829
                   Mean :2014-03-21 12:00:00
## 3rd Qu.:1.829
                   3rd Qu.:2014-03-21 12:00:00
## Max. :1.829 Max. :2014-03-21 12:00:00
tuv.spct
## Object: source_spct [3,856 x 5]
## containing 8 spectra in long form
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: data-vignettes/usrout.txt
## Measured between 2014-03-21 12:00:00 and 2014-03-21 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 3,856 x 5
##
  w.length spct.idx s.e.irrad angle
##
        <dbl> <fctr>
                        <dbl> <dbl>
## 1
        280.5
                A 3.041e-15 1.829
## 2 281.5
                    A 1.164e-13 1.829
## 3
      282.5
                   A 1.824e-12 1.829
## # ... with 3,853 more rows, and 1 more variables:
```

It is possible to extract individual spectra with subset, or as done here plot them in different panels.

```
plot(tuv.spct, annotations = c("colour.guide")) +
  facet_wrap(~date, ncol = 2)
```



The output is a single source_spct object that can be easily converted into a source_mspct object containing the individual spectra as members of the collection.

```
tuv.mspct <- subset2mspct(tuv.spct)</pre>
tuv.mspct
## Object: source_mspct [8 x 1]
## --- Member: A ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 482 x 4
## w.length s.e.irrad angle
## * <dbl> <dbl> <dbl>
                                         <time>
## 1 280.5 3.041e-15 1.829 2014-03-21 12:00:00
## 2 281.5 1.164e-13 1.829 2014-03-21 12:00:00
## 3
       282.5 1.824e-12 1.829 2014-03-21 12:00:00
## # ... with 479 more rows
## --- Member: B ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm \,
## Time unit 1s
##
## # A tibble: 482 x 4
## w.length s.e.irrad angle
                                            date
## *
      <dbl> <dbl> <dbl>
                                          <time>
## 1
       280.5 1.314e-15 13.198 2014-03-21 13:00:00
## 2
      281.5 5.415e-14 13.198 2014-03-21 13:00:00
## 3 282.5 9.039e-13 13.198 2014-03-21 13:00:00
## # ... with 479 more rows
## --- Member: C ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 482 x 4
## w.length s.e.irrad angle
## * <dbl> <dbl> <dbl>
                                         <time>
## 1 280.5 4.521e-17 28.2 2014-03-21 14:00:00
## 2 281.5 2.510e-15 28.2 2014-03-21 14:00:00
      282.5 5.413e-14 28.2 2014-03-21 14:00:00
## 3
## # ... with 479 more rows
## --- Member: D ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 482 x 4
## w.length s.e.irrad angle
                                            date
## * <dbl> <dbl> <dbl>
                                          <time>
## 1
       280.5 3.075e-20 43.202 2014-03-21 15:00:00
## 2 281.5 3.273e-18 43.202 2014-03-21 15:00:00
## 3 282.5 1.234e-16 43.202 2014-03-21 15:00:00
## # ... with 479 more rows
## --- Member: E ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit 1s
##
```

```
## # A tibble: 482 x 4
## w.length s.e.irrad angle
                                            date
## *
      <dbl> <dbl> <dbl>
       280.5 2.253e-26 58.205 2014-03-21 16:00:00
## 1
      281.5 7.751e-24 58.205 2014-03-21 16:00:00
## 3
      282.5 8.148e-22 58.205 2014-03-21 16:00:00
## # ... with 479 more rows
## --- Member: F --
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 482 x 4
## w.length s.e.irrad angle
                                            date
## * <dbl> <dbl> <dbl>
## 1
       280.5 1.929e-27 73.208 2014-03-21 17:00:00
        281.5 5.710e-25 73.208 2014-03-21 17:00:00
## 2
      282.5 5.202e-23 73.208 2014-03-21 17:00:00
## 3
## # ... with 479 more rows
## --- Member: G ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 482 x 4
## w.length s.e.irrad angle
                                            date
## *
       <dbl> <dbl> <dbl>
       280.5 4.721e-28 88.211 2014-03-21 18:00:00
## 1
## 2 281.5 1.385e-25 88.211 2014-03-21 18:00:00
## 3
      282.5 1.250e-23 88.211 2014-03-21 18:00:00
## # ... with 479 more rows
## --- Member: H ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 482 x 4
## w.length s.e.irrad angle
                                             date
## * <dbl> <dbl> <dbl>
## 1 280.5
                 0 103.213 2014-03-21 19:00:00
## 2
       281.5
                    0 103.213 2014-03-21 19:00:00
       281.5 0 103.213 2014-03-21 19:00:00 282.5 0 103.213 2014-03-21 19:00:00
## 3
## # ... with 479 more rows
## --- END ---
```

With the default of lubridate::today() for date times are 'mapped' to the current local date using the time zone of the computer as visible to R.

