GChemCalc manual

Feedback

To report a bug or make a suggestion regarding the GChemCalc application or this manual, go to theGChemCalc GChemCalc home page.

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Abstract

GChemCalc allows you to evaluate some molecular properties.

Introduction

The GChemCalc application is a simple calculator for chemistry. It parses chemical formula to calculate raw formula, molecular weights, mass composition and isotopic patterns.

Chapter 1

Getting started

1.1 To Start GChemCalc

You can start GChemCalc in the following ways:

Applications list Choose “Chemical calculator”. It might be listed either in the Education or Science category.

Command line Type **gchemcalc** [formula], then press **Return**. [Formula] stands for an optional chemical formula.

1.2 When You Start GChemCalc

When you start GChemCalc, the following window is displayed:

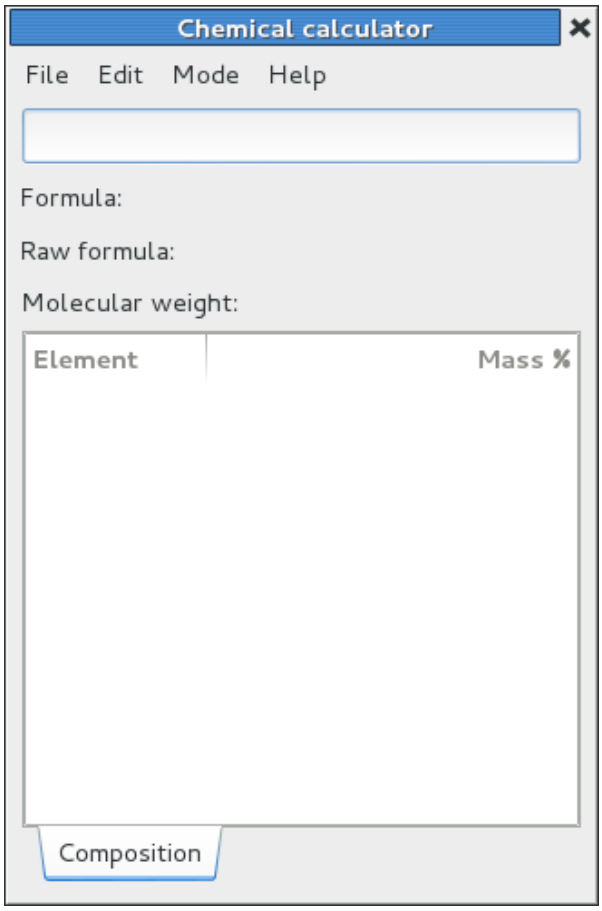

Figure 1.1: GChemCalc window

The GChemCalc window contains the following elements:

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

Formula entry This is where you can type a formula.

Results The next three lines give the entered formula as parsed by GChemCalc, the raw formula and the molecular weight.

Notebook The first page of the notebook gives the analysis as mass percent of the elements of the current formula. The second page displays the isotopic pattern. This page is hidden when the formula is empty.

Chapter 2

Usage

2.1 Entering a formula

Formulas can be entered from the command line, from GChemPaint, or directly in the formula entry.

When using the formula entry, just type a valid formula as in the following example:

