Manual for pgf-spectra 1.0

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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.

Contents

Installation and usage

pgf-spectra is placed under the terms of the LaTeX 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 pdflatex 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 pdflatex, just can simply include the style file without any option via the \usepackage command: \usepackage{pgf-spectra}

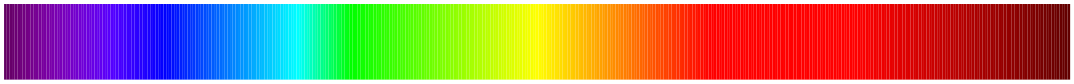
The commands

There are at this time only two commands available:

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

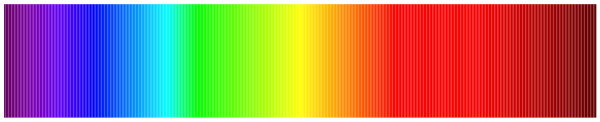
The first command is used without options to draw the visible continuous spectrum:

```
\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 'wlcolor':

```
\tikz{\foreach \x in {380,430,...,780}{
          \wlcolor{\x}
          \draw[fill=wlcolor] (.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\textwidth*

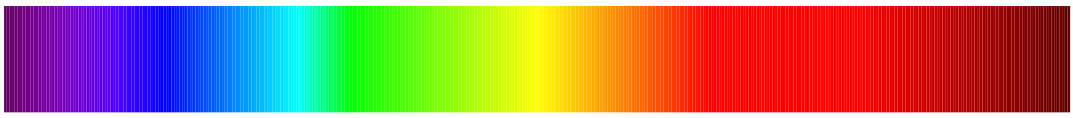
Sets the width of the spectrum.

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

height default: *1cm*

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]
```

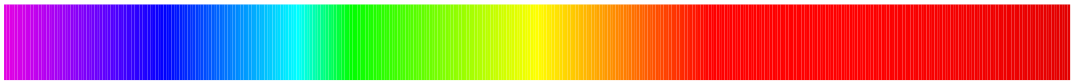
```
\pgfspectra[element=He,line intensity=100]
```

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

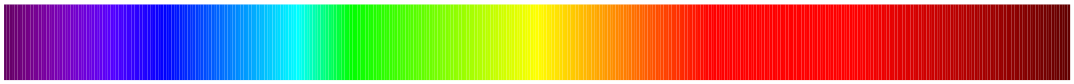
gamma default: *0.8*

Gamma color correction: any positive value.

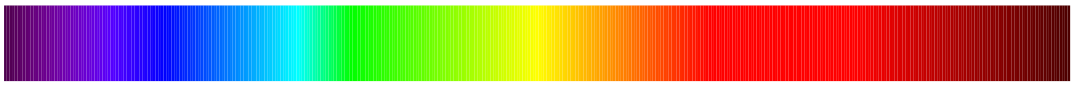
```
\pgfspectra[gamma=.1]
```



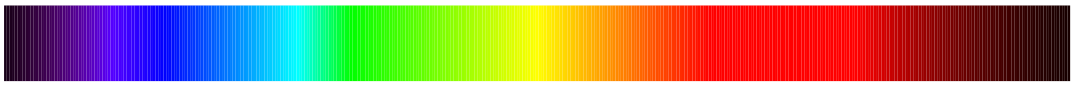
```
\pgfspectra[gamma=.8]
```



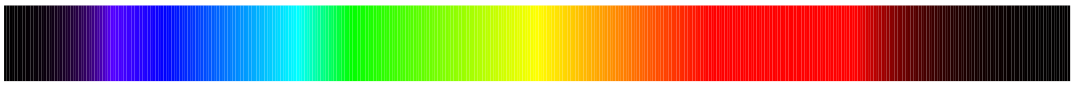
```
\pgfspectra[gamma=1]
```



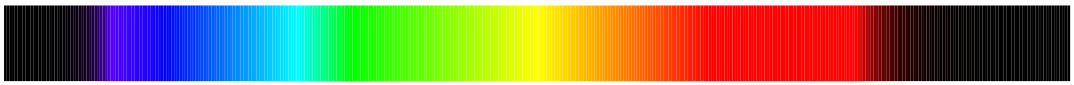
```
\pgfspectra[gamma=2]
```



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



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

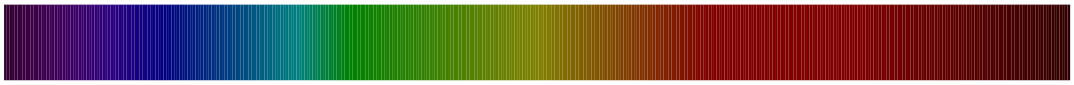


brightness default: *1*

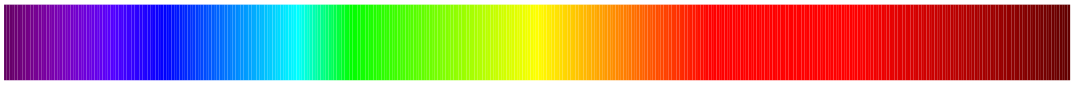
Brightness color correction as in the CMYK color model. Value between 0 and 1. Zero stands for black and one for the maximum bright. *This option only works for the continuous component of the spectra, to change the "brightness" of spectral lines use the option 'line intensity'.*

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

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



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



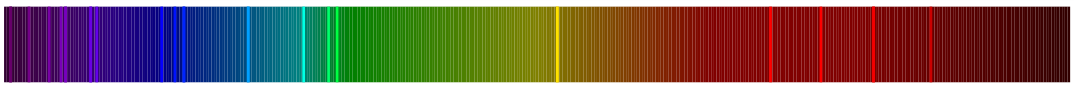
back default: *black*

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.

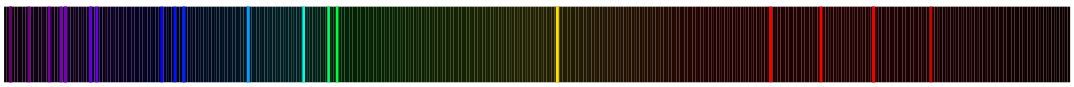
```
\pgfspectra[element=He,back=white]
```

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

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



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



lines default: *{}*

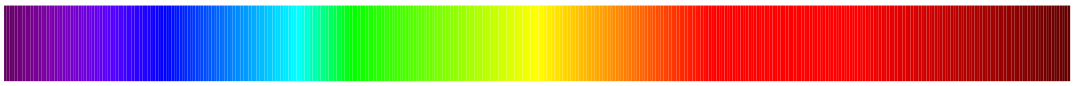
A comma separated list of wavelengths in the interval $[380; 780]\,nm$.

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

line width default: *1pt*

The width of each individual line in the spectrum.

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

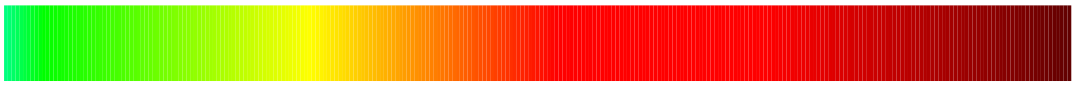