```
tuv_nd.spct <- read_tuv_usrout(file = "data-vignettes/usrout.txt")
tuv_nd.spct

## Object: source_spct [3,856 x 5]
## containing 8 spectra in long form
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: data-vignettes/usrout.txt
## Measured between 2016-07-16 12:00:00 and 2016-07-16 19:00:00 UTC</pre>
```

```
## Time unit 1s
##
## # A tibble: 3,856 x 5
## w.length spct.idx s.e.irrad angle
## <dbl> <fctr> <dbl> <dbl> <dbl>
## 1 280.5 A 3.041e-15 1.829
## 2 281.5 A 1.164e-13 1.829
## 3 282.5 A 1.824e-12 1.829
## # ... with 3,853 more rows, and 1 more variables:
## # date <time>
```

3.2 libRadtran

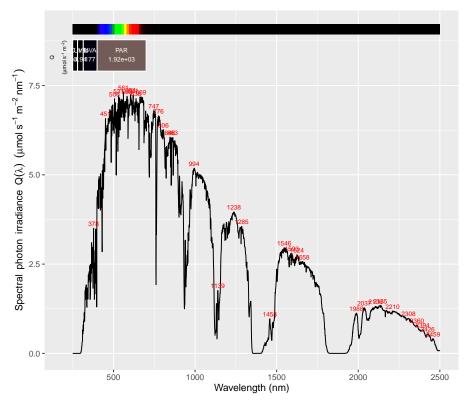
By default 'libRadtran' writes only spectral irradiances to a text file as output. This is different from 'TUV' which by default includes an extensive header with the parameter settings used for the simulation.

For reading this simple output, no special function is needed. We can use either read.table from base R. Here we read a file with two columns with wavelengths and global spectral energy irradiance (named "eglo" in libRadtran) in $mWm^{-2}nm^{-1}$. The file was created with one of the 'uvspec' examples included with libRadtran, but reducing the output to two columns.

The first few lines of the file look like this:

```
250.000 0.000000e+00
251.000 0.000000e+00
252.000 0.000000e+00
253.000 0.000000e+00
```

```
lrt.df <- read.table(file = "data-vignettes/libradtran-plain-2col.dat",</pre>
                   col.names = c("w.length", "s.e.irrad"))
summary(lrt.df)
##
                  s.e.irrad
      w.length
## Min. : 250 Min. : 0.000
## 1st Qu.:1188 1st Qu.: 3.808
## Median: 2125 Median: 23.999
## Mean :2125 Mean : 244.546
   3rd Qu.:3062
                 3rd Qu.: 264.351
## Max. :4000 Max. :1744.596
libradtran.spct <- source_spct(w.length = lrt.df$w.length,</pre>
                             s.e.irrad = lrt.df$s.e.irrad * 1e-3)
plot(libradtran.spct, range = c(250, 2500), unit.out = "photon")
```



We give two additional examples, which will most likely need some adjustment by users, as these are for output from libRadtran postprocessed to add additional information. These are included in the package because myself and collaborators use these formats heavily. In fact users could develop shell scripts or Perl scripts using the same output format.

3.3 Output enriched with time and date data

In this case the file to be read is similar as above, but including separate columns for direct and diffuse components of the spectral energy irradiance. In addition two columns, one with date strings in ISO format and one with times have been added. The file instead of containing a single spectrum, contains several spectra in long form.

The first few lines of the file look like this:

```
290.000 2015-05-19 11_00_00 0.000000e+00 0.000000e+00 291.000 2015-05-19 11_00_00 0.000000e+00 0.000000e+00 292.000 2015-05-19 11_00_00 0.000000e+00 0.000000e+00 293.000 2015-05-19 11_00_00 1.893645e-05 3.439497e-05 294.000 2015-05-19 11_00_00 1.648530e-04 2.764368e-04
```

A function is included for reading data saved in a text file in this format. It also automatically converts $mW\,m^{-2}\,nm^{-1}$ into $W\,m^{-2}\,nm^{-1}$.

