

GChemTable manual

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Abstract

GChemTable is a chemistry elements periodic table application.

Introduction

The GChemTable application is a chemical elements periodic table application. It provides scientific information on the elements and multiple table color schemes.

Chapter 1

Getting started

1.1 To Start GChemTable

You can start GChemTable in the following ways:

Applications list Choose “Periodic table of the elements”. It might be listed either in the Education or Science category.

Command line Type `gchemtable`, then press **Return**.

1.2 When You Start GChemTable

When you start GChemTable, the following window is displayed:

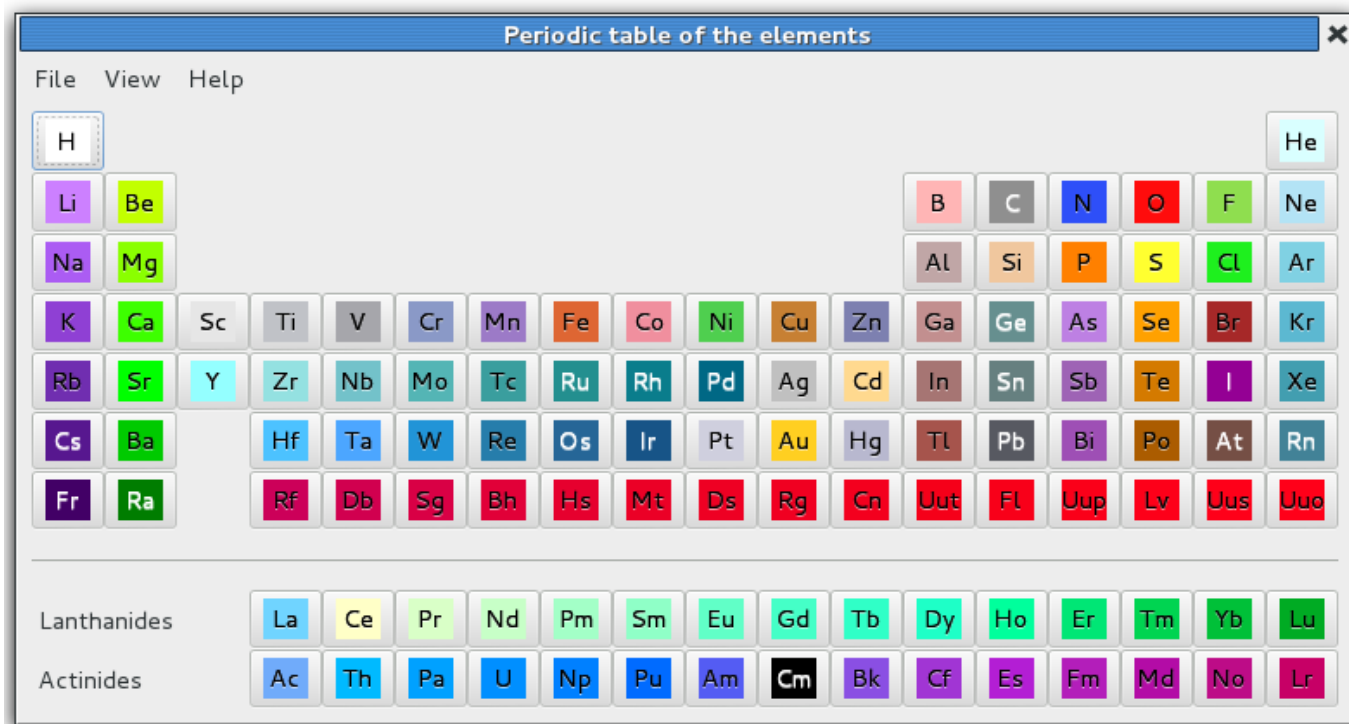


Figure 1.1: GChemTable window

The GChemTable window contains the following elements:

Menubar The menus on the menubar contain all of the commands you need to work with GChemTable.

Periodic table A periodic table of the elements. The colors used for the buttons are conventional colors for the elements. Other color schemes are also available, as explained [later](#).

When the mouse is moved over an element button, a popup window appears with some data about the element:

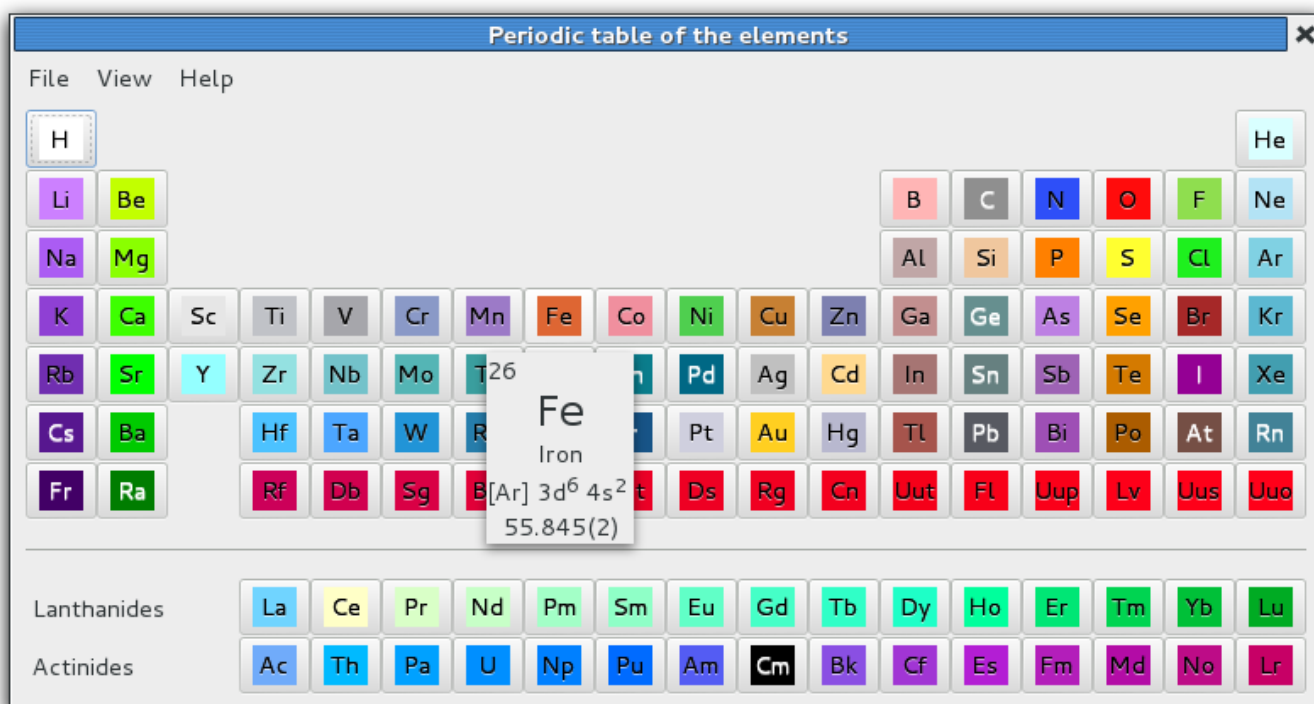


Figure 1.2: GChemTable window with an element tip.

Chapter 2

Usage

2.1 Color Schemes

Several color schemes are available:

No colors All buttons are grey.

Default Conventional colors are used.

Physical state The color of the button depends on the physical state (solid, liquid, or gas) of the element at a given temperature. This temperature can be changed using the horizontal scale.