```
\pgfspectra[line width=2pt,element=He]
```

begin default: *380*

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

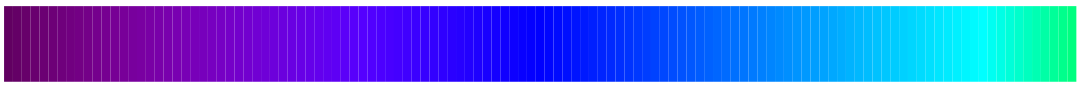
```
\pgfspectra[begin=500]
```



end default: *780*

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

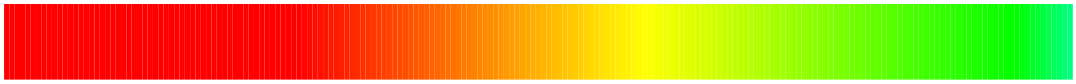
```
\pgfspectra[end=500]
```



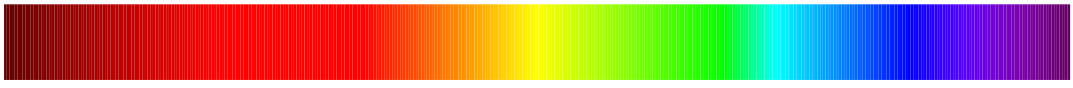
Remark: *it's obviously possible to set 'begin' and 'end' at the same time and if desired change the order of the wavelengths.*

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

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



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

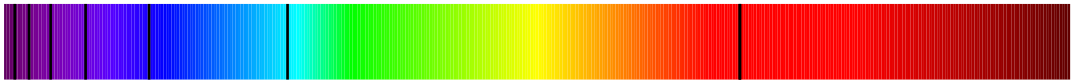


```
\pgfspectra[begin=780,end=380,element=He]
```

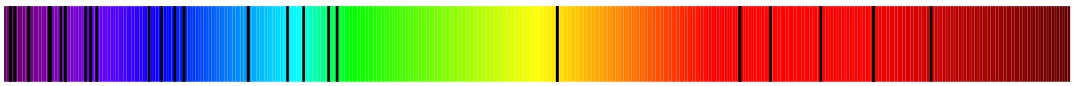
absorption default: *false*

Draws the absorption spectrum instead of the emission one.

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



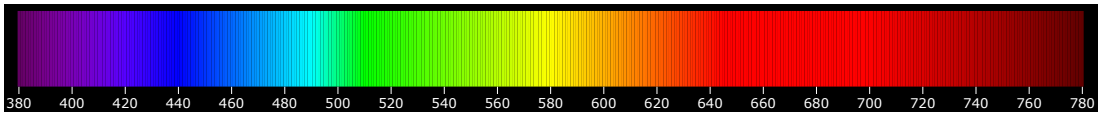
```
\pgfspectra[element={H,He},absorption]
```



axis default: *false*

Draws a nanometric axis below the spectrum.

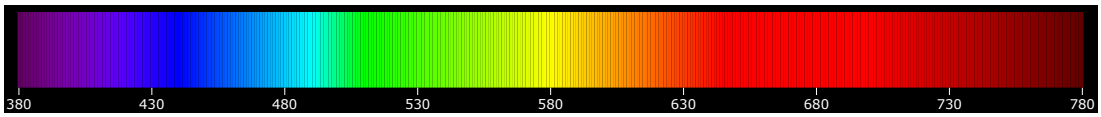
```
\pgfspectra[axis]
```



axis step default: *20*

The increment to use in the axis scale.

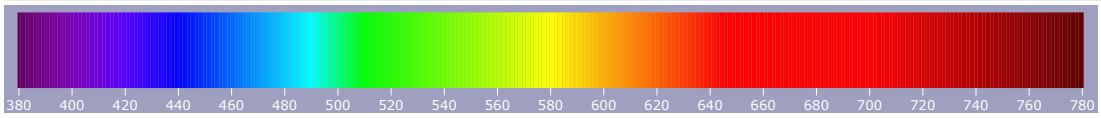
```
\pgfspectra[axis,axis step=50]
```



axis color default: *black*

The color of the axis.

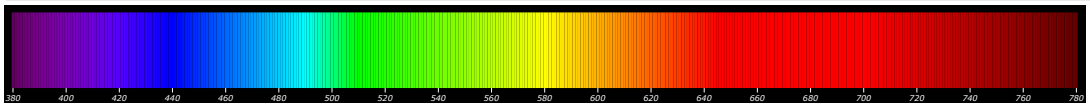
```
\pgfspectra[axis,axis color=red!50!green!50!blue!50]
```



axis font default: *\tiny*

The font specs to use in the axis.

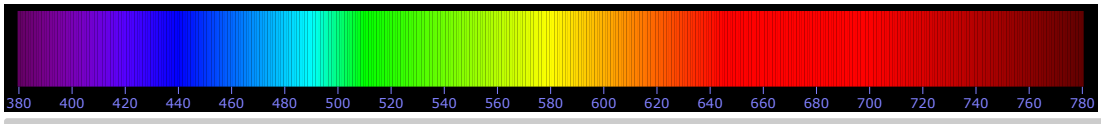
```
\pgfspectra[axis,axis font=\fontsize{3}{3}\itshape\selectfont]
```



axis font color default: *white*

The color of the font used in the axis.

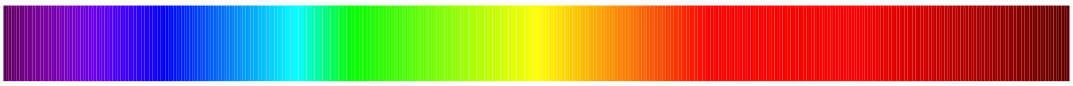
```
\pgfspectra[axis,axis font color=blue!50!white]
```



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 | *spectrum* | 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.

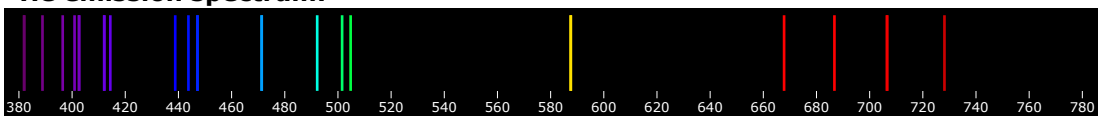
```
\pgfspectra[label,label after text=\ text,element=He]
```

Examples

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

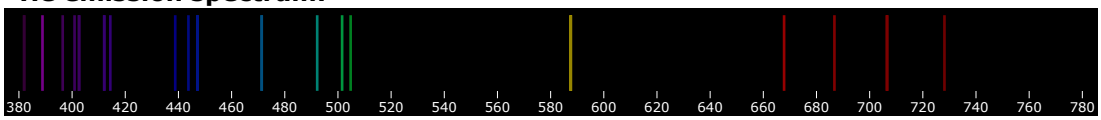
```
\pgfspectra[element=He,axis,label,label position=north west,
label after text=\ emission spectrum:]
```

He emission spectrum:




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

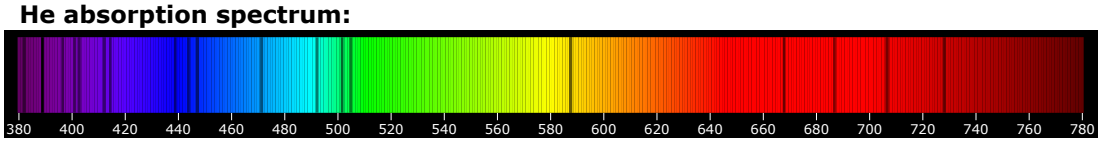
He emission spectrum:



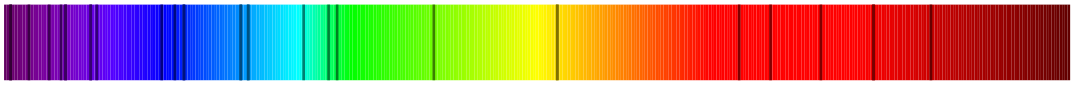

