

# Manual for pgf-spectra 1.0

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21st April 2016



## Abstract

The purpose of this package is to draw the spectrum of elements in a simple way. It's based on the package *pst-spectra* with similar options, but with some extra options. It relays on the pgf/TikZ to draw the desired spectrum, continuous or discrete. As in *pst-spectra* there are data available for the spectra of 99 elements and their ions (from the NASA database). It also allows the user to draw a spectrum with their own personal data.

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## Installation and usage

pgf-spectra is placed under the terms of the L<sup>A</sup>T<sub>E</sub>X Project Public License, version 1.3 or later (<http://www.latex-project.org/lppl.txt>). pgf-spectra loads and requires the packages *tikz* and *ifthen*.

You need to put the style file (pgf-spectra.sty) in a location where pdf<sub>l</sub>atex can find them. According to the TDS conventions this may be a subdirectory named tex/latex/pgfspectra/ or tex/latex/misc/ in your (site specific) installation tree (insert your appropriate directory delimiter instead of /, if needed).

If you are using pdf<sub>l</sub>atex, just can simply include the style file without any option via the `\usepackage` command: `\usepackage{pgf-spectra}`

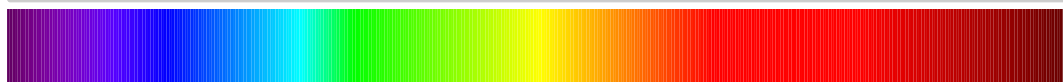
## The commands

There are at this time only two commands available:

- `\pgfspectra` or `\pgfspectra[options list]`
- and `\wcolor{\wavelength}`

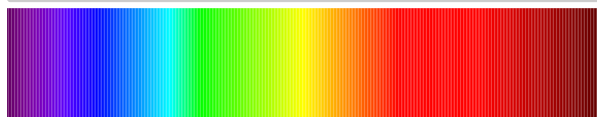
The first command is used without options to draw the visible continuous spectrum:

```
\pgfspectra
```

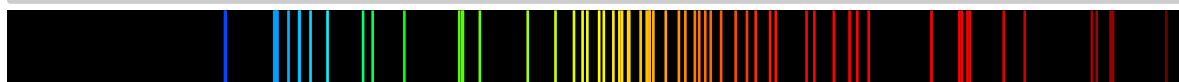


When using options a continuous or discrete spectra in the visible region can be drawn, for instance:

```
\pgfspectra[width=.5\textwidth,height=1.5cm]
```



```
\pgfspectra[width=\textwidth,element=Ne]
```



The other command is used to convert a wavelength (from 380 to 780 nanometers) to the respective color available as 'wcolor':

```
\tikz{\foreach \x in {380,430,...,780}{
  \wcolor{\x}
  \draw[fill=wcolor] (.02*\x,0) rectangle ++(1,.5)
  node[midway,font=\tiny\bfseries,text=black!50] {\x};
}}
```



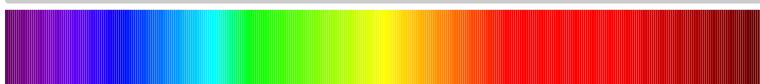
## Options

For the command `\pgfspectra` there are a set of options available to draw the spectrum as described below.

**width** default:  $0.9\textit{textwidth}$

Sets the width of the spectrum.

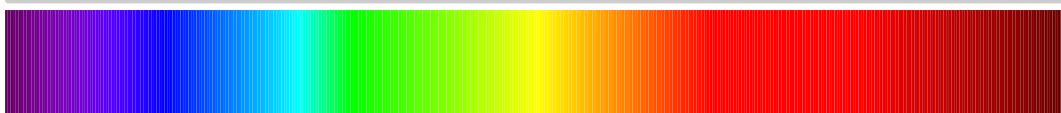
```
\pgfspectra[width=10cm]
```



**height** default:  $1\textit{cm}$

Sets the height of the spectrum.

```
\pgfspectra[height=40pt]
```



**element** default:  $NONE$

A single chemical symbol of an element or a list of chemical symbols.

```
\pgfspectra[element=H]
```



```
\pgfspectra[element={H,He}]
```



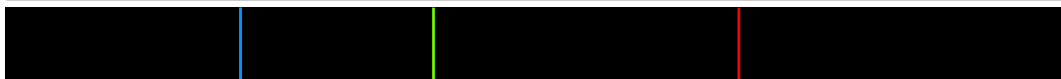
**charge** default:  $0$

The charge of the *particle* to draw the spectrum. Use 'all' to get all available lines for the element, i.e, for the atom and all the positive ions that exists in the database.

```
\pgfspectra[element=He]
```



```
\pgfspectra[element=He,charge=1]
```



```
\pgfspectra[element=He,charge=2]
```

Element "He" with charge "2" have no lines to display.

```
\pgfspectra[element=He,charge=all]
```



**Imin**

default: 0

The minimum intensity of the lines to put in the spectrum. Value from 0 to 1.

```
\pgfspectra[element=He,Imin=.5]
```



```
\pgfspectra[element=He,Imin=.05]
```

**relative intensity**

default: false

Draws the lines respecting the intensity of the observed spectrum.

```
\pgfspectra[element=He,relative intensity]
```

**relative intensity threshold**

default: 0.25

Sets the minimum intensity for the lines in the spectrum when using relative intensities. When set to 0.25 a line with real intensity 0 will have a spectral intensity of 0.25 and a line with intensity equal to the max intensity observed in that spectrum will have an intensity in the computed spectrum of 1, assuming of course an overall intensity in the range between 0 and 1.

```
\pgfspectra[element=He,relative intensity,relative intensity threshold=0]
```



```
\pgfspectra[element=He,relative intensity,relative intensity threshold=.25]
```



```
\pgfspectra[element=He,relative intensity,relative intensity threshold=.5]
```



```
\pgfspectra[element=He,relative intensity,relative intensity threshold=.75]
```



```
\pgfspectra[element=He,relative intensity,relative intensity threshold=1]
```



In fact setting the relative intensity threshold to 1 is equivalent to the spectrum without relative intensities:

```
\pgfspectra[element=He]
```



**line intensity**

default: 100

Draws all the lines with the specified intensity between 0 and 100 (as a percentage of the maximum intensity).

```
\pgfspectra[element=He,line intensity=0]
```



```
\pgfspectra[element=He,line intensity=50]
```



```
\pgfspectra[element=He,line intensity=100]
```



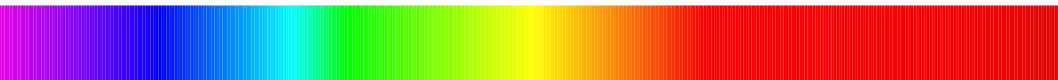
```
\pgfspectra[element=He]
```

**gamma**

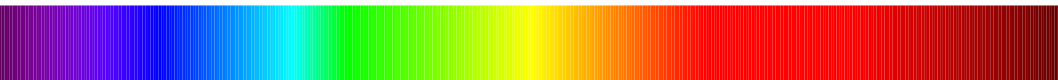
default: 0.8

Gamma color correction: any positive value.

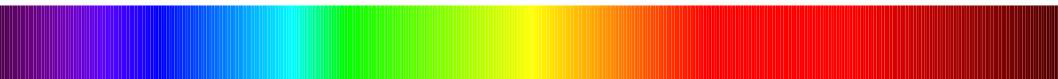
```
\pgfspectra[gamma=.1]
```



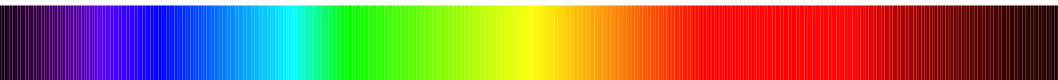
```
\pgfspectra[gamma=.8]
```



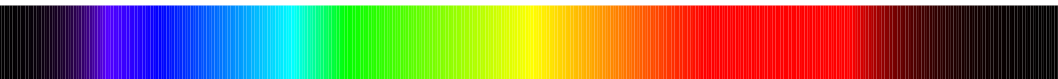
```
\pgfspectra[gamma=1]
```



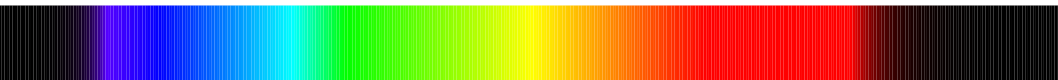
```
\pgfspectra[gamma=2]
```



```
\pgfspectra[gamma=5]
```



```
\pgfspectra[gamma=10]
```



**brightness**

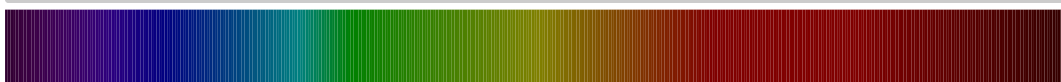
default: 1

Brightness color correction as in the CMYK color model. Value between 0 and 1. Zero stands for black and one for the maximum bright. *This option only works for the continuous component of the spectra, to change the "brightness" of spectral lines use the option 'line intensity'.*

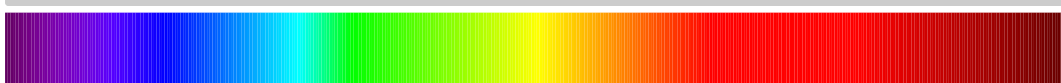
```
\pgfspectra[brightness=.1]
```



```
\pgfspectra[brightness=.5]
```



```
\pgfspectra[brightness=1]
```

**back**

default: black

Sets the background color of the spectrum. Only useful when there are spectral lines. Some shorthand are defined to put the visible region in the background: 'visible5', 'visible10', 'visible15', . . . , 'visible100'. This labels combined with the 'brightness' option makes it possible to achieve other values on the background, since the visible amount (5%,10%,. . .) is multiplied by the value of brightness.