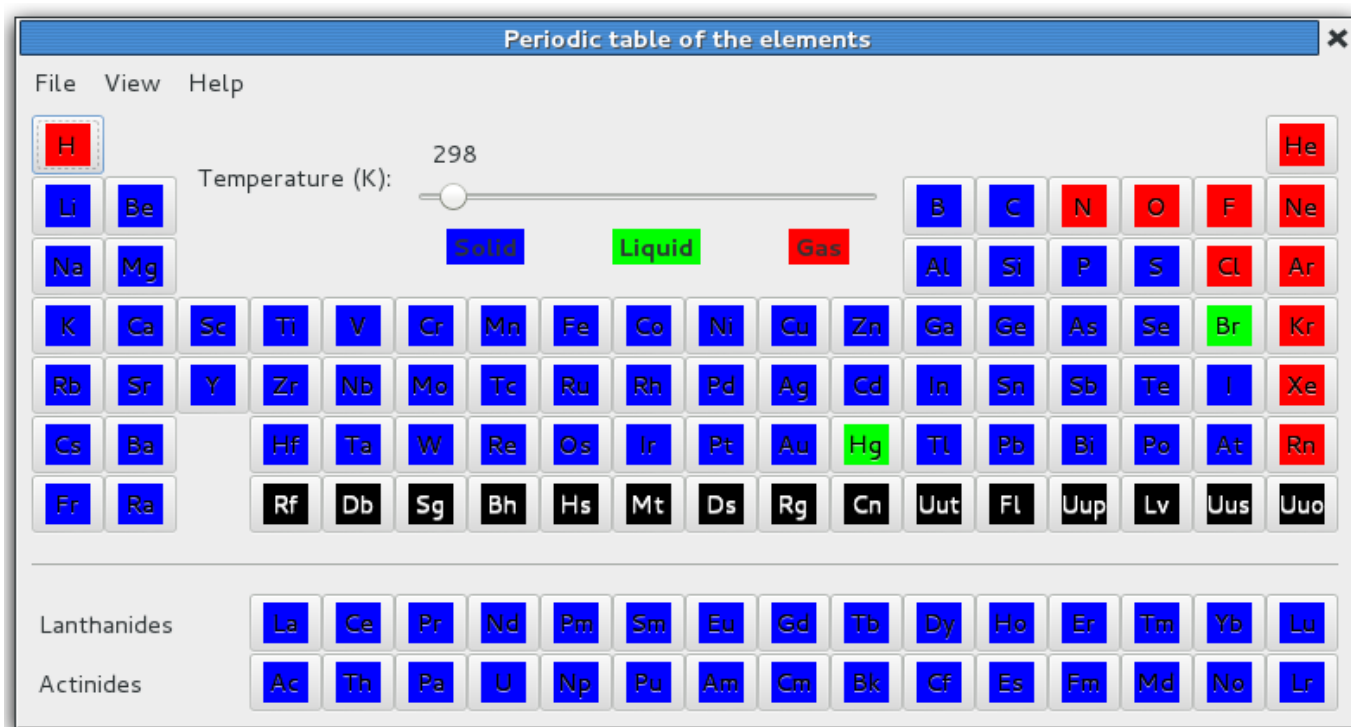


Figure 2.1: Physical state color scheme

Elements with a black background indicate that the state is unknown at the given temperature.

Family The data used are the element family as given in the [Blue Obelisk Data Repository](#).

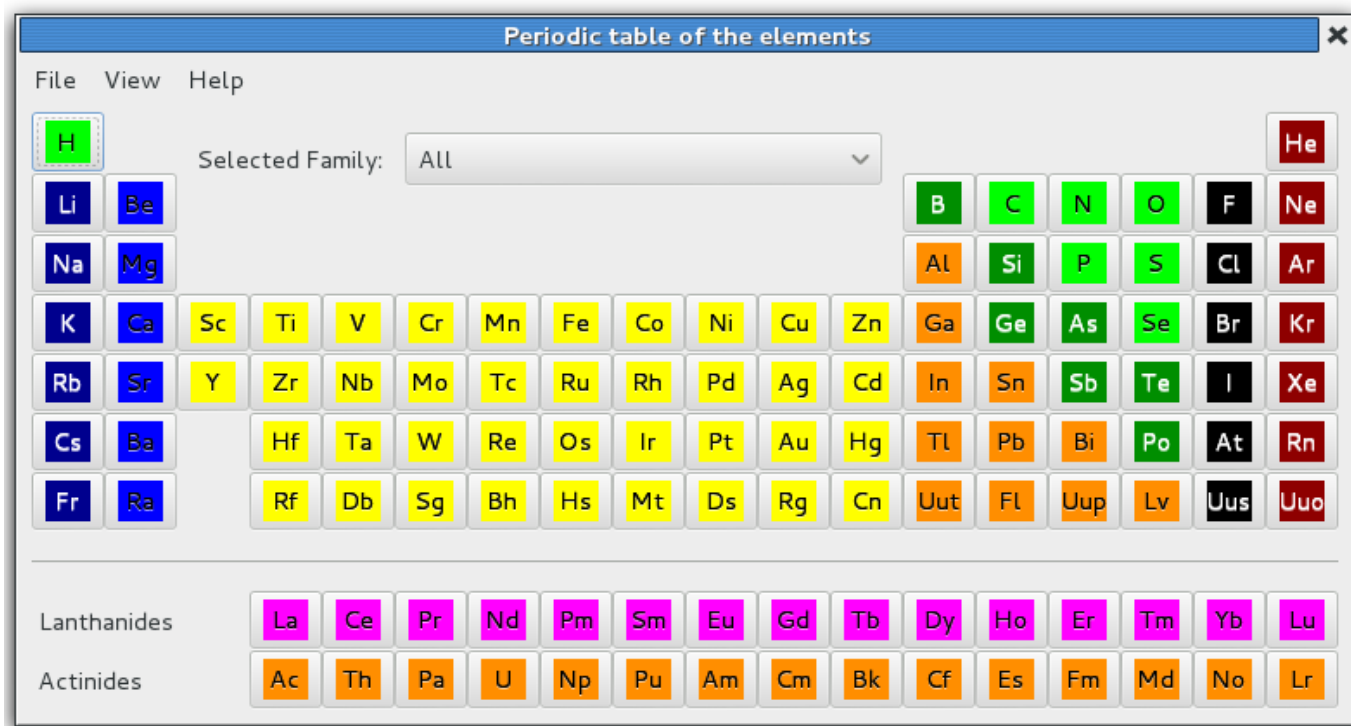


Figure 2.2: Family color scheme

If a family is selected, only elements of this family will be displayed with their family color used as a background. Other elements will have a black background.

Electronegativity The data used are the Pauling electronegativity as given in the [Blue Obelisk Data Repository](#). Colors go from red (lowest electronegativity) to blue (highest electronegativity). If no data is available in the database, the element will have a black background.