```
\pgfspectra[element=He,charge=all,line intensity=50,Imin=.05]
```

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

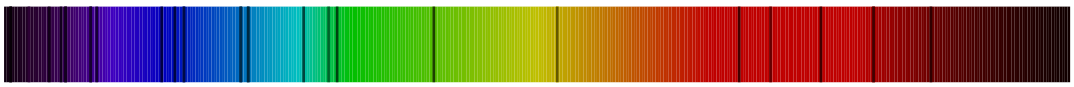
He absorption spectrum:




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



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

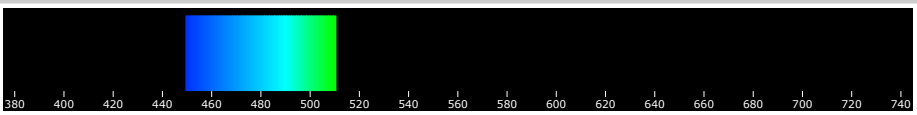


When the lines are manually inserted it's possible to use 'label before text' only with personalized text. In the next three examples 'label before text' is used to make labels for a multiple choice problem, omitting evidently the type of luminous font.

✓ Blue LED

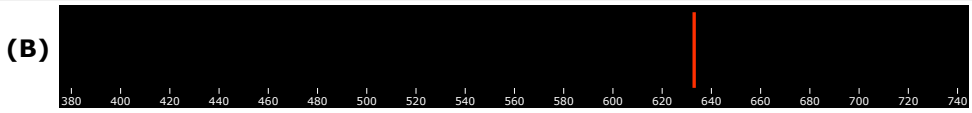
```
\pgfspectra[begin=380,end=740,lines={450,451,452,453,454,455,456,457,458,459,
460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,
479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,
498,499,500,501,502,503,504,505,506,507,508,509,510},line width=1.25pt,width=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

(A)



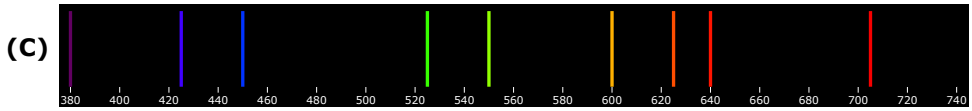
✓ Laser He-Ne

```
\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]
```



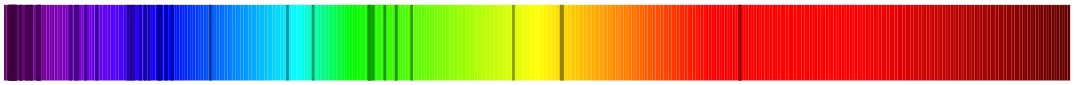
✓ Fluorescent lamp

```
\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]
```



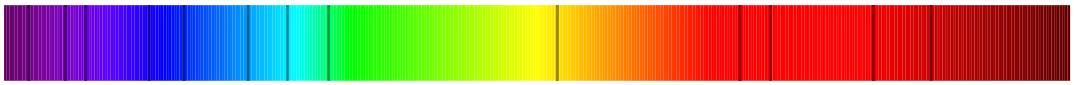
✓ Sun like spectrum

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



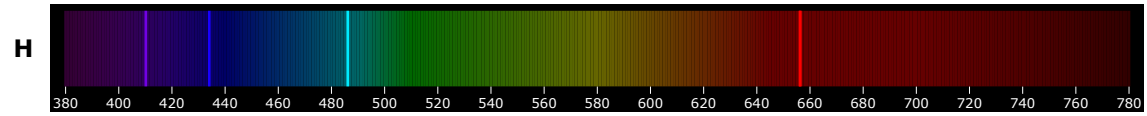
✓ Sirius like spectrum

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

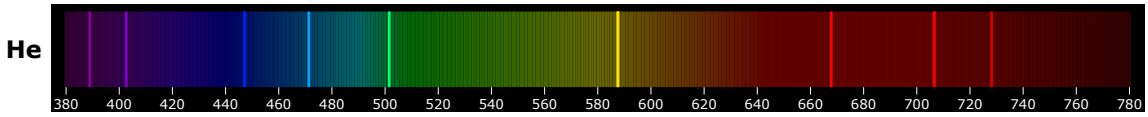


✓ “Classical” emission spectra of elements:

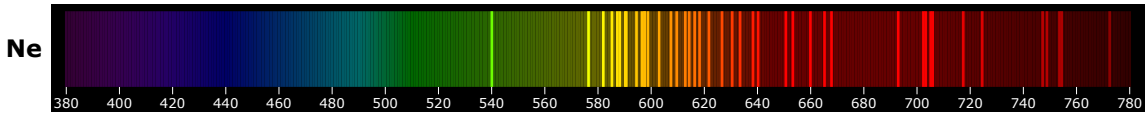
```
\pgfspectra[element=H,back=visible40,gamma=.6,label,axis,Imin=.05]
```




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




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



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}%
%%%%%%%%%%%%%%%%%%
\begin{document}
\pgfspectra[element=H,width=15cm]
\end{document}
```

The code

```
% Hugo Gomes @ 15/04/2016
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
\NeedsTeXFormat{LaTeX2e}%
\ProvidesPackage{pgf-spectra}[15/04/2016 pgf-spectra v1.0]%
\RequirePackage{tikz}%
\RequirePackage{ifthen}%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
\newif\ifwlabsorption%
\newif\ifcurelemexist%
\newif\ifwldrawaxis%
\newif\ifwlaxislabel%
\newif\ifwlintensity%
% defining PGF keys
\pgfkeys{/wl/.cd,%
element/.get=\wlelement,%
element/.store in=\wlelement,%
element/.default=NONE,%
width/.get=\wlwidth,%
width/.store in=\wlwidth,%
width/.default={0.9\textwidth},
height/.get=\wlheight,%
height/.store in=\wlheight,%
height/.default=1cm,%
back/.get=\wlback,%
back/.store in=\wlback,%
back/.default=black,%
charge/.get=\wlcharge,%
charge/.store in=\wlcharge,%
charge/.default=0,%
Imin/.get=\wlintmin,%
Imin/.store in=\wlintmin,%
Imin/.default=0,%
lines/.get=\wllines,%
lines/.store in=\wllines,%
lines/.default={},%
line width/.get=\wllinewidth,%
line width/.store in=\wllinewidth,%
line width/.default=1pt,%
begin/.get=\wlbegin,%
begin/.store in=\wlbegin,%
begin/.default=380,%
end/.get=\wlend,%
end/.store in=\wlend,%
end/.default=780,%
axis step/.get=\wlaxisstep,%
axis step/.store in=\wlaxisstep,%
axis step/.default=20,%
```

```
axis color/.get=\wlaxiscolor,%
axis color/.store in=\wlaxiscolor,%
axis color/.default=black,%
axis font/.get=\wlaxisfont,%
axis font/.store in=\wlaxisfont,%
axis font/.default={\tiny},%
axis font color/.get=\wlaxisfontcolor,%
axis font color/.store in=\wlaxisfontcolor,%
axis font color/.default=white,%
label position/.get=\wllabelposition,%
label position/.store in=\wllabelposition,%
label position/.default={west},%
label before text/.get=\wllabelbtext,%
label before text/.store in=\wllabelbtext,%
label before text/.default={},%
label after text/.get=\wllabelatext,%
label after text/.store in=\wllabelatext,%
label after text/.default={},%
label font/.get=\wllabelfont,%
label font/.store in=\wllabelfont,%
label font/.default={\bfseries\small},%
label font color/.get=\wllabelfontcolor,%
label font color/.store in=\wllabelfontcolor,%
label font color/.default=black,%
gamma/.get=\wlgamma,%
gamma/.store in=\wlgamma,%
gamma/.default=0.8,%
brightness/.get=\wlbrightness,%
brightness/.store in=\wlbrightness,%
brightness/.default=1,%
line intensity/.get=\wllineint,%
line intensity/.store in=\wllineint,%
line intensity/.default=100,%
relative intensity threshold/.get=\wlrelintthresh,%
relative intensity threshold/.store in=\wlrelintthresh,%
relative intensity threshold/.default=0.25,%
absorption/.is if=wlabsorption,%
axis/.is if=wldrawaxis,%
label/.is if=wlaxislabel,%
relative intensity/.is if=wlintensity%
}%
% setting keys with default values
\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}%
% strings for \ifx tests
\def\wlN@NE{NONE}%
\def\wl@ll{all}%
\def\wl@visible{visible}%
\def\wl@visible@list{visible,visible5,visible10,visible15,visible20,visible25,visible
  30,visible35,visible40,visible45,visible50,visible55,visible60,visible65,visible70,
  visible75,visible80,visible85,visible90,visible95,visible100}%
\def\wl@label@position@list{west,north west,north,north east,east,south east,south,
  south west}%
%%%% COMMANDS
  ------------------------------------------------------------------------------>
% \pgfspectra[options]
\def\pgfspectra{\@ifnextchar[\wl@pgfspectra@withoptions{\wl@pgfspectra@nooptions}}%
\def\wl@pgfspectra@nooptions{\wl@pgfspectra@continuous(0.9\textwidth,1cm)}%
% ##########################################################
\def\wl@pgfspectra@continuous(#1,#2){%
\begin{tikzpicture}%
\foreach \x in {380,...,780}%
        {%
        \pgfmathparse{#1/400}\edef\xscale{\pgfmathresult}\edef\wl@linewidth{\xscale pt}
        \wlcolor{\x}%
        \pgfmathparse{(\x-380)*\xscale}\edef\wl@currentx{\pgfmathresult pt}%
        \draw[wltemp,line width=\wl@linewidth] (\wl@currentx,0) -- ++(0,#2);%
```