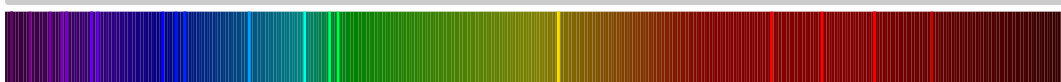
```
\pgfspectra[element=He,back=white]
```



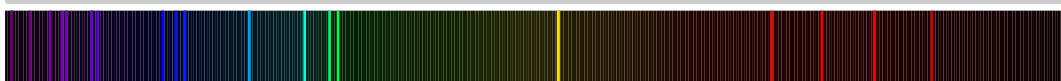
```
\pgfspectra[element=He,back=black!50]
```



```
\pgfspectra[element=He,back=visible50]
```



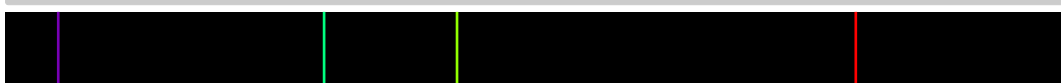
```
\pgfspectra[element=He,back=visible50,brightness=.26]
```

**lines**

default: {}

A comma separated list of wavelengths in the interval [380; 780] nm.

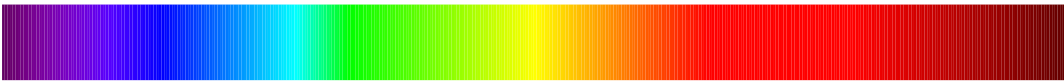
```
\pgfspectra[lines={400,500,550,700}]
```

**line width**

default: 1pt

The width of each individual line in the spectrum.

```
\pgfspectra[line width=2pt]
```



```
\pgfspectra[line width=2pt,element=He]
```

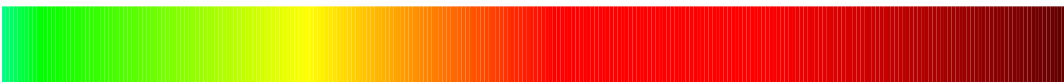


**begin**

default: 380

The starting wavelength in nanometers of the spectrum ( $380 \leq \lambda \leq 780$ ).

```
\pgfspectra[begin=500]
```

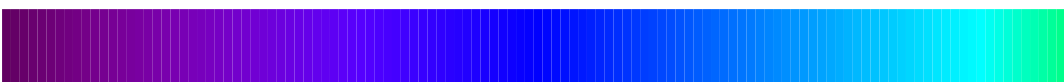


**end**

default: 780

The finishing wavelength in nanometers of the spectrum ( $380 \leq \lambda \leq 780$ ).

```
\pgfspectra[end=500]
```



**Remark:** *it's obviously possible to set 'begin' and 'end' at the same time and if desired change the order of the wavelengths.*

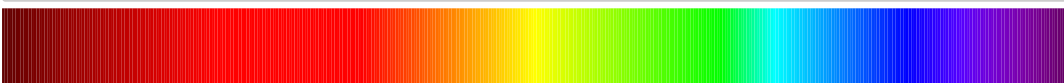
```
\pgfspectra[begin=500,end=700]
```



```
\pgfspectra[begin=700,end=500]
```



```
\pgfspectra[begin=780,end=380]
```

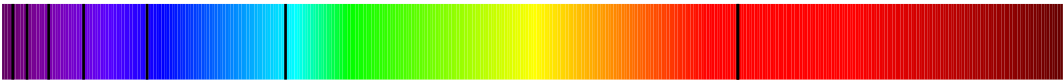
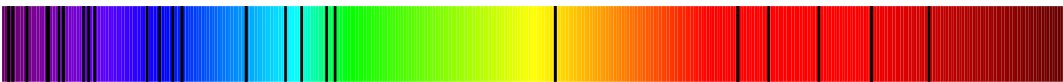


```
\pgfspectra[begin=780,end=380,element=He]
```

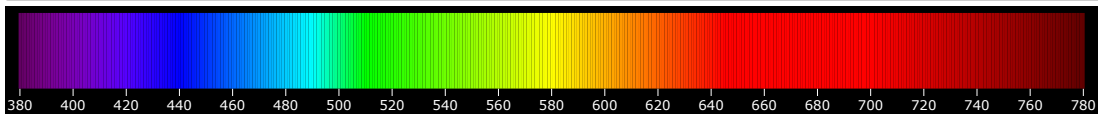


**absorption**default: *false*

Draws the absorption spectrum instead of the emission one.

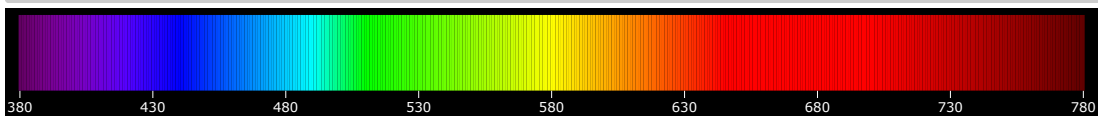
`\pgfspectra[element=H,absorption]``\pgfspectra[element={H,He},absorption]`**axis**default: *false*

Draws a nanometric axis below the spectrum.

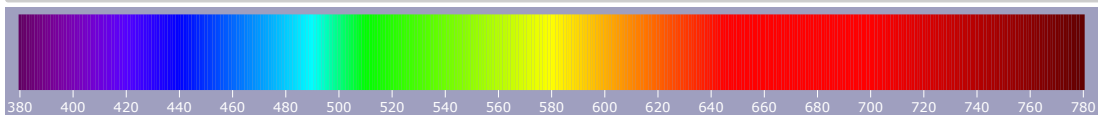
`\pgfspectra[axis]`**axis step**

default: 20

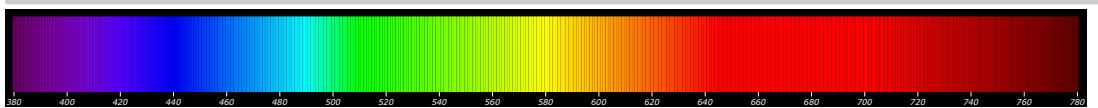
The increment to use in the axis scale.

`\pgfspectra[axis,axis step=50]`**axis color**default: *black*

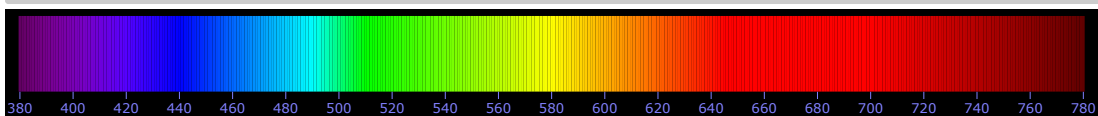
The color of the axis.

`\pgfspectra[axis,axis color=red!50!green!50!blue!50]`**axis font**default: *\tiny*

The font specs to use in the axis.

`\pgfspectra[axis,axis font=\fontsize{3}{3}\itshape\selectfont]`**axis font color**default: *white*

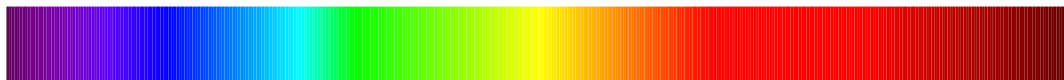
The color of the font used in the axis.