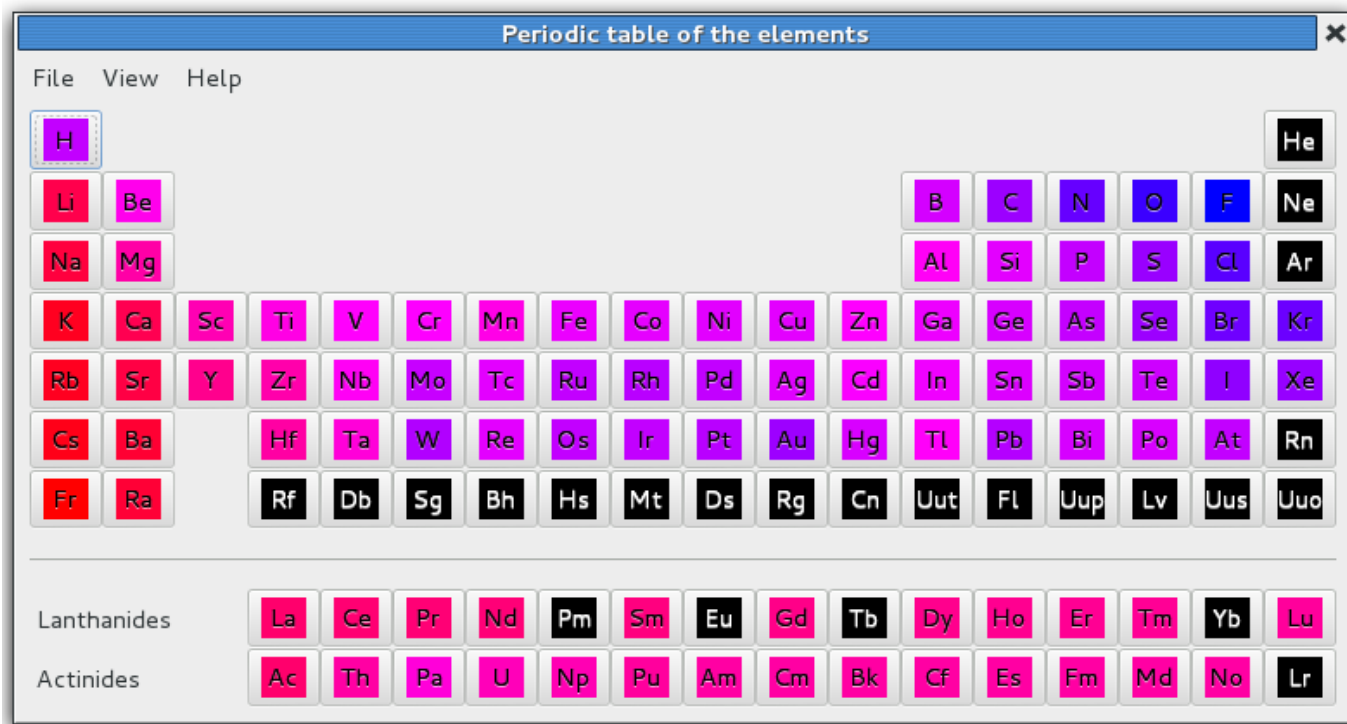


Figure 2.3: Electronegativity color scheme

Atomic radius The data used are the atomic radii as given in the [Blue Obelisk Data Repository](#). Colors go from red (lowest radius) to blue (largest radius). If no data is available in the database, the element will have a black background.

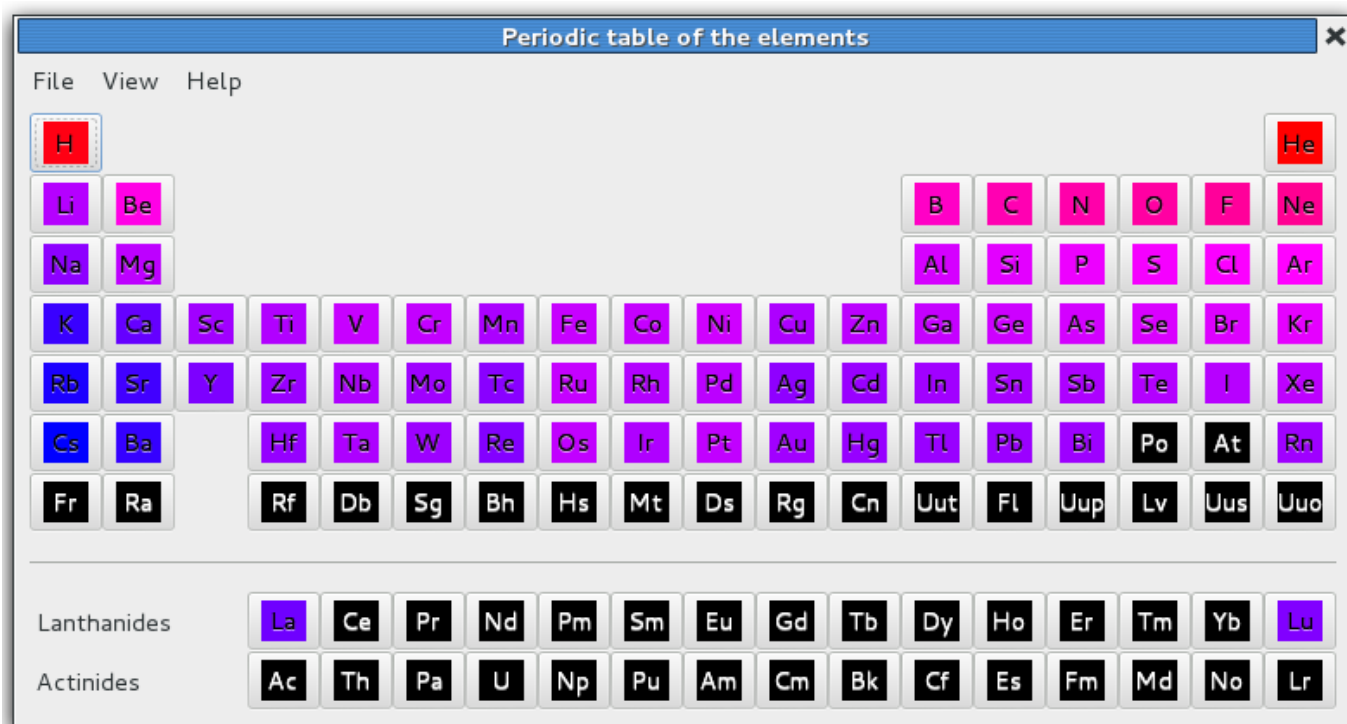


Figure 2.4: Atomic radius color scheme

Block Elements buttons are colored according to the block (s, p, d, or f) to which the element belongs

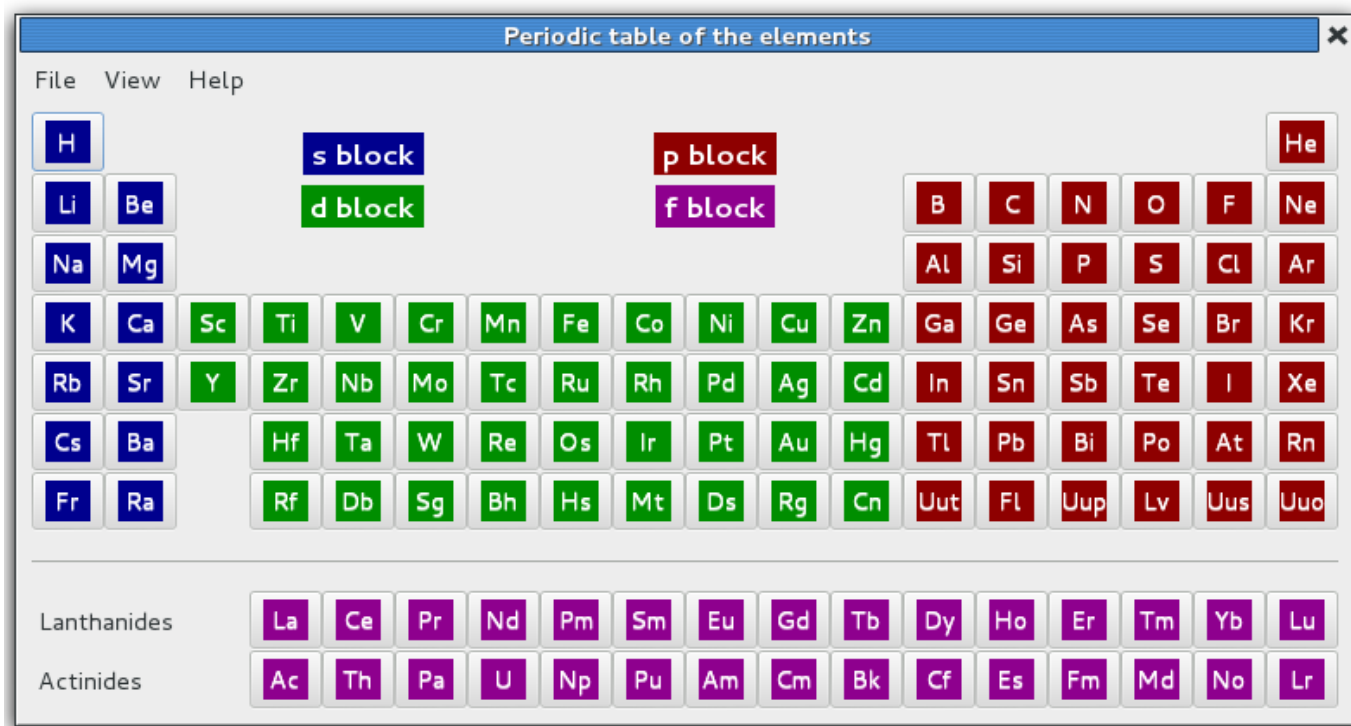


Figure 2.5: Block color scheme

2.2 Element Window

This window shows the data for an element. To display it, press the corresponding element button in the periodic table. It is possible to display several element windows at once.