```
lbr.multi.spct <- read_libradtran_vesa("data-vignettes/libradtran-multi.dat")</pre>
print(lbr.multi.spct, n = 5)
## Object: source_spct [3,055 x 5]
## containing 5 spectra in long form
## Wavelength range 290 to 900 nm, step 1 nm
## Label: libRadtran spectral simulation File: data-vignettes/libradtran-multi.dat
## Measured between 2015-05-19 11:00:00 and 2015-05-19 11:04:00 UTC
## Time unit 1s
##
## # A tibble: 3,055 x 5
##
  w.length datetime s.e.irrad.dir
##
       <dbl>
                         <time>
## 1
        290 2015-05-19 11:00:00 0.000000e+00
         291 2015-05-19 11:00:00 0.000000e+00
## 2
        292 2015-05-19 11:00:00 0.000000e+00
## 3
## 4
        293 2015-05-19 11:00:00 1.893645e-08
## 5
        294 2015-05-19 11:00:00 1.648530e-07
## # ... with 3,050 more rows, and 2 more variables:
## # s.e.irrad.diff <dbl>, s.e.irrad <dbl>
```

3.4 Scripts developed by Anders Lindfors

Functions read_fmi_cum and read_m_fmi_cum can be used to read text files output by a simulation model of solar spectral irradiance. The model was developed at the Finnish Meteorological Institute (FMI) by Dr. Anders Lindfors and collaborators and uses functions from 'libRadtran' as its engine, but saves some additional metadata to the output file.

The first few lines of the file look like this:

```
# date number_of_scans start_scan stop_scan max_time_gap max_sza_gap warnings
# 20140821 15 3:30:00 17:30:00 60 7.4
# wavelength exposure(J/m2/nm)
2900 0.00000000e+00
2910 2.93132235e-05
2920 7.23526379e-04
```

We can read an individual file into a source_spct object while adding some metadata read from the file header. In this case values are for daily global spectral energy exposures rather than irradiances. Wavelengths are expressed in Angstroms instead of nanometres.

```
z.spct <- read_fmi_cum("data-vignettes/2014-08-21_cum.hel")
class_spct(z.spct)

## [1] "source_spct" "generic_spct"
getWhenMeasured(z.spct)

## [1] "2014-08-21 UTC"

z.spct</pre>
```

```
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: data-vignettes/2014-08-21_cum.hel
## Measured on 2014-08-21 UTC
## Time unit 86400s (~1 days)
##
## # A tibble: 511 x 2
## w.length s.e.irrad
##
      <dbl>
                   <dbl>
       290 0.000000e+00
## 1
## 2 291 2.931322e-05
## 3
        292 7.235264e-04
## # ... with 508 more rows
```

With function <code>read_m_fmi_cum</code> with an "m" in the name we can read several files each containing a single spectrum. The returned object is a collection of source spectra.

```
z.mspct <- read_m_fmi_cum(c("data-vignettes/2014-08-21_cum.hel",</pre>
                             "data-vignettes/2014-08-22_cum.hel"))
class(z.mspct)
## [1] "source_mspct" "generic_mspct" "list"
getWhenMeasured(z.mspct)
## # A tibble: 2 x 2
## spct.idx when.measured
##
                 <fctr> <fctr> <time>
## 1 2014_08_21_cum.hel 2014-08-21
## 2 2014_08_22_cum.hel 2014-08-22
z.mspct
## Object: source_mspct [2 x 1]
## --- Member: 2014_08_21_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: data-vignettes/2014-08-21_cum.hel
## Measured on 2014-08-21 UTC
## Time unit 86400s (~1 days)
##
## # A tibble: 511 x 2
## w.length s.e.irrad
##
      <dbl>
                    <dbl>
## 1 290 0.000000e+00
## 2 291 2.931322e-05
## 3 292 7.235264e-04
## # ... with 508 more rows
## --- Member: 2014_08_22_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm \,
## Label: File: data-vignettes/2014-08-22_cum.hel
## Measured on 2014-08-22 UTC
## Time unit 86400s (~1 days)
##
```

Above we gave the names of the files explicitly, but as we show here, one can build on-the-fly a list of file names matching some pattern.