`\pgfspectra[axis,axis font color=blue!50!white]`**label**default: *false*

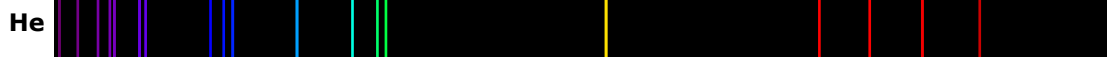
Puts a label for the spectrum.



```
\pgfspectra[label]
```



```
\pgfspectra[label,element=He]
```



**label position**

default: *west*

Sets the position of the label according to:

north west	north	north east
west	<i>spectrum</i>	east
south west	south	south east

```
\pgfspectra[label,label position=east,element=He]
```

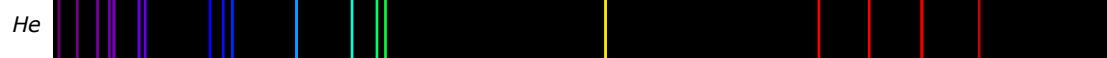


**label font**

default: `\bfseries\small`

The font specs for the label.

```
\pgfspectra[label,label font=\footnotesize\itshape,element=He]
```

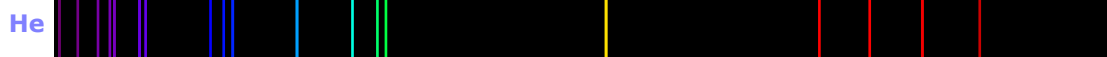


**label font color**

default: *black*

The color of the font used in the label.

```
\pgfspectra[label,label font color=blue!50!white,element=He]
```

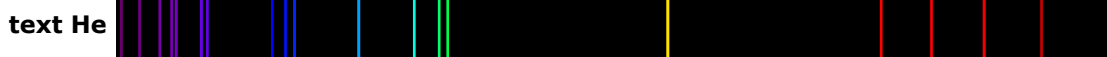


**label before text**

default: `{}`

Inserts text before the value stored in the label: if chemical symbols were provided, the label has them stored, otherwise it is empty.

```
\pgfspectra[label,label before text=text\ ,element=He]
```



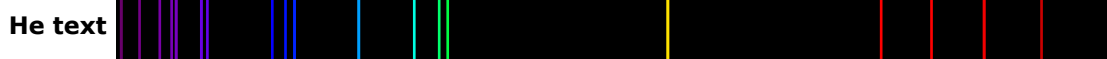
**Remark:** The `\_` is to insert a space between the text entered by user and the text stored in label.

**label after text**

default: `{}`

Inserts text after the value stored in the label: if chemical symbols were provided, the label has them stored, otherwise it is empty.

```
\pgfspectra[label,label after text=\ text,element=He]
```

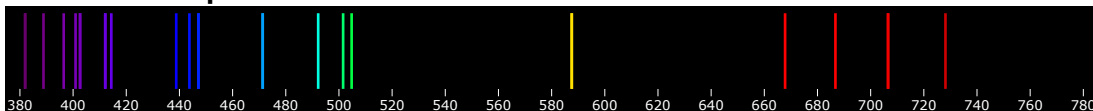


## Examples

Here are some examples for drawing some *eventually useful* spectra:

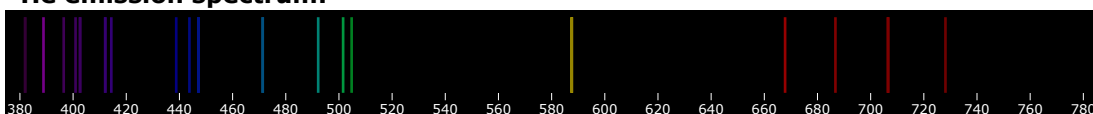
```
\pgfspectra[element=He,axis,label,label position=north west,
label after text=\ emission spectrum:]
```

He emission spectrum:



```
\pgfspectra[element=He,axis,label,label position=north west,label after text=
\ emission spectrum:,relative intensity,relative intensity threshold=.5]
```

He emission spectrum:

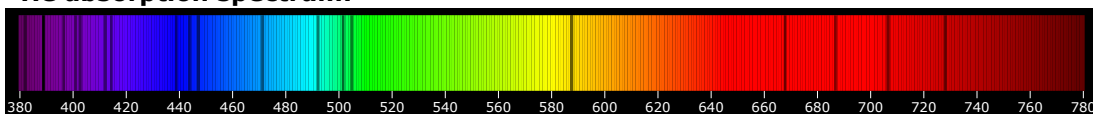


```
\pgfspectra[element=He,charge=all,line intensity=50,Imin=.05]
```

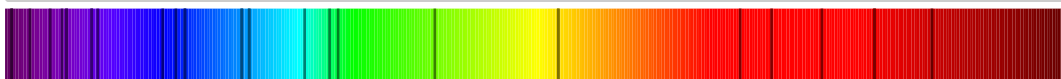


```
\pgfspectra[element=He,absorption,axis,label,label position=north west,label after text=
\ absorption spectrum:,relative intensity,relative intensity threshold=.5]
```

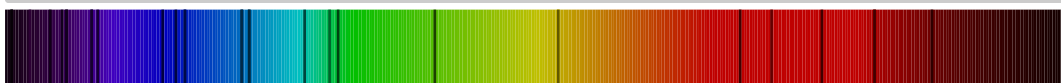
He absorption spectrum:



```
\pgfspectra[element=He,charge=all,absorption,line intensity=50]
```



```
\pgfspectra[element=He,charge=all,relative intensity,back=visible75,gamma=2]
```

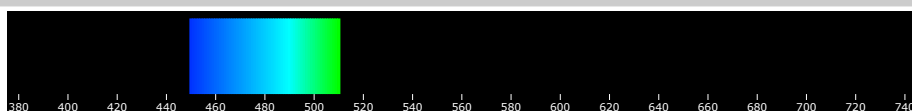


When the lines are manually inserted it's possible to use 'label before text' only with personalized text. In the next three examples 'label before text' is used to make labels for a multiple choice problem, omitting evidently the type of luminous font.

✓ Blue LED

```
\pgfspectra[begin=380,end=740,lines={450,451,452,453,454,455,456,457,458,459,
460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,
479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,
498,499,500,501,502,503,504,505,506,507,508,509,510},line width=1.25pt,width=
.75\linewidth,label,axis,label before text=(A),axis font=\fontsize{4pt}{6pt}\selectfont]
```

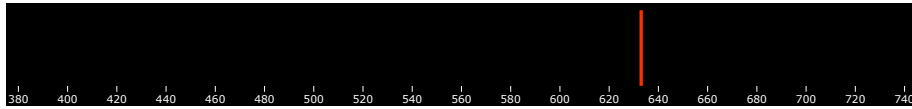
(A)



✓ Laser He-Ne

```
\pgfspectra[begin=380,end=740,lines={633},line  
width=1.25pt,width=.75\linewidth,label,axis,label before text=(B),axis  
font=\fontsize{4pt}{6pt}\selectfont]
```

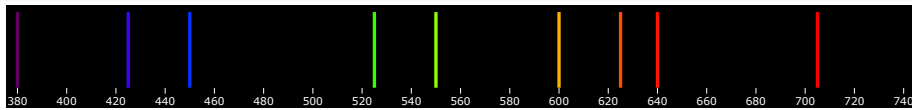
(B)



✓ Fluorescent lamp

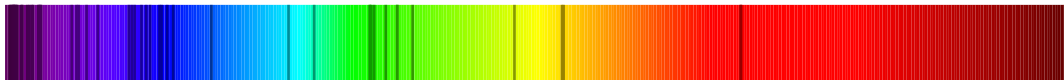
```
\pgfspectra[begin=380,end=740,lines={380,425,450,525,550,600,625,640,705},line  
width=1.25pt,width=.75\linewidth,label,axis,label before text=(C),axis  
font=\fontsize{4pt}{6pt}\selectfont]
```

(C)



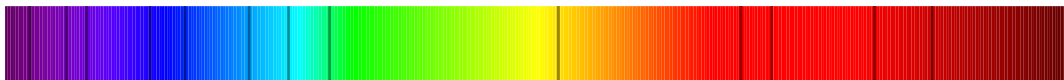
✓ Sun like spectrum

```
\pgfspectra[element={H,Fe,Mg,Na},absorption,line intensity=40,Imin=.05]
```



✓ Sirius like spectrum

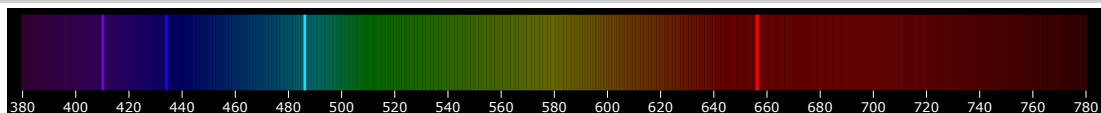
```
\pgfspectra[element={H,He},absorption,line intensity=40,Imin=.05]
```