The data are spread over several pages, the following screenshots show the various pages for iron:

Main Page

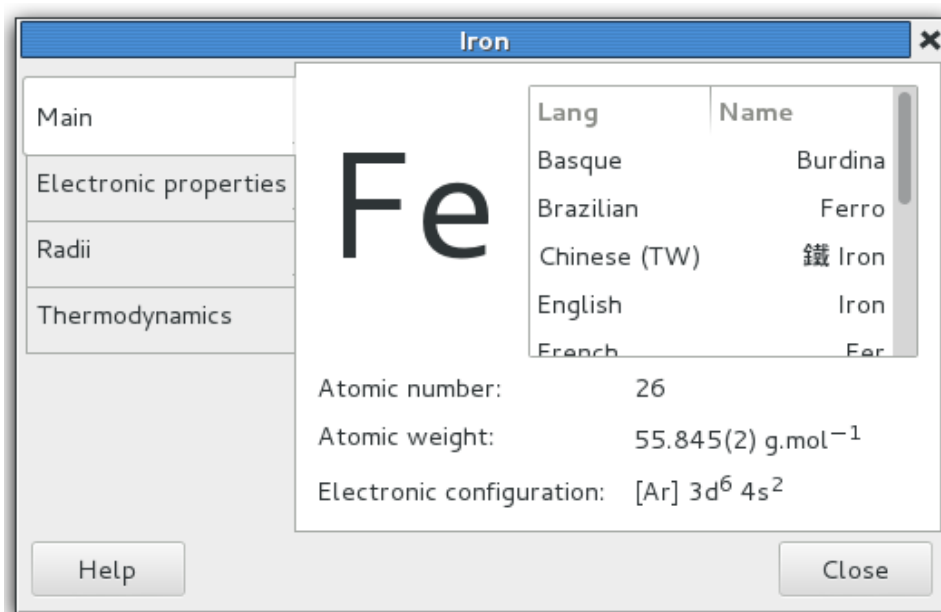


Figure 2.6: Main Page

Electronic Properties

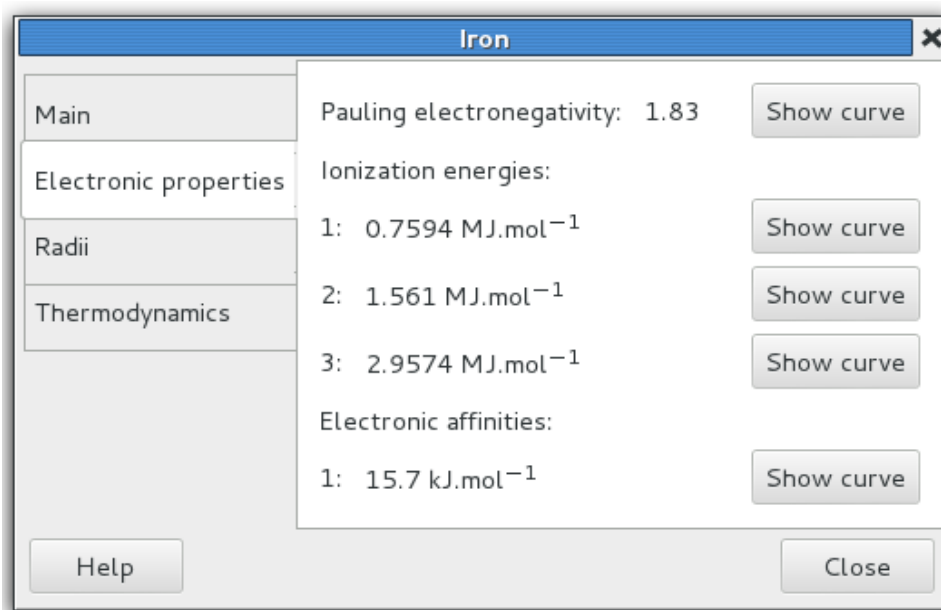


Figure 2.7: Electronic Properties Page

Radii

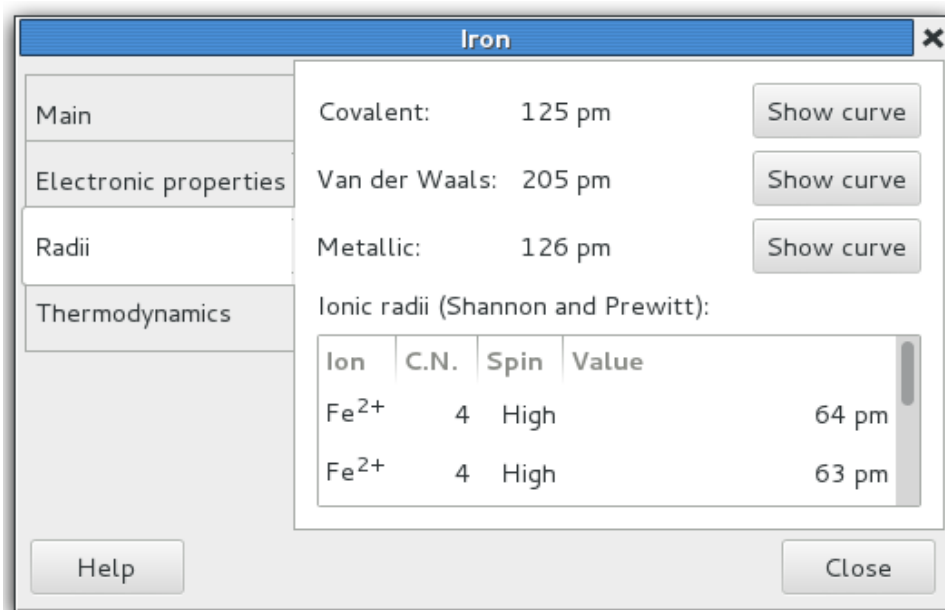


Figure 2.8: Radii Page

Thermodynamic Properties

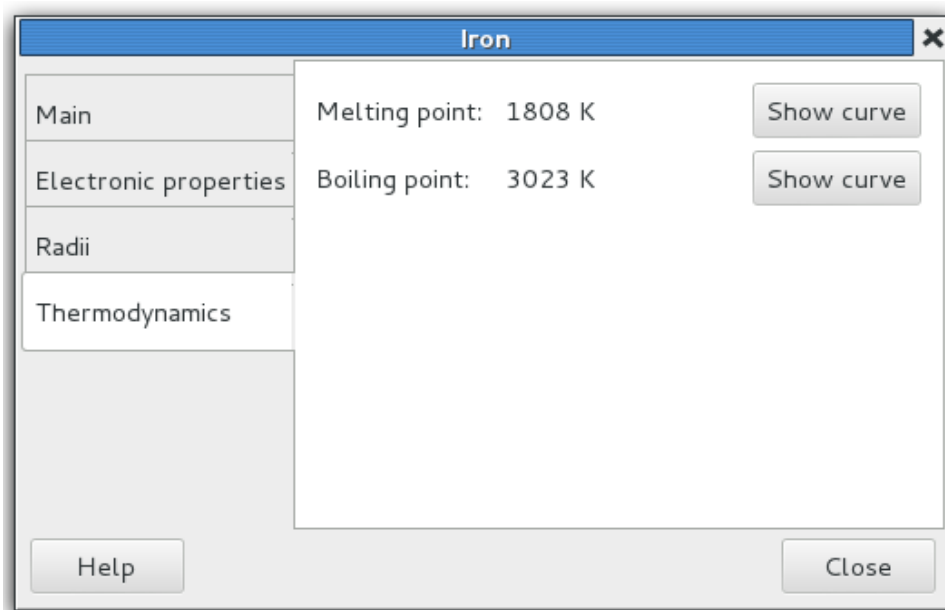


Figure 2.9: Thermodynamic Properties Page

When a Show curve button appears on the same line as data, it is possible to display a **chart** of this data as a function of the element atomic number by clicking on the button.