```
files <- system("ls ./data-vignettes/*cum.hel", intern = TRUE)</pre>
z1.mspct <- read_m_fmi_cum(files)</pre>
class(z1.mspct)
## [1] "source_mspct" "generic_mspct" "list"
getWhenMeasured(z1.mspct)
## # A tibble: 2 x 2
## spct.idx when.measured
                <fctr> <time>
## 1 2014_08_21_cum.hel 2014-08-21
## 2 2014_08_22_cum.hel 2014-08-22
z1.mspct
## Object: source_mspct [2 x 1]
## --- Member: 2014_08_21_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: ./data-vignettes/2014-08-21_cum.hel
## Measured on 2014-08-21 UTC
## Time unit 86400s (~1 days)
##
## # A tibble: 511 x 2
## w.length s.e.irrad
## <dbl>
               <dbl>
       290 0.000000e+00
291 2.931322e-05
## 1
## 2
        292 7.235264e-04
## 3
## # ... with 508 more rows
## --- Member: 2014_08_22_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: ./data-vignettes/2014-08-22_cum.hel
## Measured on 2014-08-22 UTC
## Time unit 86400s (~1 days)
##
## # A tibble: 511 x 2
## w.length s.e.irrad
```

```
## 3 292 7.213022e-04
## # ... with 508 more rows
##
## --- END ---
```

One also add a geocode at the time of import (or later).

```
z2.mspct <-
 read_m_fmi_cum(files,
               geocode = geocode("Kumpula, Helsinki, Finland",
                                source = "google"))
class(z2.mspct)
## [1] "source_mspct" "generic_mspct" "list"
getWhenMeasured(z2.mspct)
## # A tibble: 2 x 2
## spct.idx when.measured
               <fctr> <time>
## 1 2014_08_21_cum.hel 2014-08-21
## 2 2014_08_22_cum.hel 2014-08-22
getWhereMeasured(z2.mspct)
## # A tibble: 2 x 3
## spct.idx lon
                                  lat
##
               <fctr> <dbl> <dbl>
## 1 2014_08_21_cum.hel 24.96474 60.20911
## 2 2014_08_22_cum.hel 24.96474 60.20911
z2.mspct
## Object: source_mspct [2 x 1]
## --- Member: 2014_08_21_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: ./data-vignettes/2014-08-21_cum.hel
## Measured on 2014-08-21 UTC
## Measured at 60.20911 N, 24.96474 E
## Time unit 86400s (~1 days)
##
## # A tibble: 511 x 2
## w.length s.e.irrad
##
     <dbl>
               <dbl>
       290 0.000000e+00
## 1
## 2 291 2.931322e-05
        292 7.235264e-04
## 3
## # ... with 508 more rows
## --- Member: 2014_08_22_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: ./data-vignettes/2014-08-22_cum.hel
## Measured on 2014-08-22 UTC
## Measured at 60.20911 N, 24.96474 E
## Time unit 86400s (~1 days)
##
```

4 Other R packages

4.1 To R matrix

A general way of exchanging data with other R packages or for use with base R functions is to create a matrix.

Collections of spectra have a spct.byrow attribute and this is used as default, however, a value can by passed as argument to override this default.

```
z2r.mat <- mspct2mat(z2.mspct, "s.e.irrad", byrow = TRUE)
class(z2r.mat)

## [1] "matrix"

dim(z2r.mat)

## [1] 2 511

head(dimnames(z2r.mat)$spct)

## [1] "2014_08_21_cum.hel" "2014_08_22_cum.hel"</pre>
```

```
head(dimnames(z2r.mat)$w.length)

## [1] "290" "291" "292" "293" "294" "295"

head(attr(z2r.mat, "w.length"))

## [1] 290 291 292 293 294 295
```

These functions are not fully automatic, the user needs to provide the name of the variable to extract from each spectrum. If the wavelength values are not consistent among spectra, only those with the same values as the first spectrum in the collection are retained and the remaining ones dropped with a warning.

4.2 To 'hyperSpec'

Can export to "hyperSpec" objects only collections of spectra where all members have identical w.length vectors, as objects of class hypeSpec store a single vector of wavelengths for the whole collection of spectra.