```
        }%
\end{tikzpicture}%
}%
% ##########################################################
\def\wl@pgfspectra@withoptions[#1]{%
% setting default values
\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}%
% process options (key values)
\pgfkeys{/wl/.cd,#1}
% axis height
\setbox0=\hbox{\wlaxisfont\selectfont380}\edef\@wl@axis@height{\the\ht0}%
% process visible background (visible+opacity)
\wl@counta=0%
\wl@countb=-1%
\@for\@myarg:=\wl@visible@list\do{%
            \ifx\wlback\@myarg\wl@countb=\wl@counta\fi%
            \advance\wl@counta by1%
            }%
\ifnum\wl@countb=0\let\wlback\wl@visible\edef\@visible@opacity{.5}\else%
\ifnum\wl@countb>0\let\wlback\wl@visible\pgfmathparse{.05*\wl@countb}\edef\@visible@opacity{\pgfmathresult}\fi\fi%
%
    ------------------------------------------------------------------------------------------------------------------------

% if no element provided draws continuous spectrum with options or user list of lines
\ifx\wlelement\wlN@NE%no element by the user
    \ifx\wl@elt@chemsym\undefined\else\let\wl@elt@chemsym\undefined\fi
    \ifx\wllines\@empty%no lines by the user => continuous spectrum
    % draws the continuous spectrum width options (default or by the user)
    \begin{tikzpicture}%
        \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\pgfmathresult}%
        \ifwldrawaxis%draws the axis
        \wl@utils@draw@axis%
        \fi%|ifwldrawaxis
        \ifwlaxislabel%put the label
        \wl@utils@put@label%
        \fi%|ifwlaxislabel
        \wl@utils@visiblespectrum{\wlbrightness}
    \end{tikzpicture}%
    \let\wl@list@@\@empty%
    \else% lines by the user
    \edef\wl@list@@{\wllines}
    \fi%|wllines|@empty
\else%|wlelement|wlN@NE
    % else get element(s) data
    \wl@countc=0%
    \wl@countd=1%
    \@for\@myarg:=\wlelement\do{\advance\wl@countc by 1}%count number of elements
    \wl@addt@list{}{}%
    \@for\@myarg:=\wlelement\do{%
            \curelemexisttrue%
            \def\wl@elt@chemsym{NOT FOUND!}
            \def\@search@result@err{NOT FOUND!}%
            \wl@elt@data{\@myarg}\relax%
            % check if element provided exists
            \ifx\@search@result@err\wl@elt@chemsym Element\ ``\@myarg'' with charge ``\wlcharge'' not found!\curelemexistfalse\else%
            % if exists, set the wavelength's list
            \wl@set@element@list{\wl@elt@elemdata}{\wl@elt@Imax}%
            \fi%|@search@result@err|wl@elt@chemsym
            \ifcurelemexist\ifnum\wl@countd<\wl@countc\wl@addt@list{\wl@list@@}{,}\fi\fi%
            \advance\wl@countd by 1%
            }%end do
\fi%|wlelement|wlN@NE
% check if there are lines to draw and make the spectrum
```

```
    \ifx\wl@list@@\@empty\ifx\wlelement\wlN@NE\else Element\ ``\wlelement'' with charge
       ``\wlcharge'' have no lines to display.\fi\else%
        \ifwlabsorption%absortion spectrum
        \begin{tikzpicture}%
                \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\
                  pgfmathresult}%
                \ifwldrawaxis%draws the axis
                \wl@utils@draw@axis%
                \fi%|ifwldrawaxis
                \ifwlaxislabel%put the label
                \wl@utils@put@label%
                \fi%|ifwlaxislabel
                \wl@utils@visiblespectrum{\wlbrightness}%put visible spectrum in the
                  background
                % draws the lines
                \wl@utils@drawabsorptionlines%
        \end{tikzpicture}%
        \else%emission spectrum
        % draws the spectrum
        \ifx\wlback\wl@visible%visible background
        \begin{tikzpicture}%
                \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\
                  pgfmathresult}%
                \ifwldrawaxis%draws the axis
                \wl@utils@draw@axis%
                \fi%|ifwldrawaxis
                \ifwlaxislabel%put the label
                \wl@utils@put@label%
                \fi%|ifwlaxislabel
                \wl@utils@visiblespectrum{\@visible@opacity*\wlbrightness}%draws the
                  visible background
                \wl@utils@drawemissionlines% emission lines
        \end{tikzpicture}%
        \else%without visible background
        \begin{tikzpicture}%
                \pgfmathparse{\wlwidth/(abs(\wlend-\wlbegin))}\edef\xscale{\
                  pgfmathresult}%
                \ifwldrawaxis%draws the axis
                \wl@utils@draw@axis%
                \fi%|ifwldrawaxis
                \ifwlaxislabel%put the label
                \wl@utils@put@label%
                \fi%|ifwlaxislabel
                \ifnum\wlbegin>\wlend%
                    \draw[draw=none,fill=\wlback] (0,0) rectangle (-\wlwidth,\wlheight)
                      ;% background
                \else%
                    \draw[draw=none,fill=\wlback] (0,0) rectangle (\wlwidth,\wlheight);
                      % background
                \fi%
                \wl@utils@drawemissionlines% emission lines
        \end{tikzpicture}%
        \fi%|wlback|@visible
        \fi%|ifwlabsorption
    \fi% |wl@list@@|@empty
}%
% ###############################################################
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% get individual line data from one element of the array data
\def\wl@get@line@info[#1 #2 #3]{
\def\@currentline@wl{#1}% return
\def\@currentline@int{#2}% return
\def\@currentline@charge{#3}% return
}%
% ######################################################################
% ################### |wl@set@element@list ###################################
% ######################################################################
%
% |wl@set@element@list{|wl@elt@elemdata}{|wl@elt@Imax}
% RETURN: |wl@list@@ -> (wl1,wl2,...)
```