Chapter 3

Charts

3.1 Pre-defined Charts

When you click on the Show curve button in the [element window](#) you obtain a chart such as:

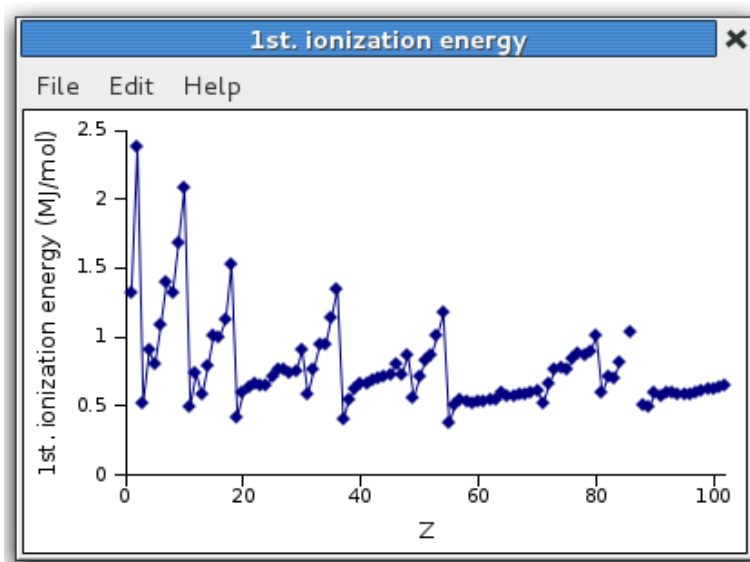


Figure 3.1: First ionization energy curve

Some charts can also be displayed by selecting one of the items in Edit → Element charts, except Custom which creates a [custom chart](#).

Consecutive points are joined by a segment. The absence of a segment means that at least one data point is missing.

Charts can be customized as explained in the [next section](#).

3.2 Customize Charts

To customize a chart, choose File → Properties in the chart window menu. The following dialog pops up:

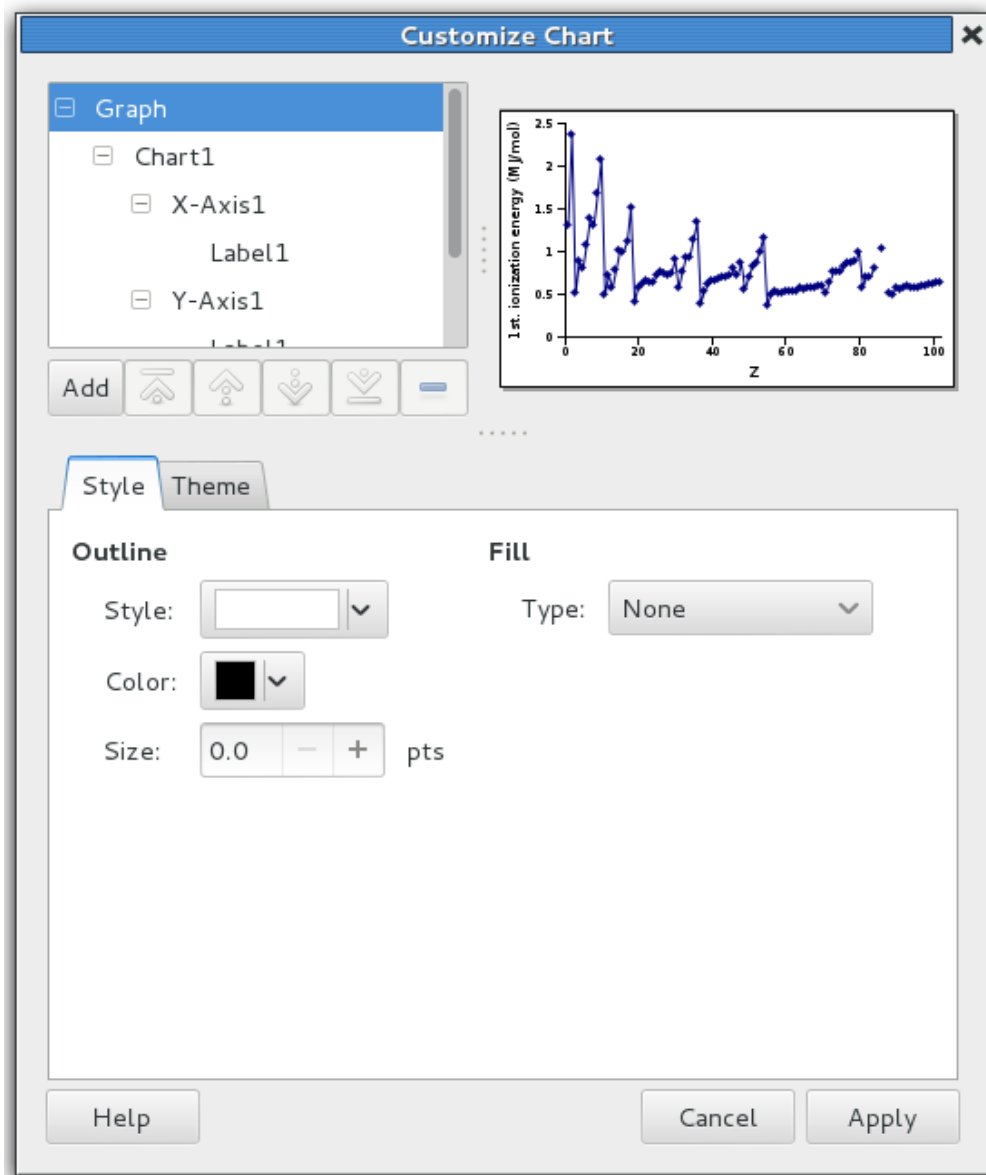


Figure 3.2: Chart properties dialog.

The main elements in this dialog are:

The graph hierarchy tree. The graph hierarchy tree (top left) displays the current graph components and their hierarchy. The hierarchy can be modified using the buttons just below it.

The graph preview. The graph preview (top right) shows the result of the modifications and displays a scaled version of the graph you will get when you apply the changes.

The Add button. The Add button allows for insertion of new components into the hierarchy. Note that the list of available components to add depends on the object selected.

The arrow buttons. The arrow buttons can be used to modify the order of child objects of the same parent. These buttons are only available when ordering makes sense for the currently selected object. If you have, say, two charts in the graph, you can change the order in the hierarchy, and this will affect the order in which they are displayed.

The Delete button. Clicking the Delete button destroys the selected graph component and all its children. The button is not available when the component can't be removed.

**Warning**

These deletions can't be undone, so be careful.

The component properties notebook. The component properties notebook (bottom) shows all the properties you can set for the current component.

**Warning**

The window title can't be changed, so if you customize a pre-defined chart, the title may no longer reflect what is displayed in the window.

GChemTable does not check the validity of the charts. It is possible add titles and labels not corresponding to the data actually used, in which case the resulting charts will not make sense.

Some features appearing in the dialog, such as error bars are not currently supported by GChemTable.

3.3 User Defined Charts

A user can create a new empty plot, and then customize it as explained in the [previous section](#).

To create a new empty plot, choose Edit+Element charts → Custom. This will open two new windows: one containing the new chart, and one containing the chart properties dialog.