```
z2.hspct <- mspct2hyperSpec(z2.mspct, "s.e.irrad")

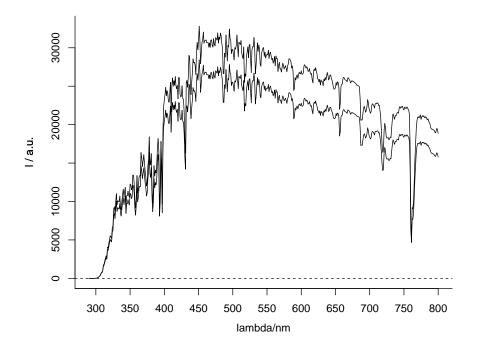
## Warning in .local(.Object, ...): Spectra in data are overwritten by argument spc.
class(z2.hspct)

## [1] "hyperSpec"

## attr(,"package")

## [1] "hyperSpec"

plot(z2.hspct)</pre>
```

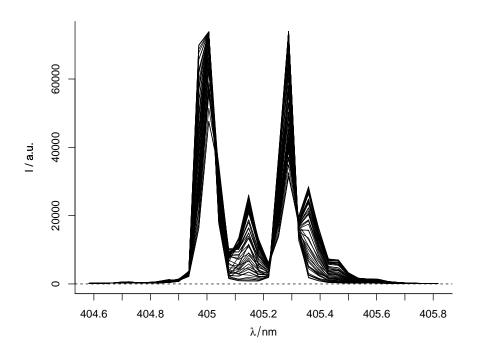


4.3 From 'hyperSpec'

Can import only data with wavelength in nanometres. Other quantities and units are not supported by the 'photobiology' classes for spectral data. See package 'hyperSpec' vignette "laser" for details on the data and the conversion of the original wavelength units into nanometres.

```
class(laser)
## [1] "hyperSpec"
## attr(,"package")
## [1] "hyperSpec"
laser
## hyperSpec object
##
      84 spectra
      2 data columns
##
      36 data points / spectrum
## wavelength: lambda/nm [numeric] 404.5828 404.6181 ... 405.8176
## data: (84 rows x 2 columns)
##
     1. t: t / s [numeric] 0 2 ... 5722
     2. spc: I / a.u. [matrix36] 164.650 179.724 ... 112.086
```

```
plot(laser)
## Warning in plotspc(x, ...): Number of spectra exceeds spc.nmax. Only the first
50 are plotted.
```



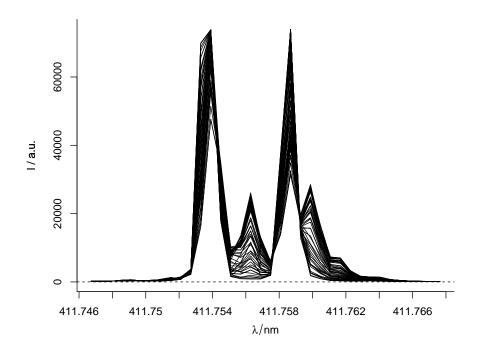
We assume here, that the quantity for the spectral emission of the laser is spectral energy irradiance, expressed in $\rm mW\,m^{-2}\,nm^{-1}$. This is likely to be wrong but for the sake of showing how the conversion takes place is irrelevant. The parameter multiplier can be passed a numeric argument to rescale the original data. The default multiplier is 1.

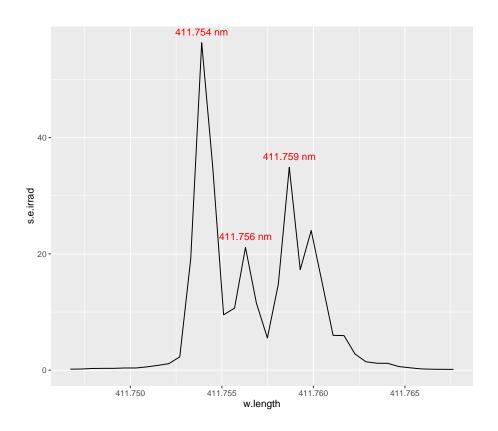
```
wl(laser) <- list (
    wl = 1e7 / (1/405e-7 - wl (laser)),
    label = expression (lambda / nm)
)
laser

## hyperSpec object
## 84 spectra
## 2 data columns
## 36 data points / spectrum
## wavelength: lambda/nm [numeric] 411.7467 411.7473 ... 411.7677
## data: (84 rows x 2 columns)
## 1. t: t / s [numeric] 0 2 ... 5722
## 2. spc: I / a.u. [matrix36] 164.650 179.724 ... 112.086</pre>
```