```
%            or if relative intensity true (between 0 and 1)
%                 |wl@list@@ -> (wl1/int1,wl2/int2,...)
%
\newif\ifwl@first% for first ocurrence of Imin
\def\wl@set@element@list#1#2{% |wl@elt@Imax
\wl@firsttrue%
\wl@counta=0%
\wl@countb=1%
\pgfmathparse{int(\wlintmin*100)}\edef\wl@intmin{\pgfmathresult}%intensity percentage
\ifnum\wl@intmin=0% include all intensities
\ifx\wl@ll\wlcharge%ALL lines
\@for\@myarg:=#1\do{\advance\wl@counta by 1}%count all entries
        \ifwlintensity%
        \@for\@myarg:=#1%
        \do{%
        \expandafter\wl@get@line@info\@myarg%
        \pgfmathparse{\wlrelintthresh+(1-\wlrelintthresh)*\@currentline@int/#2}\edef\
          wl@intensity@to@list{\pgfmathresult}%
        \ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl/\
          wl@intensity@to@list,}\else%
        \wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list}\fi%
        \advance\wl@countb by 1%
        }%END do
        \else%
        \@for\@myarg:=#1%
        \do{%
        \expandafter\wl@get@line@info\@myarg%
        \ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl,}\else%
        \wl@addt@list{\wl@list@@}{\@currentline@wl}\fi%
        \advance\wl@countb by 1%
        }%END do
        \fi%
\else% lines for one specific charge
\@for\@myarg:=#1\do{\expandafter\wl@get@line@info\@myarg\ifx\@currentline@charge\
  wlcharge\advance\wl@counta by 1\fi}%count only if is the desired charge
        \ifwlintensity%
        \@for\@myarg:=#1%
        \do{%
        \expandafter\wl@get@line@info\@myarg%
        \pgfmathparse{\wlrelintthresh+(1-\wlrelintthresh)*\@currentline@int/#2}\edef\
          wl@intensity@to@list{\pgfmathresult}%
        \ifx\@currentline@charge\wlcharge%add to list if is the desired charge
            \ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl/\
              wl@intensity@to@list,}\else%
            \wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list}\fi%
        \advance\wl@countb by 1%
        \fi%
        }%END do
        \else%
        \@for\@myarg:=#1%
        \do{%
        \expandafter\wl@get@line@info\@myarg%
        \ifx\@currentline@charge\wlcharge%add to list if is the desired charge
            \ifnum\wl@countb<\wl@counta\wl@addt@list{\wl@list@@}{\@currentline@wl,}\
              else%
            \wl@addt@list{\wl@list@@}{\@currentline@wl}\fi%
        \advance\wl@countb by 1%
        \fi%
        }%END do
        \fi%
\fi%
\else%|wlintmin>0 & |wlintmin<1
\ifnum\wl@intmin>100\else%
\pgfmathparse{\wlintmin*#2}\edef\wl@actual@int{\pgfmathresult}%
\ifx\wl@ll\wlcharge%ALL lines
\@for\@myarg:=#1\do{\advance\wl@counta by 1}%count all entries
        \ifwlintensity%
        \@for\@myarg:=#1%
        \do{%
        \expandafter\wl@get@line@info\@myarg%
```

```
          \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\relax\edef\
            wl@int@result{\pgfmathresult}%
          \ifnum\wl@int@result=1%
              \pgfmathparse{\wlrelintthresh+(1-\wlrelintthresh)*\@currentline@int/#2}\
                edef\wl@intensity@to@list{\pgfmathresult}%
              \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list
                }\else%
              \wl@addt@list{\wl@list@@}{,\@currentline@wl/\wl@intensity@to@list}\fi%
              \ifwl@first\wl@firstfalse\fi%
          \fi%
          \advance\wl@countb by 1%
          }%END do
          \else%
          \@for\@myarg:=#1%
          \do{%
          \expandafter\wl@get@line@info\@myarg%
          \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\relax\edef\
            wl@int@result{\pgfmathresult}%
          \ifnum\wl@int@result=1%
              \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl}\else%
              \wl@addt@list{\wl@list@@}{,\@currentline@wl}\fi%
              \ifwl@first\wl@firstfalse\fi%
          \fi%
          \advance\wl@countb by 1%
          }%END do
          \fi%
  \else% lines for one specific charge
  \@for\@myarg:=#1\do{\expandafter\wl@get@line@info\@myarg\ifx\@currentline@charge\
    wlcharge\advance\wl@counta by 1\fi}%count only if is the desired charge
          \ifwlintensity%
          \@for\@myarg:=#1%
          \do{%
          \expandafter\wl@get@line@info\@myarg%
          \ifx\@currentline@charge\wlcharge%add to list if is the desired charge
              \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\edef\wl@int@result
                {\pgfmathresult}%
              \ifnum\wl@int@result=1%
              \pgfmathparse{\wlrelintthresh+(1-\wlrelintthresh)*\@currentline@int/#2}\
                edef\wl@intensity@to@list{\pgfmathresult}%
              \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl/\wl@intensity@to@list
                }\else%
              \wl@addt@list{\wl@list@@}{,\@currentline@wl/\wl@intensity@to@list}\fi%
              \ifwl@first\wl@firstfalse\fi%
          \fi%
          \advance\wl@countb by 1%
          \fi%
          }%END do
          \else%
          \@for\@myarg:=#1%
          \do{%
          \expandafter\wl@get@line@info\@myarg%
          \ifx\@currentline@charge\wlcharge%add to list if is the desired charge
              \pgfmathparse{notless(\@currentline@int,\wl@actual@int)}\edef\wl@int@result
                {\pgfmathresult}%
              \ifnum\wl@int@result=1%
              \ifwl@first\wl@addt@list{\wl@list@@}{\@currentline@wl}\else%
              \wl@addt@list{\wl@list@@}{,\@currentline@wl}\fi%
              \ifwl@first\wl@firstfalse\fi%
          \fi%
          \advance\wl@countb by 1%
          \fi%
          }%END do
          \fi%
  \fi%
  \fi%
  \fi%
  }%
  % add to list
  \def\wl@addt@list#1#2{\edef\wl@list@@{#1#2}}
  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
% internal utils ---------------------------------------------------------------------------------------------------%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
\def\wl@utils@draw@axis{%
                \ifnum\wlbegin>\wlend%
                \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);%
                \pgfmathparse{\wlend+\wlaxisstep}\pgfmathparse{int(\pgfmathresult)}
                \edef\@axis@list{\wlend,\pgfmathresult,...,\wlbegin}
                \foreach \x in \@axis@list%
                {%
                \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\pgfmathresult pt}%
                \draw[\wlaxisfontcolor,line width=.25pt] (\wl@currentx,-.75*\@wl@axis@height) -- ++(0,.75*\@wl@axis@height);
                \node[\wlaxisfontcolor,font=\wlaxisfont,above,inner sep=0pt] at (\wl@currentx,-2.25*\@wl@axis@height) {\x};
                }%
                \else%
                \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);%
                \pgfmathparse{\wlbegin+\wlaxisstep}\pgfmathparse{int(\pgfmathresult)}
                \edef\@axis@list{\wlbegin,\pgfmathresult,...,\wlend}
                \foreach \x in \@axis@list%
                {%
                \pgfmathparse{(\x-\wlbegin)*\xscale}\edef\wl@currentx{\pgfmathresult pt}%
                \draw[\wlaxisfontcolor,line width=.25pt] (\wl@currentx,-.75*\@wl@axis@height) -- ++(0,.75*\@wl@axis@height);
                \node[\wlaxisfontcolor,font=\wlaxisfont,above,inner sep=0pt] at (\wl@currentx,-2.25*\@wl@axis@height) {\x};
                }%
                \fi%
}%
\def\wl@utils@put@label{%
                \ifx\wl@elt@chemsym\undefined\def\wl@elt@chemsym{}\fi%
                \wl@get@label@position%
                \ifnum\wlbegin>\wlend%
                        \ifcase\wl@label@position%
                        %west
                            \ifwldrawaxis%\ifwlaxislabel%
                            \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};%
                            \else%
                            \node[\wllabelfontcolor,font=\wllabelfont,left,minimum width=2em,align=right] at (-\wlwidth,0.5*\wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                            \fi%
                        \or%north west
                        \node[\wllabelfontcolor,font=\wllabelfont,above right,inner xsep=0pt] at (-\wlwidth,\wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                        \or%north
                        \node[\wllabelfontcolor,font=\wllabelfont,above] at (-0.5*\wlwidth,\wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                        \or%north east
                        \node[\wllabelfontcolor,font=\wllabelfont,above left,inner xsep=0pt] at (0,\wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                        \or%east
                            \ifwldrawaxis%
                            \node[\wllabelfontcolor,font=\wllabelfont,right] at (1.5*\@wl@axis@height,0.5*\wlheight) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                            \else%
```