✓ "Classical" emission spectra of elements:

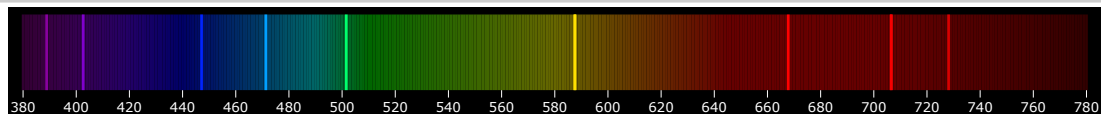
```
\pgfspectra[element=H,back=visible40,gamma=.6,label,axis,Imin=.05]
```

H



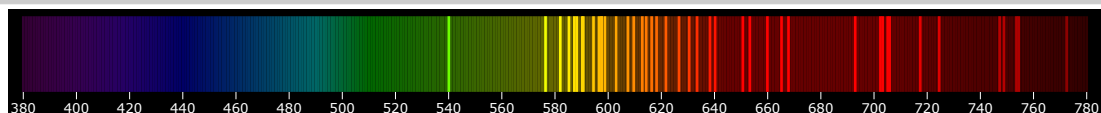
```
\pgfspectra[element=He,back=visible40,gamma=.6,label,axis,Imin=.05]
```

He



```
\pgfspectra[element=Ne,back=visible40,gamma=.6,label,axis,Imin=.05]
```

Ne



## Recommendations and known issues

The code could be a bit slow, so if there are many spectra to draw, the time consumption to get them could be high. In that case it's preferable to compile individual spectrum via the *preview* package, for later inclusion with `\includegraphics{<filename>.pdf}`:

```
% <filename>.tex
\documentclass{article}
\usepackage{pgf-spectra}
\usepackage[active,tightpage]{preview}
\PreviewEnvironment{tikzpicture}
\setlength\PreviewBorder{1pt}%
XXXXXXXXXXXXXXXXXXXX
\begin{document}
\pgfspectra[element=H,width=15cm]
\end{document}
```