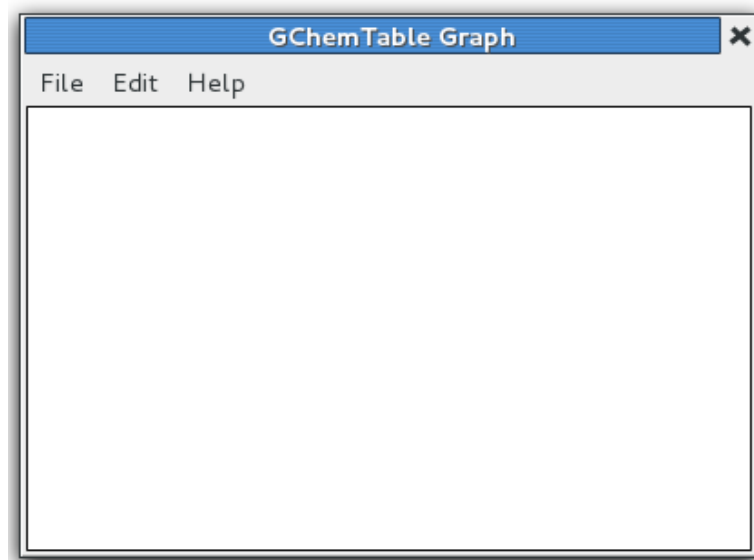


Figure 3.3: New empty chart window

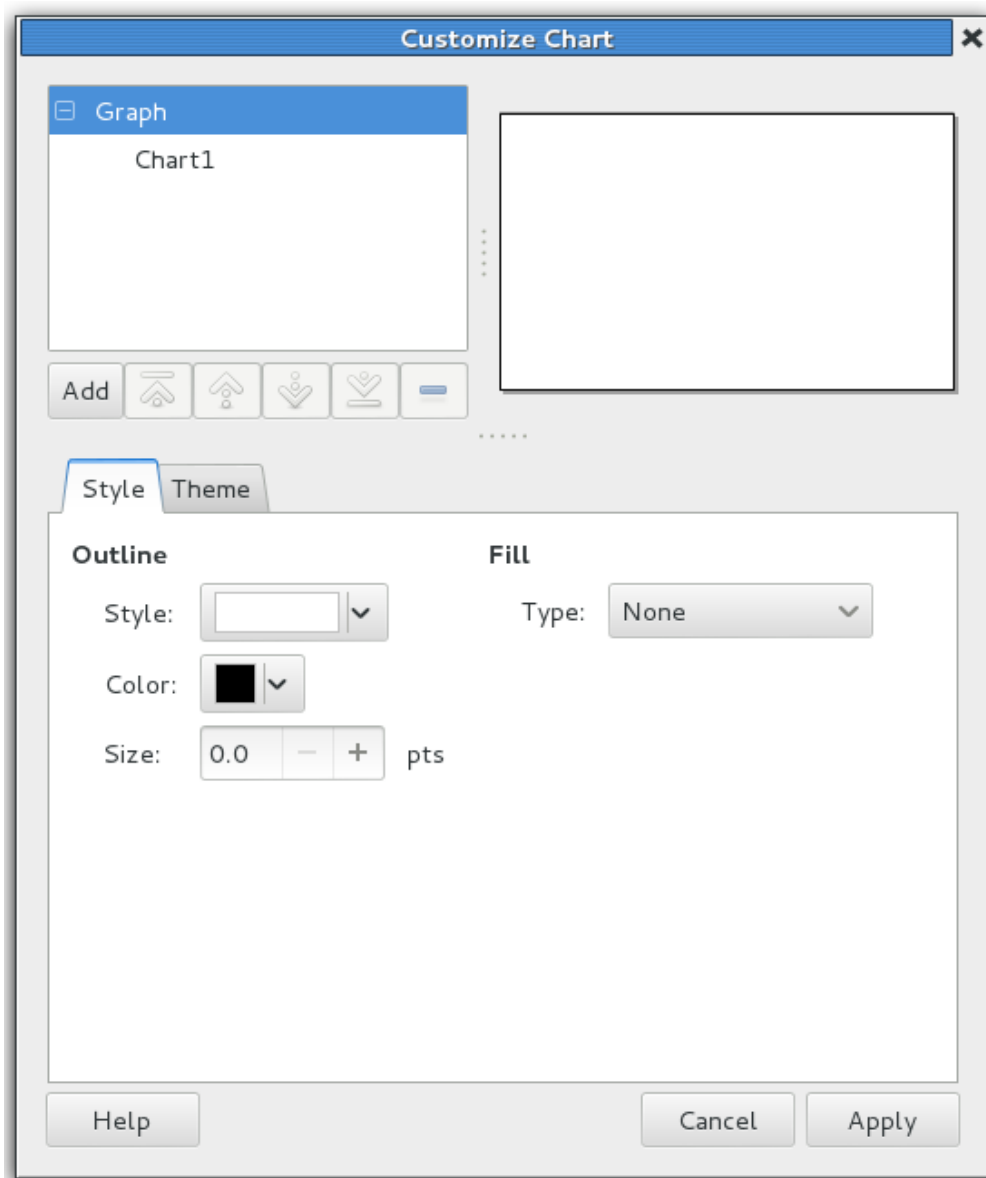


Figure 3.4: New empty chart properties dialog

The graph contains just one empty chart. In most cases, the first thing to do is to add a new plot using the Add button as seen in next screenshot:

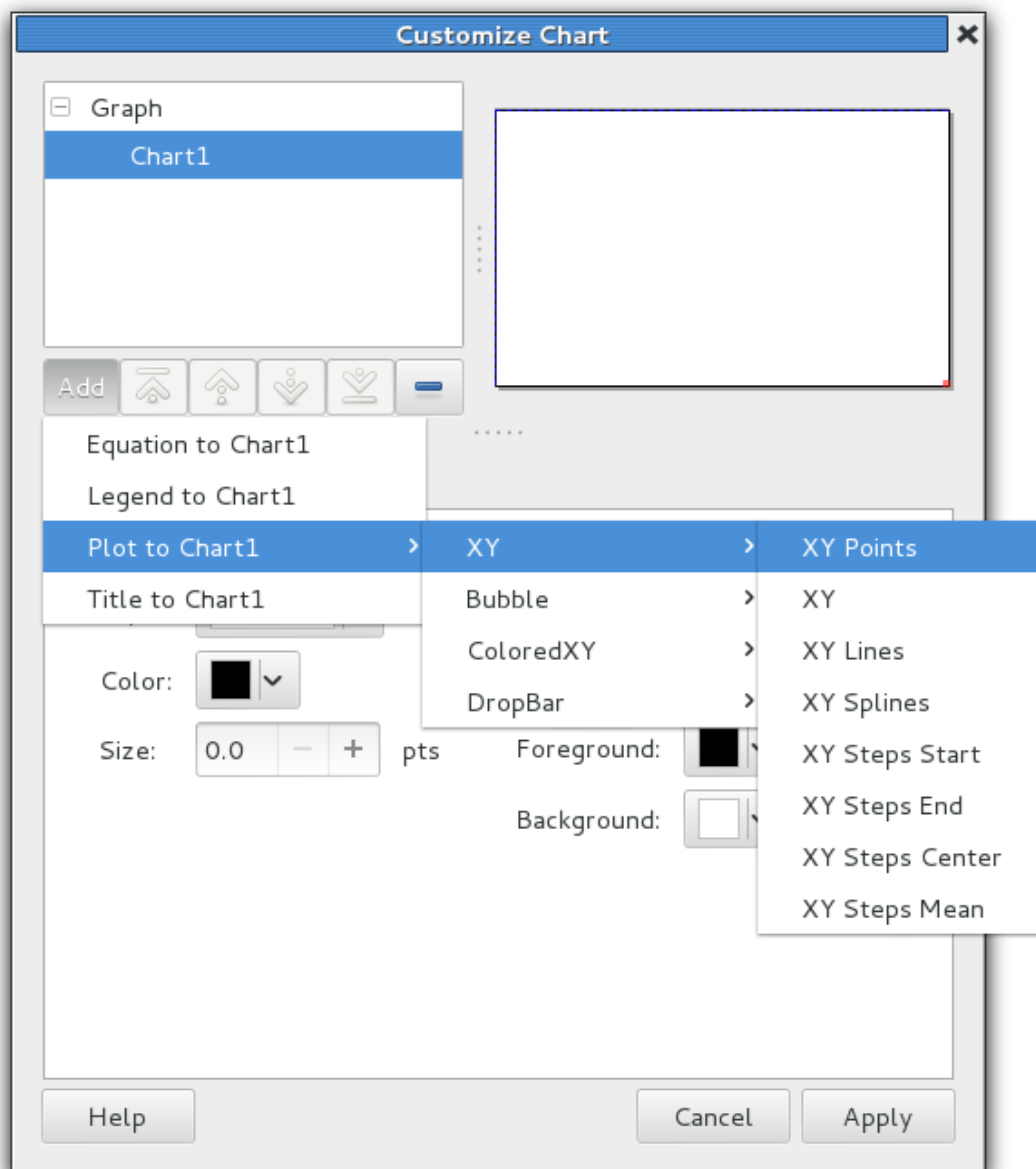


Figure 3.5: Adding a plot

This adds not only a plot, but also a backplane, the two needed axes, and a data series to the plot.

You can then select the data to use for the new series. Only predefined data vectors can be used. If X values are not selected, an integer series starting from 0 will be used; that is the atomic number minus one.

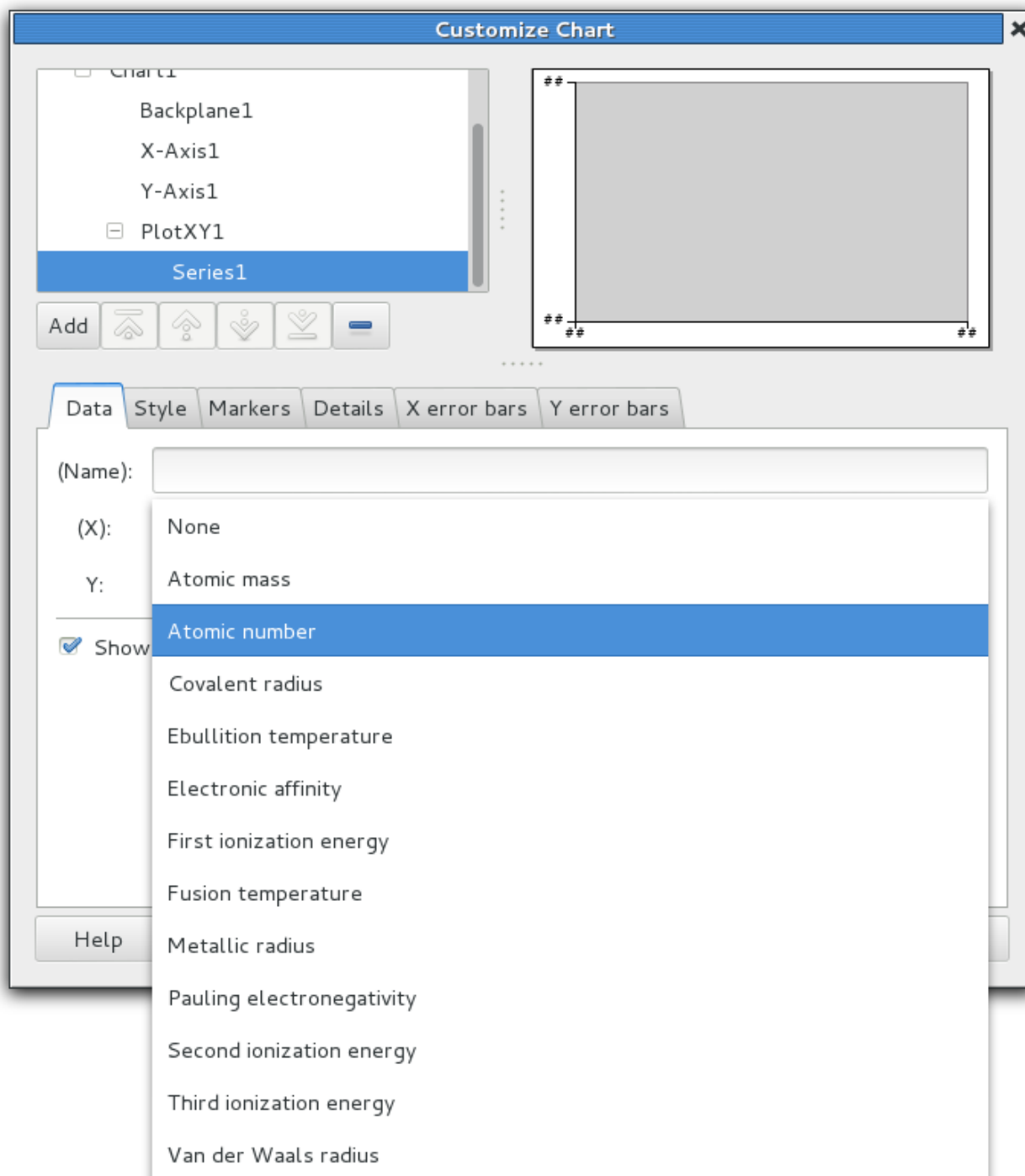


Figure 3.6: Data selection

Further customization is explained in the [previous section](#).

3.4 To Copy a Chart

To copy the chart, choose Edit → Copy and then paste into the target application. Charts will be copied as native graphs to Abiword or as svg or png data to other applications which support such formats.

3.5 To Export a Chart as an Image

To export the displayed chart to an image, use File → Save As Image.

Available formats are SVG, EPS, PS, PDF, and formats that support writing in GdkPixbuf.

To choose a format, you can use an appropriate file name extension, or explicitly select a format in the combo box. With the first method, if GChemTable does not recognize an extension, the exported file will be a SVG file. GChemTable will add an extension to the file name if needed.

You might change the default width and height of the exported image using the appropriate entries.

Postscript and PDF files can also be produced using the **FilePrint... command**.

3.6 To Print a Chart

To print the chart, choose File → Print....

File → Preview opens a window with a preview of the printed output.

To tune the printed output, choose File → Page setup... as explained below.

3.6.1 The page setup dialog.

The first tab of the dialog concerns the paper and margins setup. Headers and footers are not supported in the version of GChemTable