```
## Warning in plotspc(x, ...): Number of spectra exceeds spc.nmax. Only the first
50 are plotted.

laser.mspct <-
   hyperSpec2mspct(laser, "source_spct", "s.e.irrad", multiplier = 1e-3)
ggplot(laser.mspct[[1]]) +
   geom_line() +
   stat_peaks(geom = "text", vjust = -1, label.fmt = "%.6g nm", color = "red")</pre>
```





4.4 From 'colorSpec'

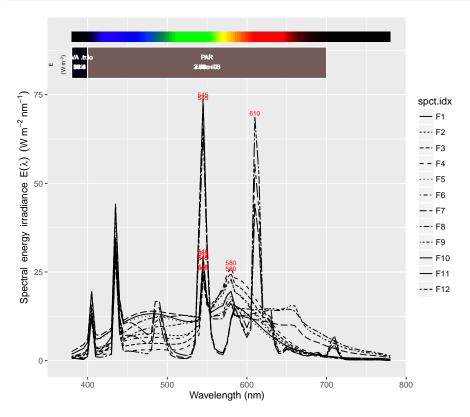
```
fluorescent.mspct <- colorSpec2mspct(Fs.5nm)</pre>
print(fluorescent.mspct, n = 3, n.members = 3)
## Object: source_mspct [12 x 1]
## --- Member: F1 --
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm
## Time unit 1s
##
## # A tibble: 81 x 2
##
   w.length s.e.irrad
       <dbl> <dbl>
               1.87
## 1
        380
## 2
         385
                  2.36
        390
                  2.94
## 3
## # ... with 78 more rows
## --- Member: F2 ---
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm \,
## Time unit 1s
##
## # A tibble: 81 x 2
```

```
## w.length s.e.irrad
## <dbl> <dbl>
## 1
       380
                1.18
       385
## 2
                1.48
## 3
       390 1.84
## # ... with 78 more rows
## --- Member: F3 ---
## Object: source_spct [81 x 2]
\mbox{\tt \#\#} Wavelength range 380 to 780 nm, step 5 nm
## Time unit 1s
##
## # A tibble: 81 x 2
## w.length s.e.irrad
    <dbl> <dbl>
##
## 1 380 0.82
## 2 385 1.02
## 3 390 1.26
## 3
        390
                1.26
## # ... with 78 more rows
## .....
## 9 other member spectra not shown
##
## --- END ---
```

```
colorSpec2mspct(Hoya)
## Object: filter_mspct [4 x 1]
## --- Member: R-60 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
## # A tibble: 46 x 2
## w.length Tfr
## <dbl> <dbl>
       300 0
310 0
## 1
       310
## 2
## 3
       320
## # ... with 43 more rows
## --- Member: G-533 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm \,
##
## # A tibble: 46 x 2
##
  w.length Tfr
##
     <dbl> <dbl>
## 1
       300 0
## 2 310 0
## 3
       320
              0
## # ... with 43 more rows
## --- Member: B-440 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm \,
##
## # A tibble: 46 x 2
## w.length Tfr
## <dbl> <dbl>
## 1 300 0
```

```
## 2 310 0
## 3
        320
                  0
## # ... with 43 more rows ## --- Member: LB-120 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm \,
##
## # A tibble: 46 x 2
##
               Tfr
   w.length
##
        <dbl> <dbl>
          300 0.00003
## 1
## 2
          310 0.00580
## 3
          320 0.08100
## # ... with 43 more rows
## --- END ---
```

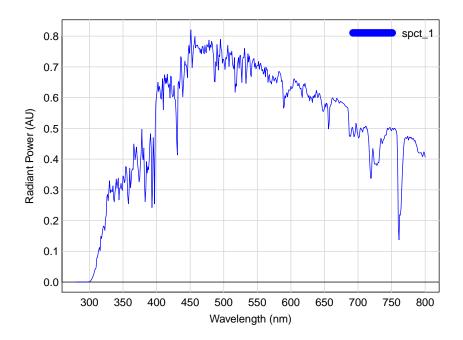
```
fluorescent.spct <- colorSpec2spct(Fs.5nm)
plot(fluorescent.spct) + aes(linetype = spct.idx)</pre>
```