## The code

```
1 % Hugo Gomes @ 15/04/2016
2 XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
3 \NeedsTeXFormat{LaTeX2e}%
4 \ProvidesPackage{pgf-spectra}[15/04/2016 pgf-spectra v1.0]%
5 \RequirePackage{tikz}%
6 \RequirePackage{ifthen}%
7 XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
8 \newif\ifwlaborption%
9 \newif\ifcurelemexist%
10 \newif\ifwldrawaxis%
11 \newif\ifwlaxislabel%
12 \newif\ifwlintensity%
13 % defining PGF keys
14 \pgfkeys{/wl/.cd,%
15 element/.get=\wlelement,%
16 element/.store in=\wlelement,%
17 element/.default=NONE,%
18 width/.get=\wlwidth,%
19 width/.store in=\wlwidth,%
20 width/.default={0.9\textwidth},
21 height/.get=\wlheight,%
22 height/.store in=\wlheight,%
23 height/.default=1cm,%
24 back/.get=\wlback,%
25 back/.store in=\wlback,%
26 back/.default=black,%
27 charge/.get=\wlcharge,%
28 charge/.store in=\wlcharge,%
29 charge/.default=0,%
30 Imin/.get=\wlintmin,%
31 Imin/.store in=\wlintmin,%
32 Imin/.default=0,%
33 lines/.get=\wllines,%
34 lines/.store in=\wllines,%
35 lines/.default={},%
36 line width/.get=\wllinewidth,%
37 line width/.store in=\wllinewidth,%
38 line width/.default=1pt,%
39 begin/.get=\wlbegin,%
40 begin/.store in=\wlbegin,%
41 begin/.default=380,%
42 end/.get=\wlend,%
43 end/.store in=\wlend,%
44 end/.default=780,%
45 axis step/.get=\wlaxisstep,%
46 axis step/.store in=\wlaxisstep,%
47 axis step/.default=20,%
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48 axis color/.get=\wlabelcolor,%
49 axis color/.store in=\wlabelcolor,%
50 axis color/.default=black,%
51 axis font/.get=\wlabelfont,%
52 axis font/.store in=\wlabelfont,%
53 axis font/.default={\tiny},%
54 axis font color/.get=\wlabelfontcolor,%
55 axis font color/.store in=\wlabelfontcolor,%
56 axis font color/.default=white,%
57 label position/.get=\wlabelposition,%
58 label position/.store in=\wlabelposition,%
59 label position/.default={west},%
60 label before text/.get=\wlabelbtext,%
61 label before text/.store in=\wlabelbtext,%
62 label before text/.default={},%
63 label after text/.get=\wlabelatext,%
64 label after text/.store in=\wlabelatext,%
65 label after text/.default={},%
66 label font/.get=\wlabelfont,%
67 label font/.store in=\wlabelfont,%
68 label font/.default={\bfseries\small},%
69 label font color/.get=\wlabelfontcolor,%
70 label font color/.store in=\wlabelfontcolor,%
71 label font color/.default=black,%
72 gamma/.get=\wlabelgamma,%
73 gamma/.store in=\wlabelgamma,%
74 gamma/.default=0.8,%
75 brightness/.get=\wlabelbrightness,%
76 brightness/.store in=\wlabelbrightness,%
77 brightness/.default=1,%
78 line intensity/.get=\wlabelint,%
79 line intensity/.store in=\wlabelint,%
80 line intensity/.default=100,%
81 relative intensity threshold/.get=\wlabelrelintthresh,%
82 relative intensity threshold/.store in=\wlabelrelintthresh,%
83 relative intensity threshold/.default=0.25,%
84 absorption/.is if=wlabelabsorption,%
85 axis/.is if=wlabeldrawaxis,%
86 label/.is if=wlabelaxislabel,%
87 relative intensity/.is if=wlabelintensity%
88 }%
89 % setting keys with default values
90 \pgfkeys{/wl/.cd,element,width,height,back,charge,Imin,lines,line width,begin,end,%
91 axis color,axis font,axis font color,axis step,label position,label before text,label
92 after text,label font,label font color,gamma,brightness,line intensity,%
93 relative intensity threshold,absorption=false,axis=false,label=false,relative intensity
94 =false}%
95 % strings for ifx tests
96 \def\wlabel@none{NONE}%
97 \def\wlabel@all{all}%
98 \def\wlabel@visible{visible}%
99 \def\wlabel@visible@list{visible,visible5,visible10,visible15,visible20,visible25,visible
100 30,visible35,visible40,visible45,visible50,visible55,visible60,visible65,visible70,
101 visible75,visible80,visible85,visible90,visible95,visible100}%
102 \def\wlabel@label@position@list{west,north west,north,north east,east,south east,south,
103 south west}%
104 %%%% COMMANDS
105 ----->
106 % \pgfspectra[options]
107 \def\pgfspectra{@ifnextchar[\wlabel@pgfspectra@withoptions{\wlabel@pgfspectra@nooptions}}%
108 \def\wlabel@pgfspectra@nooptions{\wlabel@pgfspectra@continuous(0.9\textwidth,1cm)}%
109 % #####
110 \def\wlabel@pgfspectra@continuous(#1,#2){%
111 \begin{tikzpicture}%
112 \foreach \x in {380,...,780}%
113 {%
114 \pgfmathparse{#1/400}\edef\xscale{\pgfmathresult}\edef\wlabel@linewidth{\xscale pt}%
115 \wlabel@color{\x}%
116 \pgfmathparse{(\x-380)*\xscale}\edef\wlabel@currentx{\pgfmathresult pt}%
117 \draw[\wlabel@temp,line width=\wlabel@linewidth] (\wlabel@currentx,0) -- ++(0,#2);%

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112     }%
113 \end{tikzpicture}%
114 }%
115 % #####
116 \def\wl@pgfspectra@withoptions[#1]{%
117 % setting default values
118 \pgfkeys{/wl/.cd,element,width,height,back,charge,Imin,lines,line width,begin,end,axis
    color,axis font,axis font color,axis step,label position,label before text,label
    after text,label font,label font color,gamma,brightness,line intensity,relative
    intensity threshold,absorption=false,axis=false,label=false,relative intensity=false}
    %
119 % process options (key values)
120 \pgfkeys{/wl/.cd,#1}
121 % axis height
122 \setbox0=\hbox{\wlaxisfont\selectfont380}\edef\@wl@axis@height{\the\ht0}%
123 % process visible background (visible+opacity)
124 \wl@counta=0%
125 \wl@countb=-1%
126 \@for\@myarg:=\wl@visible@list\do{%
127     \ifx\wlback\@myarg\wl@countb=\wl@counta\fi%
128     \advance\wl@counta by1%
129 }%
130 \ifnum\wl@countb=0\let\wlback\wl@visible\edef\@visible@opacity{.5}\else%
131 \ifnum\wl@countb>0\let\wlback\wl@visible\pgfmathparse{.05*\wl@countb}\edef\
    @visible@opacity{\pgfmathresult}\fi\fi%
132 %
-----
133 % if no element provided draws continuous spectrum with options or user list of lines
134 \ifx\wlelement\wlN@NE%no element by the user
135     \ifx\wl@elt@chemsym\undefined\else\let\wl@elt@chemsym\undefined\fi
136     \ifx\wl@lines@empty%no lines by the user => continuous spectrum
137     % draws the continuous spectrum width options (default or by the user)
138     \begin{tikzpicture}%
139         \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\pgfmathresult}%
140         \ifwldrawaxis%draws the axis
141             \wl@utils@draw@axis%
142             \fi%|ifwldrawaxis
143             \ifwlaxislabel%put the label
144             \wl@utils@put@label%
145             \fi%|ifwlaxislabel
146             \wl@utils@visiblespectrum{\wlbrightness}
147         \end{tikzpicture}%
148         \let\wl@list@@@empty%
149         \else% lines by the user
150         \edef\wl@list@@{\wl@lines}
151         \fi%|wl@lines|empty
152 \else%|wlelement|wlN@NE
153     % else get element(s) data
154     \wl@countc=0%
155     \wl@countd=1%
156     \@for\@myarg:=\wlelement\do{\advance\wl@countc by 1}%count number of elements
157     \wl@addt@list{}{}%
158     \@for\@myarg:=\wlelement\do{%
159         \curelemexisttrue%
160         \def\wl@elt@chemsym{NOT FOUND!}
161         \def\@search@result@err{NOT FOUND!}%
162         \wl@elt@data{\@myarg}\relax%
163         % check if element provided exists
164         \ifx\@search@result@err\wl@elt@chemsym Element\ ‘\@myarg’ with charge ‘\
            wlcharge’ not found!\curelemexistfalse\else%
165             % if exists, set the wavelength's list
166             \wl@set@element@list{\wl@elt@elemdata}{\wl@elt@Imax}%
167             \fi%|\@search@result@err|\wl@elt@chemsym
168             \ifcurelemexist\ifnum\wl@countd<\wl@countc\wl@addt@list{\wl@list@@}{,}\fi\
                fi%
169             \advance\wl@countd by 1%
170         }%end do
171 \fi%|wlelement|wlN@NE
172 % check if there are lines to draw and make the spectrum

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173 \ifx\wl@list@@\@empty\ifx\wlelement\wlN@NE\else Element\ ‘\wlelement’ with charge
‘\wlcharge’ have no lines to display.\fi\else%
174 \ifwlaborption%absortion spectrum
175 \begin{tikzpicture}%
176 \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\
pgfmathresult}%
177 \ifwldrawaxis%draws the axis
178 \wl@utils@draw@axis%
179 \fi%|ifwldrawaxis
180 \ifwlaxislabel%put the label
181 \wl@utils@put@label%
182 \fi%|ifwlaxislabel
183 \wl@utils@visiblespectrum{\wlbrightness}%put visible spectrum in the
background
% draws the lines
184 \wl@utils@drawabsorptionlines%
185 \end{tikzpicture}%
186 \else%emission spectrum
187 % draws the spectrum
188 \ifx\wlback\wl@visible%visible background
189 \begin{tikzpicture}%
190 \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\
pgfmathresult}%
191 \ifwldrawaxis%draws the axis
192 \wl@utils@draw@axis%
193 \fi%|ifwldrawaxis
194 \ifwlaxislabel%put the label
195 \wl@utils@put@label%
196 \fi%|ifwlaxislabel
197 \wl@utils@visiblespectrum{@visible@opacity*\wlbrightness}%draws the
visible background
198 \wl@utils@drawemissionlines% emission lines
199 \end{tikzpicture}%
200 \else%without visible background
201 \begin{tikzpicture}%
202 \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\
pgfmathresult}%
203 \ifwldrawaxis%draws the axis
204 \wl@utils@draw@axis%
205 \fi%|ifwldrawaxis
206 \ifwlaxislabel%put the label
207 \wl@utils@put@label%
208 \fi%|ifwlaxislabel
209 \ifnum\wlbegin>\wlend%
210 \draw[draw=none,fill=\wlback] (0,0) rectangle (-\wlwidth,\wlheight)
211 ;% background
212 \else%
213 \draw[draw=none,fill=\wlback] (0,0) rectangle (\wlwidth,\wlheight);
% background
214 \fi%
215 \wl@utils@drawemissionlines% emission lines
216 \end{tikzpicture}%
217 \fi%|wlback|@visible
218 \fi%|ifwlaborption
219 \fi% |wl@list@@|@empty
220 }%
221 % #####
222 % #####
223 % get individual line data from one element of the array data
224 \def\wl@get@line@info[#1 #2 #3]{
225 \def\@currentline@wl{#1}% return
226 \def\@currentline@int{#2}% return
227 \def\@currentline@charge{#3}% return
228 }%
229 % #####
230 % ##### \wl@set@element@list #####
231 % #####
232 %
233 % \wl@set@element@list{\wl@elt@elemdata}{\wl@elt@Imax}
234 % RETURN: \wl@list@@ -> (wl1,wl2,...)

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235 %           or if relative intensity true (between 0 and 1)
236 %           |wl@list@@ -> (wl1/int1,wl2/int2,...)
237 %
238 \newif\ifwl@first% for first occurrence of Imin
239 \def\wl@set@element@list#1#2{% |wl@elt@I_max
240 |wl@firsttrue%
241 |wl@counta=0%
242 |wl@countb=1%
243 |pgfmathparse{int(\wlintmin*100)}\edef\wl@intmin{\pgfmathresult}%intensity percentage
244 |ifnum\wl@intmin=0% include all intensities
245 |ifx\wl@ll\wlcharge%ALL lines
246 |@for\@myarg:=#1\do{\advance\wl@counta by 1}%count all entries
247 |   |ifwl@intensity%
248 |   |@for\@myarg:=#1%
249 |   |do{%
250 |   |   |expandafter\wl@get@line@info\@myarg%
251 |   |   |pgfmathparse{\wlrelinthresh+(1-\wlrelinthresh)*\@currentline@int/#2}\edef\
252 |   |   |wl@intensity@to@list{\pgfmathresult}%
253 |   |   |ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl/\
254 |   |   |wl@intensity@to@list,}\else%
255 |   |   |   |wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list}\fi%
256 |   |   |   |advance\wl@countb by 1%
257 |   |   |   |}%END do
258 |   |   |   |else%
259 |   |   |   |@for\@myarg:=#1%
260 |   |   |   |do{%
261 |   |   |   |   |expandafter\wl@get@line@info\@myarg%
262 |   |   |   |   |ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl,}\else%
263 |   |   |   |   |   |wl@addt@list{\wl@list@@}{\@currentline@wl}\fi%
264 |   |   |   |   |advance\wl@countb by 1%
265 |   |   |   |   |}%END do
266 |   |   |   |   |fi%
267 |   |   |   |}%END do
268 |   |   |   |else%
269 |   |   |   |@for\@myarg:=#1%
270 |   |   |   |do{%
271 |   |   |   |   |expandafter\wl@get@line@info\@myarg%
272 |   |   |   |   |pgfmathparse{\wlrelinthresh+(1-\wlrelinthresh)*\@currentline@int/#2}\edef\
273 |   |   |   |   |wl@intensity@to@list{\pgfmathresult}%
274 |   |   |   |   |ifx\@currentline@charge\wlcharge%add to list if is the desired charge
275 |   |   |   |   |ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl/\
276 |   |   |   |   |wl@intensity@to@list,}\else%
277 |   |   |   |   |   |wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list}\fi%
278 |   |   |   |   |advance\wl@countb by 1%
279 |   |   |   |   |fi%
280 |   |   |   |   |}%END do
281 |   |   |   |   |else%
282 |   |   |   |   |@for\@myarg:=#1%
283 |   |   |   |   |do{%
284 |   |   |   |   |   |expandafter\wl@get@line@info\@myarg%
285 |   |   |   |   |   |ifx\@currentline@charge\wlcharge%add to list if is the desired charge
286 |   |   |   |   |   |ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl,}\
287 |   |   |   |   |   |else%
288 |   |   |   |   |   |   |wl@addt@list{\wl@list@@}{\@currentline@wl}\fi%
289 |   |   |   |   |   |advance\wl@countb by 1%
290 |   |   |   |   |   |fi%
291 |   |   |   |   |   |}%END do
292 |   |   |   |   |fi%
293 |   |   |   |}%END do
294 |   |   |}%END do
295 |   |   |else%
296 |   |   |@for\@myarg:=#1\do{\advance\wl@counta by 1}%count all entries
297 |   |   |   |ifwl@intensity%
298 |   |   |   |@for\@myarg:=#1%
299 |   |   |   |do{%
300 |   |   |   |   |expandafter\wl@get@line@info\@myarg%

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```

299 \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\relax\edef\
300 \wl@int@result{\pgfmathresult}%
301 \ifnum\wl@int@result=1%
302 \pgfmathparse{\wl@relintthresh+(1-\wl@relintthresh)*\@currentline@int/#2}\
303 \edef\wl@intensity@to@list{\pgfmathresult}%
304 \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list
305 }\else%
306 \wl@addt@list{\wl@list@@}{,\@currentline@wl/\wl@intensity@to@list}\fi%
307 \ifwl@first\wl@firstfalse\fi%
308 \fi%
309 \advance\wl@countb by 1%
310 }%END do
311 \else%
312 \for\@myarg:=#1%
313 \do{%
314 \expandafter\wl@get@line@info\@myarg%
315 \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\relax\edef\
316 \wl@int@result{\pgfmathresult}%
317 \ifnum\wl@int@result=1%
318 \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl}\else%
319 \wl@addt@list{\wl@list@@}{,\@currentline@wl}\fi%
320 \ifwl@first\wl@firstfalse\fi%
321 \fi%
322 \advance\wl@countb by 1%
323 }%END do
324 \fi%
325 \else% lines for one specific charge
326 \for\@myarg:=#1\do{\expandafter\wl@get@line@info\@myarg\ifx\@currentline@charge\
327 \wlcharge\advance\wl@counta by 1\fi}%count only if is the desired charge
328 \ifwl@intensity%
329 \@for\@myarg:=#1%
330 \do{%
331 \expandafter\wl@get@line@info\@myarg%
332 \ifx\@currentline@charge\wlcharge%add to list if is the desired charge
333 \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\edef\wl@int@result
334 {\pgfmathresult}%
335 \ifnum\wl@int@result=1%
336 \pgfmathparse{\wl@relintthresh+(1-\wl@relintthresh)*\@currentline@int/#2}\
337 \edef\wl@intensity@to@list{\pgfmathresult}%
338 \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list
339 }\else%
340 \wl@addt@list{\wl@list@@}{,\@currentline@wl/\wl@intensity@to@list}\fi%
341 \ifwl@first\wl@firstfalse\fi%
342 \fi%
343 \advance\wl@countb by 1%
344 \fi%
345 }%END do
346 \else%
347 \for\@myarg:=#1%
348 \do{%
349 \expandafter\wl@get@line@info\@myarg%
350 \ifx\@currentline@charge\wlcharge%add to list if is the desired charge
351 \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\edef\wl@int@result
352 {\pgfmathresult}%
353 \ifnum\wl@int@result=1%
354 \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl}\else%
355 \wl@addt@list{\wl@list@@}{,\@currentline@wl}\fi%
356 \ifwl@first\wl@firstfalse\fi%
357 \fi%
358 \advance\wl@countb by 1%
359 \fi%
360 }%END do
361 \fi%
362 \fi%
363 \fi%
364 \fi%
365 \fi%
366 }%
367 % add to list
368 \def\wl@addt@list#1#2{\edef\wl@list@@{#1#2}}
369 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

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360 % internal utils
-----
361 %
362 \def\wl@utils@draw@axis{%
363     \ifnum\wlbegin>\wlend%
364     \draw[draw=none,fill=\wlaxiscolor] ([xshift={1.5*\wl@axis@height}]0,\
        wlheight+2.5pt) rectangle ([xshift={-1.5*\wl@axis@height}]-\wlwidth
        ,-2.5*\wl@axis@height);%
365     \pgfmathparse{\wlend+\wlaxisstep}\pgfmathresult}
366     \edef\@axis@list{\wlend,\pgfmathresult,...,\wlbegin}
367     \foreach \x in \@axis@list%
368     {%
369     \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\pgfmathresult pt}%
370     \draw[\wlaxisfontcolor,line width=.25pt] (\wl@currentx,-.75*\
        @wl@axis@height) -- ++(0,.75*\wl@axis@height);
371     \node[\wlaxisfontcolor,font=\wlaxisfont,above,inner sep=0pt] at (\
        wl@currentx,-2.25*\wl@axis@height) {\x};
372     }%
373     \else%
374     \draw[draw=none,fill=\wlaxiscolor] ([xshift={-1.5*\wl@axis@height}]0,\
        wlheight+2.5pt) rectangle ([xshift={1.5*\wl@axis@height}]\wlwidth
        ,-2.5*\wl@axis@height);%
375     \pgfmathparse{\wlbegin+\wlaxisstep}\pgfmathresult}
376     \edef\@axis@list{\wlbegin,\pgfmathresult,...,\wlend}
377     \foreach \x in \@axis@list%
378     {%
379     \pgfmathparse{(\x-\wlbegin)*\xscale}\edef\wl@currentx{\pgfmathresult pt
        }%
380     \draw[\wlaxisfontcolor,line width=.25pt] (\wl@currentx,-.75*\
        @wl@axis@height) -- ++(0,.75*\wl@axis@height);
381     \node[\wlaxisfontcolor,font=\wlaxisfont,above,inner sep=0pt] at (\
        wl@currentx,-2.25*\wl@axis@height) {\x};
382     }%
383     \fi%
384 }%
385 \def\wl@utils@put@label{%
386     \ifx\wl@elt@chemsym\undefined\def\wl@elt@chemsym{}\fi%
387     \wl@get@label@position%
388     \ifnum\wlbegin>\wlend%
389         \ifcase\wl@label@position%
390             %west
391             \ifwldrawaxis%\ifwlabel%
392             \node[\wllabelfontcolor,font=\wllabelfont,left,minimum
                width=2em,align=right] at (-1.5*\wl@axis@height-\wlwidth
                ,0.5*\wlheight) {\wllabelbtext\wl@elt@chemsym\
                wllabelatext};%
393             \else%
394             \node[\wllabelfontcolor,font=\wllabelfont,left,minimum
                width=2em,align=right] at (-\wlwidth,0.5*\wlheight) {\
                wllabelbtext\wl@elt@chemsym\wllabelatext};%
395             \fi%
396             \or%north west
397             \node[\wllabelfontcolor,font=\wllabelfont,above right,inner
                xsep=0pt] at (-\wlwidth,\wlheight) {\wllabelbtext\
                wl@elt@chemsym\wllabelatext};%
398             \or%north
399             \node[\wllabelfontcolor,font=\wllabelfont,above] at (-0.5*\
                wlwidth,\wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext
                };%
400             \or%north east
401             \node[\wllabelfontcolor,font=\wllabelfont,above left,inner xsep
                =0pt] at (0,\wlheight) {\wllabelbtext\wl@elt@chemsym\
                wllabelatext};%
402             \or%east
403             \ifwldrawaxis%
404             \node[\wllabelfontcolor,font=\wllabelfont,right] at (1.5*\
                @wl@axis@height,0.5*\wlheight) {\wllabelbtext\
                wl@elt@chemsym\wllabelatext};%
405             \else%

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406         \node[\wllabelfontcolor,font=\wllabelfont,right] at
         (0,0.5*\wlheight) {\wllabelbtext\wl@elt@chemsym\
         wllabelatext};%
407     \fi%
408 \or%south east
409     \ifwldrawaxis%
410     \node[\wllabelfontcolor,font=\wllabelfont,below left,inner
         xsep=0pt] at (0,-2.5*\@wl@axis@height) {\wllabelbtext\
         wl@elt@chemsym\wllabelatext};%
411     \else%
412     \node[\wllabelfontcolor,font=\wllabelfont,below left,inner
         xsep=0pt] at (0,0) {\wllabelbtext\wl@elt@chemsym\
         wllabelatext};%
413     \fi%
414 \or%south
415     \ifwldrawaxis%
416     \node[\wllabelfontcolor,font=\wllabelfont,below] at (-0.5*\
         wlwidth,-2.5*\@wl@axis@height) {\wllabelbtext\
         wl@elt@chemsym\wllabelatext};%
417     \else%
418     \node[\wllabelfontcolor,font=\wllabelfont,below] at (-0.5*\
         wlwidth,0) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
419     \fi%
420 \or%south west
421     \ifwldrawaxis%
422     \node[\wllabelfontcolor,font=\wllabelfont,below right,inner
         xsep=0pt] at (-1.5*\@wl@axis@height-\wlwidth,-2.5*\
         @wl@axis@height) {\wllabelbtext\wl@elt@chemsym\
         wllabelatext};%
423     \else%
424     \node[\wllabelfontcolor,font=\wllabelfont,below right,inner
         xsep=0pt] at (-\wlwidth,0) {\wllabelbtext\wl@elt@chemsym
         \wllabelatext};%
425     \fi%
426 \else%
427     \fi%
428     \ifcase\wl@label@position%
429     %west
430     \ifwldrawaxis%
431     \node[\wllabelfontcolor,font=\wllabelfont,left,minimum
         width=2em,align=right] at (-1.5*\@wl@axis@height,0.5*\
         wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
432     \else%
433     \node[\wllabelfontcolor,font=\wllabelfont,left,minimum
         width=2em,align=right] at (0,0.5*\wlheight) {\
         wllabelbtext\wl@elt@chemsym\wllabelatext};%
434     \fi%
435     \or%north west
436     \node[\wllabelfontcolor,font=\wllabelfont,above right,inner
         xsep=0pt] at (0,\wlheight) {\wllabelbtext\wl@elt@chemsym\
         wllabelatext};%
437     \or%north
438     \node[\wllabelfontcolor,font=\wllabelfont,above] at (0.5*\
         wlwidth,\wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext
         };%
439     \or%north east
440     \node[\wllabelfontcolor,font=\wllabelfont,above left,inner xsep
         =0pt] at (\wlwidth,\wlheight) {\wllabelbtext\wl@elt@chemsym\
         wllabelatext};%
441     \or%east
442     \ifwldrawaxis%
443     \node[\wllabelfontcolor,font=\wllabelfont,right] at ([
         xshift={1.5*\@wl@axis@height}]\wlwidth,0.5*\wlheight) {\
         wllabelbtext\wl@elt@chemsym\wllabelatext};%
444     \else%
445     \node[\wllabelfontcolor,font=\wllabelfont,right] at (\
         wlwidth,0.5*\wlheight) {\wllabelbtext\wl@elt@chemsym\
         wllabelatext};%
446     \fi%
447     \or%south east