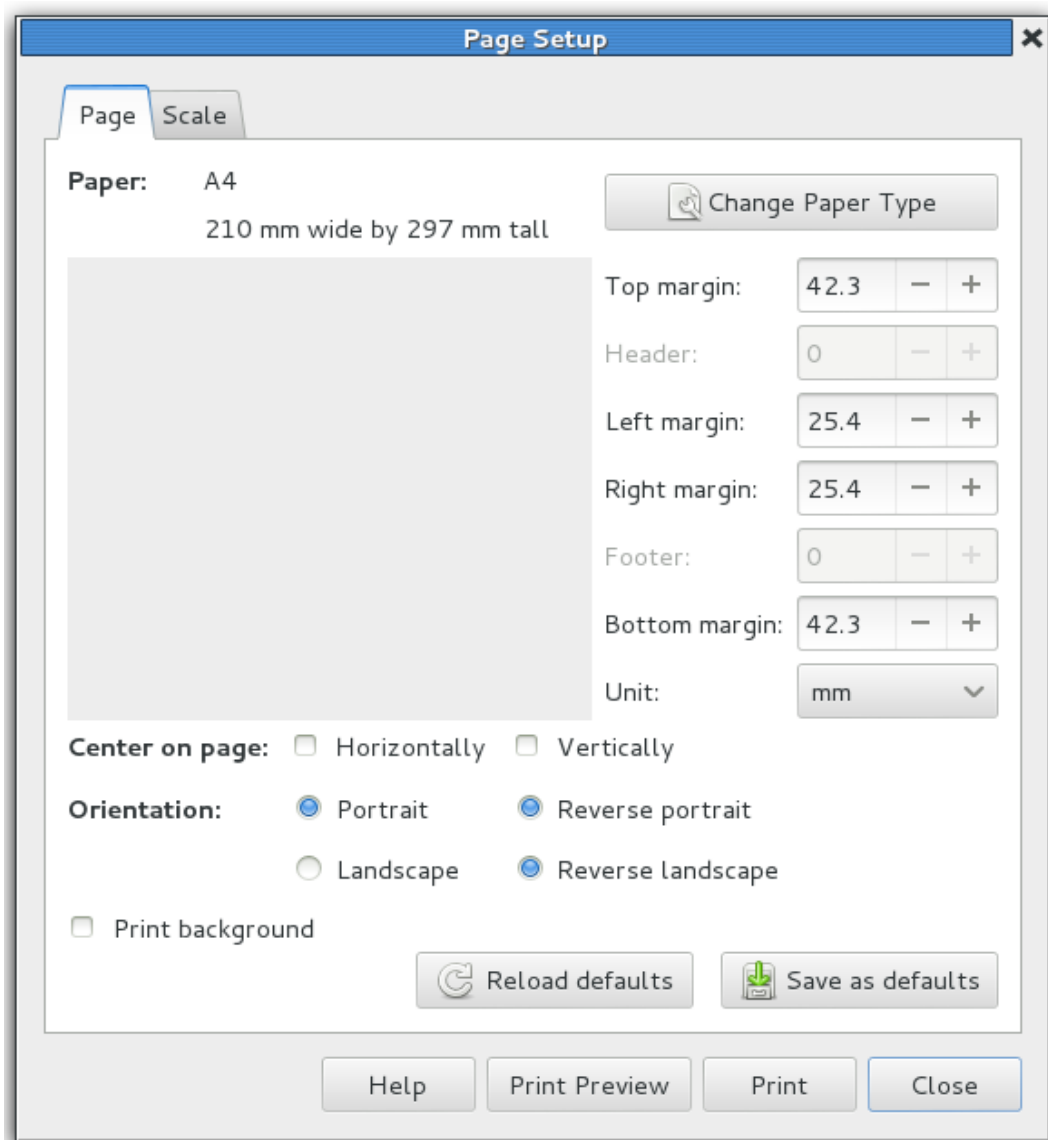


Figure 3.7: The Page Setup tab.

The second tab allows you to choose the scale of the output. With no scaling or scaling at 100%, the output will have the same size in points as the size in pixels on the screen. If you choose automatic scaling, you can make the output fill the available space either horizontally, vertically, or both (unchecking both options is equivalent to no scaling).

Printing to more than one page is not supported in this version of GChemTable

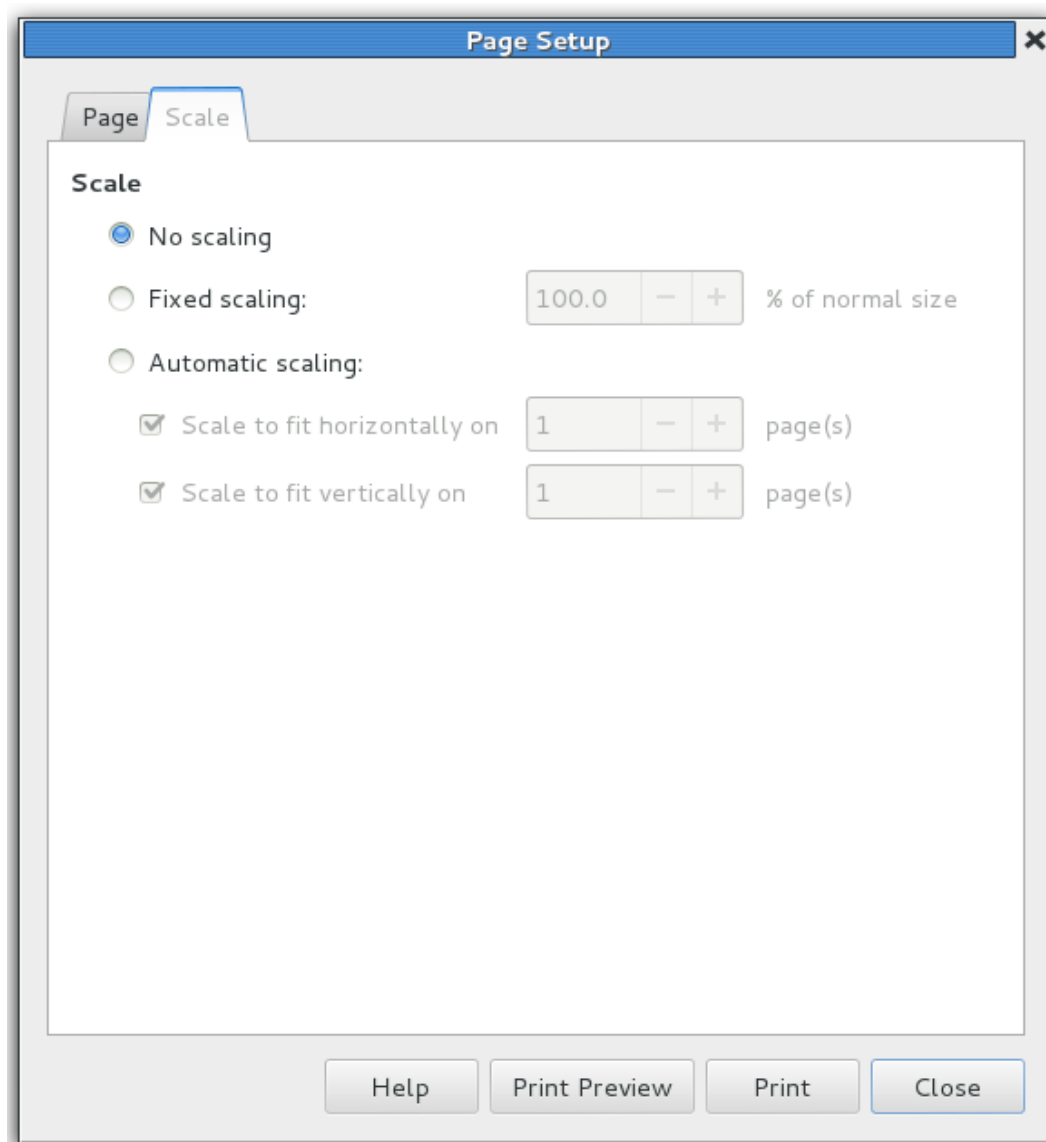


Figure 3.8: The Print Scale tab.

Chapter 4

Support.

4.1 To Ask a Question

If you choose Help → Ask a question, your mail client should pop up with a new message to the [Gnome Chemistry Utils mailing list](#).

Another way to get some help is to connect on the [#gchemutils](#) IRC channel on the irc.gimp.net network and ask your question there (if you are not alone on the channel).

4.2 To Find the Gnome Chemistry Utils on the Web.

If you choose Help → Gnome Chemistry Utils on the web, the default web browser should pop up and display the main page for the Gnome Chemistry Utils.

The main page is <http://gchemutils.nongnu.org> and the project page at Savannah <http://savannah.nongnu.org/projects/gchemutils>.

4.3 To Report a Bug

To report a bug, you must use the bug page for the Gnome Chemistry Utils at Savannah. You can access it by choosing Help → Report Bugs (hopefully you'll have only one at a time to report).

You can also use a web browser to go to the bug report page address directly. The bug repository is at <https://savannah.nongnu.org/bugs/?group=gchemutils>

Chapter 5

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