```
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                     \fi%
427                 \else%
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
```

```
                                \ifwldrawaxis%
                                \node[\wllabelfontcolor,font=\wllabelfont,below left,inner xsep=0pt] at (\wlwidth,-2.5*\@wl@axis@height) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                                \else%
                                \node[\wllabelfontcolor,font=\wllabelfont,below left,inner xsep=0pt] at (\wlwidth,0) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                                \fi%
                            \or%south
                                \ifwldrawaxis%
                                \node[\wllabelfontcolor,font=\wllabelfont,below] at (0.5*\wlwidth,-2.5*\@wl@axis@height) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                                \else%
                                \node[\wllabelfontcolor,font=\wllabelfont,below] at (0.5*\wlwidth,0) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                                \fi%
                            \or%south west
                                \ifwldrawaxis%
                                \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};%
                                \else%
                                \node[\wllabelfontcolor,font=\wllabelfont,below right,inner xsep=0pt] at (0,0) {\wllabelbtext\wl@elt@chemsym\wllabelatext};%
                                \fi%
                            \fi%
                    \fi%
}%
\def\wl@utils@visiblespectrum#1{%
                    \pgfmathparse{int(#1*100)}\edef\wl@bright{\pgfmathresult}
                    \ifnum\wlbegin>\wlend%
                        \foreach \x in {\wlend,...,\wlbegin}%
                        {%
                        \wlcolor{\x}%
                        \colorlet{wlcolor}{wltemp!\wl@bright!black}% ??? !black
                        \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\pgfmathresult pt}%
                        \edef\wl@linewidth{\xscale pt}%
                        \draw[wlcolor,line width=\wl@linewidth] (\wl@currentx,0) -- ++(0,\wlheight);%
                        }%
                    \else%
                        \foreach \x in {\wlbegin,...,\wlend}%
                        {%
                        \wlcolor{\x}%
                        \colorlet{wlcolor}{wltemp!\wl@bright!black}% ??? !black
                        \pgfmathparse{(\x-\wlbegin)*\xscale}\edef\wl@currentx{\pgfmathresult pt}%
                        \edef\wl@linewidth{\xscale pt}%
                        \draw[wlcolor,line width=\wl@linewidth] (\wl@currentx,0) -- ++(0,\wlheight);%
                        }%
                    \fi%
}%
\def\wl@utils@drawabsorptionlines{%
                    \ifnum\wlbegin>\wlend%
                        \ifwlintensity%
                            \foreach \x/\y in \wl@list@@%
                            {%
                            \pgfmathparse{notless(\x,\wlend)}\edef\wl@x@nl{\pgfmathresult}%
                            \pgfmathparse{notgreater(\x,\wlbegin)}\edef\wl@x@ng{\pgfmathresult}
                            \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\pgfmathresult}%
                            \ifnum\wl@plot@point=1%
```