```

```

448         \ifwldrawaxis%
449         \node [\wllabelfontcolor,font=\wllabelfont,below left,inner
           xsep=0pt] at (\wlwidth,-2.5*\wl@axis@height) {\
           wllabelbtext\wl@elt@chemsym\wllabelatext};%
450         \else%
451         \node [\wllabelfontcolor,font=\wllabelfont,below left,inner
           xsep=0pt] at (\wlwidth,0) {\wllabelbtext\wl@elt@chemsym\
           wllabelatext};%
452         \fi%
453     \or%south%
454         \ifwldrawaxis%
455         \node [\wllabelfontcolor,font=\wllabelfont,below] at (0.5*\
           wlwidth,-2.5*\wl@axis@height) {\wllabelbtext\
           wl@elt@chemsym\wllabelatext};%
456         \else%
457         \node [\wllabelfontcolor,font=\wllabelfont,below] at (0.5*\
           wlwidth,0) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
458         \fi%
459     \or%south west%
460         \ifwldrawaxis%
461         \node [\wllabelfontcolor,font=\wllabelfont,below right,inner
           xsep=0pt] at (-1.5*\wl@axis@height,-2.5*\
           \wl@axis@height) {\wllabelbtext\wl@elt@chemsym\
           wllabelatext};%
462         \else%
463         \node [\wllabelfontcolor,font=\wllabelfont,below right,inner
           xsep=0pt] at (0,0) {\wllabelbtext\wl@elt@chemsym\
           wllabelatext};%
464         \fi%
465     \fi%
466 }%
467
468 \def\wl@utils@visiblespectrum#1{%
469     \pgfmathparse{int(#1*100)}\edef\wl@bright{\pgfmathresult}
470     \ifnum\wlbegin>\wlend%
471         \foreach \x in {\wlend,...,\wlbegin}%
472             {%
473             \wlcOLOR{\x}%
474             \colorlet{\wlcOLOR}{\wltmp!\wl@bright!black}% ??? !black
475             \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\pgfmathresult
           pt}%
476             \edef\wl@linewidth{\xscale pt}%
477             \draw[\wlcOLOR,line width=\wl@linewidth] (\wl@currentx,0) -- ++(0,\
           wlheight);%
478             }%
479     \else%
480     \foreach \x in {\wlbegin,...,\wlend}%
481         {%
482         \wlcOLOR{\x}%
483         \colorlet{\wlcOLOR}{\wltmp!\wl@bright!black}% ??? !black
484         \pgfmathparse{(\x-\wlbegin)*\xscale}\edef\wl@currentx{\
           pgfmathresult pt}%
485         \edef\wl@linewidth{\xscale pt}%
486         \draw[\wlcOLOR,line width=\wl@linewidth] (\wl@currentx,0) -- ++(0,\
           wlheight);%
487         }%
488     \fi%
489 }%
490 \def\wl@utils@drawabsorptionlines{%
491     \ifnum\wlbegin>\wlend%
492     \ifwlintensity%
493         \foreach \x/\y in \wl@list@%
494             {%
495             \pgfmathparse{notless(\x,\wlend)}\edef\wl@x@nl{\pgfmathresult}%
496             \pgfmathparse{notgreater(\x,\wlbegin)}\edef\wl@x@ng{\
           pgfmathresult}
497             \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
           pgfmathresult}%
498             \ifnum\wl@plot@point=1%