```
colorSpec2chroma_spct(xyz1931.5nm)
## Object: chroma_spct [81 x 4]
```

4.5 To 'colorSpec'

```
sun.cspec <- spct2colorSpec(sun.spct)
plot(sun.cspec, col = "blue")</pre>
```



```
##
## colorSpec (yellow_gel.spct)

##
## colorSpec object. The organization is 'vector'. Object size is 11488 bytes.
## the object describes 1 transparent materials, and the quantity is 'transmittance'.
## Wavelength range: 190 to 800 nm. Step size is 1 nm.
##
```

```
## 1 spectra
## 611 data points / spectrum
##
## Material Min Max LambdaMax Integral
## 1 spct_1 1e-05 0.9025 768.5 260.3194
```

4.6 From 'pavo'

In this example we convert an rspec object from package 'pavo' into a collection of spectra and then we plot it with ggplot methods from package 'ggspectra' (an extension to 'ggplot2'). The data are the spectral reflectance of the plumage from seven different individual birds of the same species, measured in three different body parts.

We convert the data into a collection of spectra, and calculate summaries for three spectra.

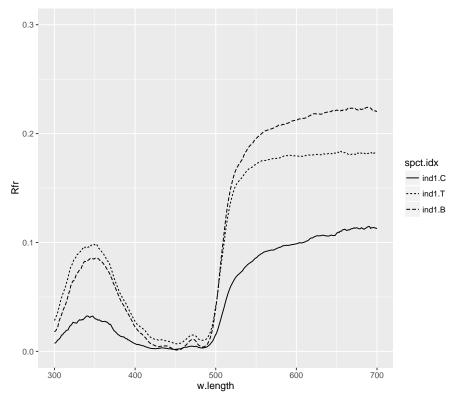
```
sicalis.mspct <- rspec2mspct(sicalis, "reflector_spct", "Rpc")
summary(sicalis.mspct[[1]])

## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## w.length Rfr</pre>
```

```
## Min. :300 Min. :0.001798
## 1st Qu.:400 1st Qu.:0.008288
## Median :500
                 Median :0.031709
## Mean :500 Mean :0.052848
## 3rd Qu.:600 3rd Qu.:0.098775
## Max. :700 Max. :0.114807
summary(sicalis.mspct[[2]])
## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
                     Rfr
##
      w.length
## Min. :300 Min. :0.006783
## 1st Qu.:400 1st Qu.:0.030112
## Median :500 Median :0.096994
## Mean :500 Mean :0.105449
## 3rd Qu.:600 3rd Qu.:0.179691
## Max. :700 Max. :0.183823
summary(sicalis.mspct[[3]])
## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
##
      w.length
                     Rfr
## Min. :300 Min. :0.001191
## 1st Qu.:400 1st Qu.:0.022293
## Median:500 Median:0.085235
## Mean :500 Mean :0.116253
## 3rd Qu.:600 3rd Qu.:0.212554
## Max. :700 Max. :0.224162
```

We convert the subset of the collection corresponding to the first individual into a single spectra object for plotting with ggplot.

```
ggplot(rbindspct(sicalis.mspct[1:3])) +
  aes(linetype = spct.idx) +
  ylim(0,0.3) +
  geom_line()
```



Here we extract the "crown" data from all individuals and plot these spectra in a single plot.

```
print(sicalis.mspct[c(TRUE, FALSE, FALSE)])
## Object: reflector_mspct [7 x 1]
## --- Member: ind1.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm \,
##
## # A tibble: 401 x 2
##
    w.length
                     Rfr
##
        <dbl>
                    <dbl>
## 1
         300 0.007594984
         301 0.007727841
## 2
         302 0.008288000
## # ... with 398 more rows
## --- Member: ind2.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm \,
##
## # A tibble: 401 x 2
##
     w.length
##
        <dbl>
                    <dbl>
## 1
         300 0.002971167
## 2 301 0.002326722
```