```
                        \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\
                          pgfmathresult pt}%
                        \pgfmathparse{int(\y*100)}\edef\wl@black{\pgfmathresult}
                        \wlcolor{\x}
                        \colorlet{wlcolor}{black!\wl@black!wltemp}
                        \draw[wlcolor,line width=\wllinewidth] (\wl@currentx,0) --
                          ++(0,\wlheight);%
                        \fi%
                        }%
                    \else%
                        \foreach \x in \wl@list@@%
                        {%
                        \pgfmathparse{notless(\x,\wlend)}\edef\wl@x@nl{\pgfmathresult}%
                        \pgfmathparse{notgreater(\x,\wlbegin)}\edef\wl@x@ng{\
                          pgfmathresult}
                        \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
                          pgfmathresult}%
                        \ifnum\wl@plot@point=1%
                        \pgfmathparse{(\wlend-\x)*\xscale}\edef\wl@currentx{\
                          pgfmathresult pt}%
                        \wlcolor{\x}
                        \colorlet{wlcolor}{black!\wllineint!wltemp}
                        \draw[wlcolor,line width=\wllinewidth] (\wl@currentx,0) --
                          ++(0,\wlheight);%
                        \fi%
                        }%
                    \fi%
                \else%
                    \ifwlintensity%
                        \foreach \x/\y in \wl@list@@%
                        {%
                        \pgfmathparse{notless(\x,\wlbegin)}\edef\wl@x@nl{\pgfmathresult
                          }%
                        \pgfmathparse{notgreater(\x,\wlend)}\edef\wl@x@ng{\
                          pgfmathresult}
                        \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
                          pgfmathresult}%
                        \ifnum\wl@plot@point=1%
                        \pgfmathparse{(\x-\wlbegin)*\xscale}\edef\wl@currentx{\
                          pgfmathresult pt}%
                        \pgfmathparse{int(\y*100)}\edef\wl@black{\pgfmathresult}
                        \wlcolor{\x}
                        \colorlet{wlcolor}{black!\wl@black!wltemp}
                        \draw[wlcolor,line width=\wllinewidth] (\wl@currentx,0) --
                          ++(0,\wlheight);%
                        \fi%
                        }%
                    \else%
                        \foreach \x in \wl@list@@%
                        {%
                        \pgfmathparse{notless(\x,\wlbegin)}\edef\wl@x@nl{\pgfmathresult
                          }%
                        \pgfmathparse{notgreater(\x,\wlend)}\edef\wl@x@ng{\
                          pgfmathresult}
                        \pgfmathparse{and(\wl@x@nl,\wl@x@ng)}\edef\wl@plot@point{\
                          pgfmathresult}%
                        \ifnum\wl@plot@point=1%
                        \pgfmathparse{(\x-\wlbegin)*\xscale}\edef\wl@currentx{\
                          pgfmathresult pt}%
                        \wlcolor{\x}
                        \colorlet{wlcolor}{black!\wllineint!wltemp}
                        \draw[wlcolor,line width=\wllinewidth] (\wl@currentx,0) --
                          ++(0,\wlheight);%
                        \fi%
                        }%
                    \fi%
                \fi%
}%
\def\wl@utils@drawemissionlines{%
                \ifnum\wlbegin>\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}{wltemp!\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}{wltemp!\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}{wltemp!\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}{wltemp!\wllineint!black}
```

```
                        \draw[wlcolor,line width=\wllinewidth] (\wl@currentx,0) --
                          ++(0,\wlheight);%
                        \fi%
                        }%
                \fi%
                \fi%
}
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% return: integer with position (e.g. '0' for west, ... )
\def\wl@get@label@position{%
\wl@countc=0%
\@for\@mylabel:=\wl@label@position@list%
            \do{%
            \ifx\@mylabel\wllabelposition\edef\wl@label@position{\the\wl@countc}\fi%
            \advance\wl@countc by1%
            }%
}%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
% nm2rgb convert nanometer wavelength to rgb
% (380 <= Lambda <= 780 ) -> r,g,b on stack
%
% BASED on FORTRAN Code
% RGB VALUES FOR VISIBLE WAVELENGTHS by Dan Bruton (astro@tamu.edu)
% This program can be found at
% http://www.physics.sfasu.edu/astro/color.html
% and was last updated on February 20, 1996.
% The spectrum is generated using approximate RGB values for visible
% wavelengths between 380 nm and 780 nm.
% The red, green and blue values (RGB) are
% assumed to vary linearly with wavelength (for GAMMA=1).
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
\newdimen\wl%wavlength
\newdimen\wl@i%intensity
\newdimen\wl@gamma%gamma
\newdimen\wlc@lorr%red (0. - 1)
\newdimen\wlc@lorg%green (0. - 1)
\newdimen\wlc@lorb%blue (0. - 1) % wavelength to rgb values
\newcount\wl@counta% tmp counter
\newcount\wl@countb% tmp counter
\newcount\wl@countc% tmp counter
\newcount\wl@countd% tmp counter
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% \wlcolor{wavelength}
\def\wlcolor#1{%
\wl=#1pt%
\wl@gamma=\wlgamma pt%
% compute the rgb components
\ifdim\wl<380pt\\ Err: wavelength must be graeter or equal to 380nm\else%
\ifdim\wl<440pt\wlc@lorr=440pt\advance\wlc@lorr by-\wl\divide\wlc@lorr by60\wlc@lorg=0
  pt\wlc@lorb=1pt\else%
\ifdim\wl<490pt\wlc@lorr=0pt\wlc@lorg=\wl\advance\wlc@lorg by-440pt\divide\wlc@lorg by
  50\wlc@lorb=1pt\else%
\ifdim\wl<510pt\wlc@lorr=0pt\wlc@lorg=1pt\wlc@lorb=510pt\advance\wlc@lorb by-\wl\divide
  \wlc@lorb by20\else%
\ifdim\wl<580pt\wlc@lorr=\wl\advance\wlc@lorr by-510pt\divide\wlc@lorr by70\wlc@lorg=1
  pt\wlc@lorb=0pt\else%
\ifdim\wl<645pt\wlc@lorr=1pt\wlc@lorg=645pt\advance\wlc@lorg by-\wl\divide\wlc@lorg by
  65\wlc@lorb=0pt\else%
\ifdim\wl<780.00001pt\wlc@lorr=1pt\wlc@lorg=0pt\wlc@lorb=0pt\else%
\\ Err: wavelength must be lesser or equal to 780nm%
\fi\fi\fi\fi\fi\fi\fi%
% intensity correction at vision limits
\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%
\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%
```

```
\wl@i=1pt%
\fi\fi%
%apply intensity at vision limits correction and  gamma
\pgfmathparse{\wlc@lorr*\wl@i^\wl@gamma}\edef\wl@red{\pgfmathresult}%
\pgfmathparse{\wlc@lorg*\wl@i^\wl@gamma}\edef\wl@green{\pgfmathresult}%
\pgfmathparse{\wlc@lorb*\wl@i^\wl@gamma}\edef\wl@blue{\pgfmathresult}%
\definecolor{wltemp}{rgb}{\wl@red,\wl@green,\wl@blue}%
\colorlet{wlcolor}{wltemp}
}%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
\def\wl@elt@search#1#2#3#4{%
% #1 Chemical Symbol, entered by USER
% #2 Chemical Symbol to compare to, e.g. Na
% #3 Emission Lines Data (or error message)
% #4 Imax
\ifthenelse{\equal{\expandafter\noexpand#1}{\expandafter\noexpand#2}}%
        {% true
        \def\wl@elt@chemsym{#2}%  set chemical symbol
        \def\wl@elt@elemdata{#3}%  set element lines data
        \def\wl@elt@Imax{#4}%  set element Imax
        }%
        {}% false
}%
\input{spectra.data.tex}
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
\endinput
```