```

```

499     \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\
500     pgfmathresult pt}%
501     \pgfmathparse{int(\y*100)}\edef\wl@black{\pgfmathresult}
502     \wcolor{\x}
503     \colorlet{\wcolor}{black!\wl@black!wltemp}
504     \draw[\wcolor,line width=\wllinewidth] (\wl@currentx,0) --
505     ++(0,\wlheight);%
506     \fi%
507     }%
508     \else%
509     \foreach \x in \wl@list@@%
510     {%
511     \pgfmathparse{notless(\x,\wlend)}\edef\wl@x@nl{\pgfmathresult}%
512     \pgfmathparse{notgreater(\x,\wlbeg)}\edef\wl@x@ng{\
513     pgfmathresult}
514     \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
515     pgfmathresult}%
516     \ifnum\wl@plot@point=1%
517     \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\
518     pgfmathresult pt}%
519     \wcolor{\x}
520     \colorlet{\wcolor}{black!\wllineint!wltemp}
521     \draw[\wcolor,line width=\wllinewidth] (\wl@currentx,0) --
522     ++(0,\wlheight);%
523     \fi%
524     }%
525     \fi%
526     \else%
527     \ifwlintensity%
528     \foreach \x/\y in \wl@list@@%
529     {%
530     \pgfmathparse{notless(\x,\wlbeg)}\edef\wl@x@nl{\pgfmathresult}
531     }%
532     \pgfmathparse{notgreater(\x,\wlend)}\edef\wl@x@ng{\
533     pgfmathresult}
534     \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
535     pgfmathresult}%
536     \ifnum\wl@plot@point=1%
537     \pgfmathparse{(\x-\wlbeg)*\xscale}\edef\wl@currentx{\
538     pgfmathresult pt}%
539     \pgfmathparse{int(\y*100)}\edef\wl@black{\pgfmathresult}
540     \wcolor{\x}
541     \colorlet{\wcolor}{black!\wl@black!wltemp}
542     \draw[\wcolor,line width=\wllinewidth] (\wl@currentx,0) --
543     ++(0,\wlheight);%
544     \fi%
545     }%
546     \else%
547     \foreach \x in \wl@list@@%
548     {%
549     \pgfmathparse{notless(\x,\wlbeg)}\edef\wl@x@nl{\pgfmathresult}
550     }%
551     \pgfmathparse{notgreater(\x,\wlend)}\edef\wl@x@ng{\
552     pgfmathresult}
553     \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
554     pgfmathresult}%
555     \ifnum\wl@plot@point=1%
556     \pgfmathparse{(\x-\wlbeg)*\xscale}\edef\wl@currentx{\
557     pgfmathresult pt}%
558     \wcolor{\x}
559     \colorlet{\wcolor}{black!\wllineint!wltemp}
560     \draw[\wcolor,line width=\wllinewidth] (\wl@currentx,0) --
561     ++(0,\wlheight);%
562     \fi%
563     }%
564     \fi%
565     \fi%
566     }%
567     \def\wl@utils@drawemissionlines{%
568     \ifnum\wlbeg>\wlend%