```
## 3 302 0.003227833
## # ... with 398 more rows
## --- Member: ind3.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
## w.length
##
      <dbl>
                   <dbl>
       300 0.0005947619
## 2 301 0.0000000000
## 3
        302 0.0011853968
## # ... with 398 more rows
## --- Member: ind4.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm \,
## # A tibble: 401 x 2
## w.length Rfr
##
     <dbl>
       300 0.003750159
## 1
## 2
         301 0.003465714
       302 0.004133333
## 3
## # ... with 398 more rows
## --- Member: ind5.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
## w.length Rfr
##
      <dbl>
                  <dbl>
## 1
        300 0.004225349
        301 0.005361222
## 2
## 3
       302 0.006554556
## # ... with 398 more rows
## --- Member: ind6.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm \,
##
## # A tibble: 401 x 2
## w.length Rfr
##
      <dbl>
       300 0.0006326984
## 1
## 2
       301 0.0006136508
## 3
       302 0.0001934921
## # ... with 398 more rows
## --- Member: ind7.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
## w.length
                  Rfr
##
     <dbl>
                   <dbl>
       300 0.001680730
## 1
     301 0.001043270
302 0.001702476
## 2
## 3
## # ... with 398 more rows
```

```
##
## --- END ---

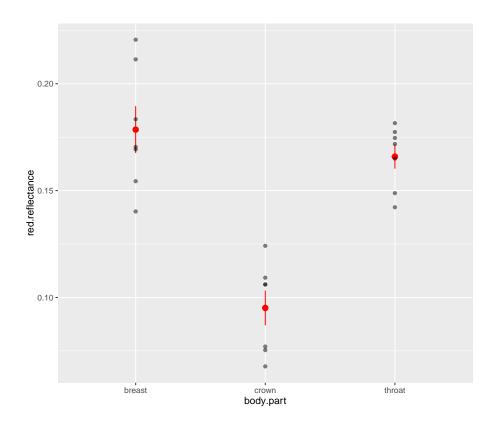
ggplot(rbindspct(sicalis.mspct[c(TRUE, FALSE, FALSE)])) +
   aes(linetype = spct.idx) +
   ylim(0,0.15) +
   geom_line() +
   ggtitle("'crown' reflectance spectra")
```

'crown' reflectance spectra 0.15 spct.idx 0.10 ---- ind1.C ---- ind2.C --· ind3.C 쟊 - - ind4.C ···· ind5.C · - · ind6.C 0.05 -- ind7.C 0.00 -500 300 400 600 700 w.length

We calculate the mean reflectance in wavebands corresponding to ISO colors obtaining a data frame. We then add to this returned data frame a factor indicating the body parts.

```
refl.by.band <- reflectance(sicalis.mspct, w.band = list(Red(), Green(), Blue(), UVA()))
refl.by.band$body.part <- c("crown", "throat", "breast")

refl.red <- reflectance(sicalis.mspct, w.band = Red())
names(refl.red)[2] <- "red.reflectance"
refl.red$body.part <- c("crown", "throat", "breast")
ggplot(refl.red, aes(x = body.part, y = red.reflectance)) +
    stat_summary(fun.data = "mean_se", color = "red") +
    geom_point(alpha = 0.5)</pre>
```



5 Dealing with odd and bad data

5.1 Using locales

Most functions in this package have a parameter locale, that accepts readr::locole objects as arguments. At the moment only the time zone and decimal mark are respected. This allows files using comma for decimal marker be easily imported, or the dates and times in the input file be interpreted in a given time zone. Setting the correct time zone is very important to avoid errors. Time coordinates are always stored in the created objects using universal time coordinates ("UTC").

5.2 Overriding default metadata

We revisit now the Jaz irradiance data to show how the metadata can be changed by the user if needed (e.g. clock settings at the time of data acquisition were wrong).

A variable with the user supplied date and time data, or the date read from the header (the text itself) not the file date as the file date may not reflect the creation date and time.

5.3 Adding additional metadata

When can add a geocode, either directly by giving latitude and longitude coordinates or by generating it from a Google maps search using function ggmap::geocode() as shown here.

```
## Object: source_spct [2,048 x 2]
## Wavelength range 188.82523 to 1033.1483 nm, step 0.357056 to 0.459625 nm
## Label: File: data-vignettes/spectrum.JazIrrad
## Measured on 2015-02-03 09:44:41 UTC
## Measured at 60.22515 N, 25.02006 E
## Time unit 1s
##
## # A tibble: 2,048 x 2
## w.length s.e.irrad
## <dbl> <dbl>
## 1 188.8252
## 2 189.2849
                     0
              0
## 3 189.7444
## # ... with 2,045 more rows
getWhereMeasured(jaz04.spct)
## lon
                 lat
## 1 25.02006 60.22515
```