```

```

553 \ifwlintensity%
554 \foreach \x/\y in \wl@list@%
555 {%
556 \wlcOLOR{\x}%
557 \pgfmathparse{notless(\x,\wlend)}\edef\wl@x@nl{\pgfmathresult}%
558 \pgfmathparse{notgreater(\x,\wlbegIn)}\edef\wl@x@ng{\
pgfmathresult}
559 \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
pgfmathresult}%
560 \ifnum\wl@plot@point=1%
561 \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\
pgfmathresult pt}%
562 \pgfmathparse{int(\y*100)}\edef\wl@black{\pgfmathresult}
563 \colorlet{\wlcOLOR}{\wltmp!\wl@black!black}
564 \draw[\wlcOLOR,line width=\wllinewidth] (\wl@currentx,0) --
++(0,\wlheight);%
565 \fi%
566 }%
567 \else%
568 \foreach \x in \wl@list@%
569 {%
570 \wlcOLOR{\x}%
571 \pgfmathparse{notless(\x,\wlend)}\edef\wl@x@nl{\pgfmathresult}%
572 \pgfmathparse{notgreater(\x,\wlbegIn)}\edef\wl@x@ng{\
pgfmathresult}
573 \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
pgfmathresult}%
574 \ifnum\wl@plot@point=1%
575 \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\
pgfmathresult pt}%
576 \colorlet{\wlcOLOR}{\wltmp!\wllineint!black}
577 \draw[\wlcOLOR,line width=\wllinewidth] (\wl@currentx,0) --
++(0,\wlheight);%
578 \fi%
579 }%
580 \fi%
581 \else%
582 \ifwlintensity%
583 \foreach \x/\y in \wl@list@%
584 {%
585 \wlcOLOR{\x}%
586 \pgfmathparse{notless(\x,\wlbegIn)}\edef\wl@x@nl{\pgfmathresult
}%
587 \pgfmathparse{notgreater(\x,\wlend)}\edef\wl@x@ng{\
pgfmathresult}
588 \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
pgfmathresult}%
589 \ifnum\wl@plot@point=1%
590 \pgfmathparse{(\x-\wlbegIn)*\xscale}\edef\wl@currentx{\
pgfmathresult pt}%
591 \pgfmathparse{int(\y*100)}\edef\wl@black{\pgfmathresult}
592 \colorlet{\wlcOLOR}{\wltmp!\wl@black!black}
593 \draw[\wlcOLOR,line width=\wllinewidth] (\wl@currentx,0) --
++(0,\wlheight);%
594 \fi%
595 }%
596 \else%
597 \foreach \x in \wl@list@%
598 {%
599 \wlcOLOR{\x}%
600 \pgfmathparse{notless(\x,\wlbegIn)}\edef\wl@x@nl{\pgfmathresult
}%
601 \pgfmathparse{notgreater(\x,\wlend)}\edef\wl@x@ng{\
pgfmathresult}
602 \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
pgfmathresult}%
603 \ifnum\wl@plot@point=1%
604 \pgfmathparse{(\x-\wlbegIn)*\xscale}\edef\wl@currentx{\
pgfmathresult pt}%
605 \colorlet{\wlcOLOR}{\wltmp!\wllineint!black}

```

```

606             \draw[wlcolor,line width=\wllinewidth] (\wl@currentx,0) --
              ++(0,\wlheight);%
607             \fi%
608             }%
609         \fi%
610         \fi%
611     }
612     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
613     % return: integer with position (e.g. '0' for west, ... )
614     \def\wl@get@label@position{%
615         \wl@countc=0%
616         \@for\@mylabel:=\wl@label@position@list%
617             \do{%
618                 \ifx\@mylabel\wllabelposition\edef\wl@label@position{\the\wl@countc}\fi%
619                 \advance\wl@countc by1%
620             }%
621     }%
622     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
623     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
624     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
625     %
626     % nm2rgb convert nanometer wavelength to rgb
627     % (380 <= Lambda <= 780 ) -> r,g,b on stack
628     %
629     % BASED on FORTRAN Code
630     % RGB VALUES FOR VISIBLE WAVELENGTHS by Dan Bruton (astro@tamu.edu)
631     % This program can be found at
632     % http://www.physics.sfasu.edu/astro/color.html
633     % and was last updated on February 20, 1996.
634     % The spectrum is generated using approximate RGB values for visible
635     % wavelengths between 380 nm and 780 nm.
636     % The red, green and blue values (RGB) are
637     % assumed to vary linearly with wavelength (for GAMMA=1).
638     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
639     \newdimen\wl#wavelength
640     \newdimen\wl#i#intensity
641     \newdimen\wl@gamma#gamma
642     \newdimen\wlc@lorr#red (0. - 1)
643     \newdimen\wlc@lorg#green (0. - 1)
644     \newdimen\wlc@lorb#blue (0. - 1) % wavelength to rgb values
645     \newcount\wl@counta# tmp counter
646     \newcount\wl@countb# tmp counter
647     \newcount\wl@countc# tmp counter
648     \newcount\wl@countd# tmp counter
649     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
650     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
651     % |wlcolor{wavelength}
652     \def\wlcolor#1{%
653         \wl=#1pt%
654         \wl@gamma=\wlgamma pt%
655         % compute the rgb components
656         \ifdim\wl<380pt\ Err: wavelength must be greater or equal to 380nm\else%
657         \ifdim\wl<440pt\wlc@lorr=440pt\advance\wlc@lorr by-\wl\divide\wlc@lorr by60\wlc@lorg=0
        pt\wlc@lorb=1pt\else%
658         \ifdim\wl<490pt\wlc@lorr=0pt\wlc@lorg=\wl\advance\wlc@lorg by-440pt\divide\wlc@lorg by
        50\wlc@lorb=1pt\else%
659         \ifdim\wl<510pt\wlc@lorr=0pt\wlc@lorg=1pt\wlc@lorb=510pt\advance\wlc@lorb by-\wl\divide
        \wlc@lorb by20\else%
660         \ifdim\wl<580pt\wlc@lorr=\wl\advance\wlc@lorr by-510pt\divide\wlc@lorr by70\wlc@lorg=1
        pt\wlc@lorb=0pt\else%
661         \ifdim\wl<645pt\wlc@lorr=1pt\wlc@lorg=645pt\advance\wlc@lorg by-\wl\divide\wlc@lorg by
        65\wlc@lorb=0pt\else%
662         \ifdim\wl<780.00001pt\wlc@lorr=1pt\wlc@lorg=0pt\wlc@lorb=0pt\else%
663         \ Err: wavelength must be lesser or equal to 780nm%
664         \fi\fi\fi\fi\fi\fi\fi%
665         % intensity correction at vision limits
666         \ifdim\wl>700pt\wl#i=780pt\advance\wl#i by-\wl\divide\wl#i by80\multiply\wl#i by7\
        advance\wl#i by3pt\divide\wl#i by10\else%
667         \ifdim\wl<420pt\wl#i=\wl\advance\wl#i by-380pt\divide\wl#i by40\multiply\wl#i by7\
        advance\wl#i by3pt\divide\wl#i by10\else%

```

```

668 \wl@i=1pt%
669 \fi\fi%
670 %apply intensity at vision limits correction and gamma
671 \pgfmathparse{\wlc@lorr*\wl@i^\wl@gamma}\edef\wl@red{\pgfmathresult}%
672 \pgfmathparse{\wlc@lorg*\wl@i^\wl@gamma}\edef\wl@green{\pgfmathresult}%
673 \pgfmathparse{\wlc@lorb*\wl@i^\wl@gamma}\edef\wl@blue{\pgfmathresult}%
674 \definecolor{wltemp}{rgb}{\wl@red,\wl@green,\wl@blue}%
675 \colorlet{wlcolor}{wltemp}
676 }%
677 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
678 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
679 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
680 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
681 \def\wl@elt@search#1#2#3#4{%
682 % #1 Chemical Symbol, entered by USER
683 % #2 Chemical Symbol to compare to, e.g. Na
684 % #3 Emission Lines Data (or error message)
685 % #4 Imax
686 \ifthenelse{\equal{\expandafter\noexpand#1}{\expandafter\noexpand#2}}%
687     {% true
688         \def\wl@elt@chemsym{#2}% set chemical symbol
689         \def\wl@elt@elemdata{#3}% set element lines data
690         \def\wl@elt@Imax{#4}% set element Imax
691     }%
692     {% false
693 }%
694 \input{spectra.data.tex}
695 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
696 \endinput

```