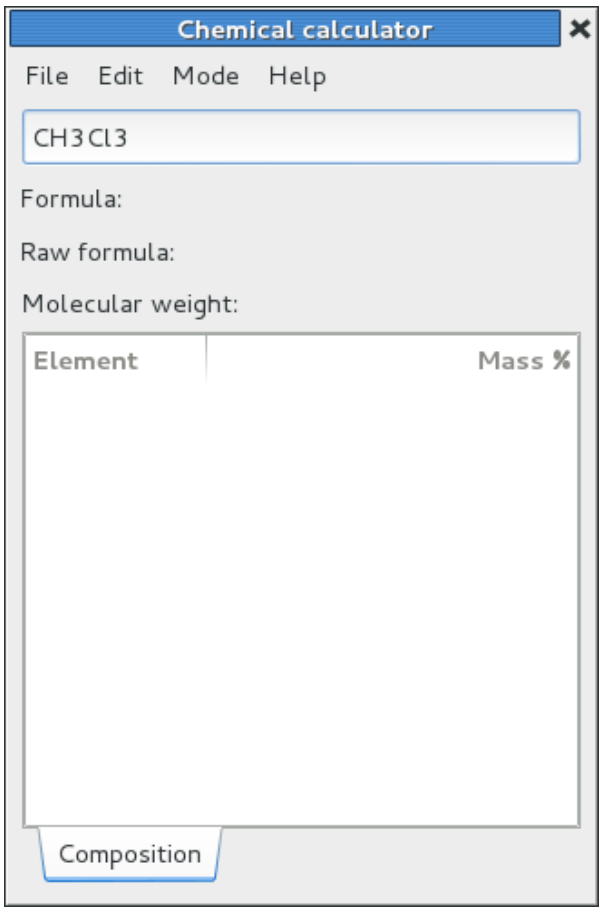

Figure 2.1: Entering a formula

After validating, if the formula has been succesfully parsed, you get:

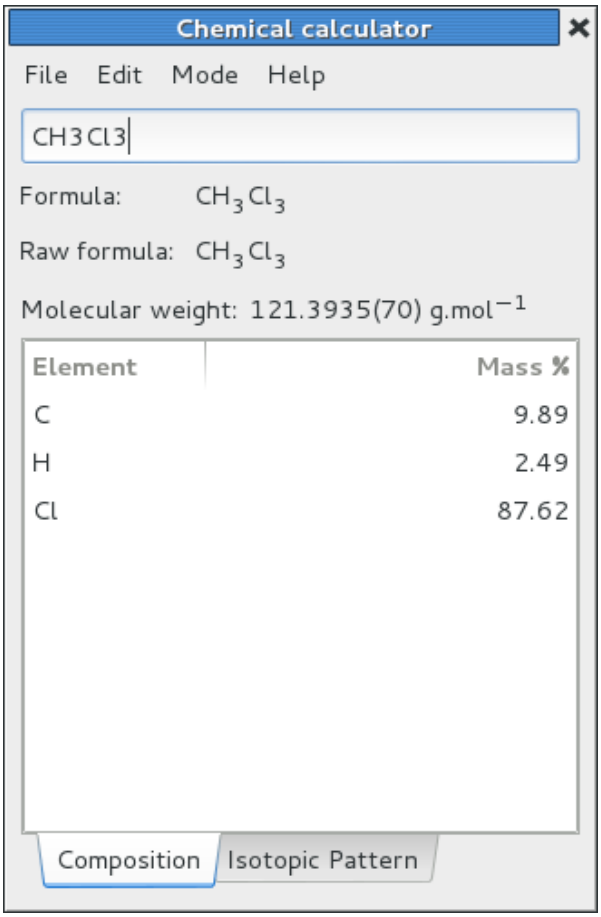

Figure 2.2: Results

The isotopic pattern is displayed on the second page of the notebook:

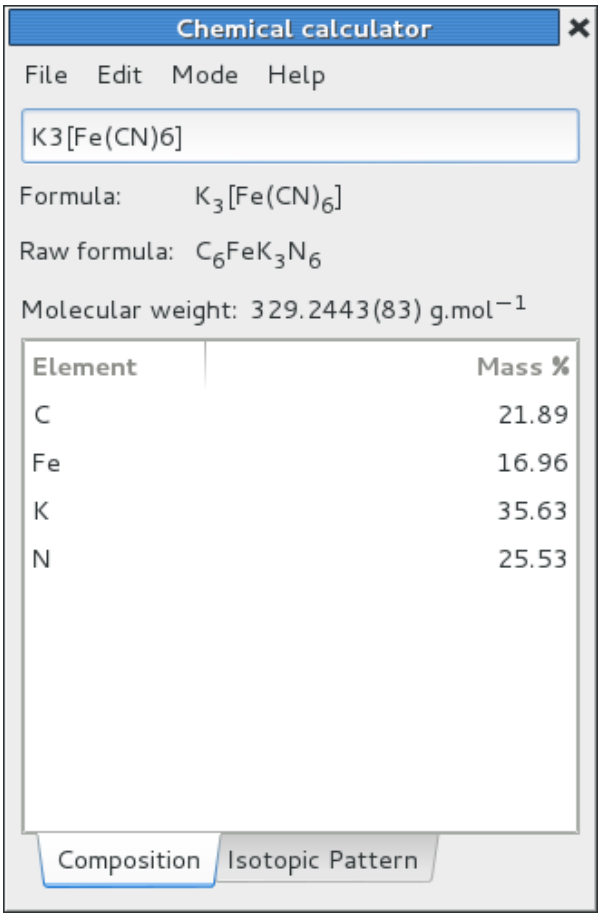

Figure 2.3: Isotopic pattern

If an error occurs while parsing the formula, a message box will pop up and the cursor will be moved in the entry to the error position.

2.2 Features

GChemCalc supports parenthesis and brackets to any level provided each one is matched as in the following example:

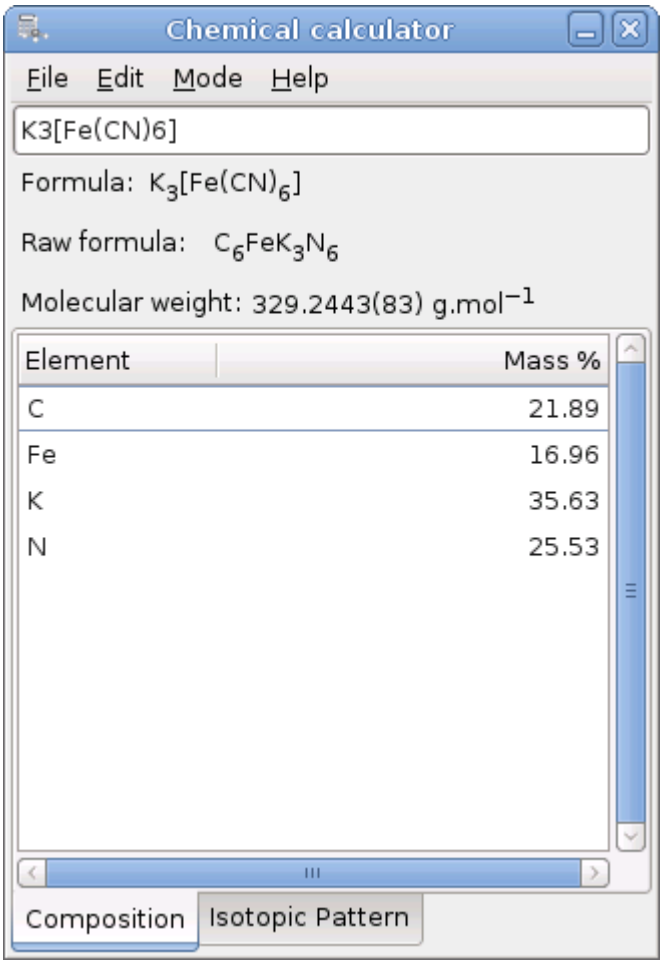

Figure 2.4: Using parenthesis and brackets

Abbreviations such as "Ph" for a phenyl substituant are supported.

This is also true for abbreviations such as Pr which might represent either a praseodymium atom or a propyl group. Three options are available in the Mode menu:

Guess GChemCalc try to guess if the symbol represents an atom or a group, PrCl is analyzed as propyl chloride, while $PrCl_3$ is praseodymium chloride; however, this method might fail in some cases such as $PrPr_3$ which will not be recognized as trypropylpraseodymium, at least with this version of GChemCalc.

Atom Ambiguous symbols are interpreted as atoms.

Nickname Ambiguous symbols are interpreted as groups.

Custom nicknames can be defined using the GChemPaint application.

2.3 To Print the Isotopic Pattern Graph

To print a isotopic pattern graph, choose File → Print....

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

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

2.3.1 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 GChemCalc

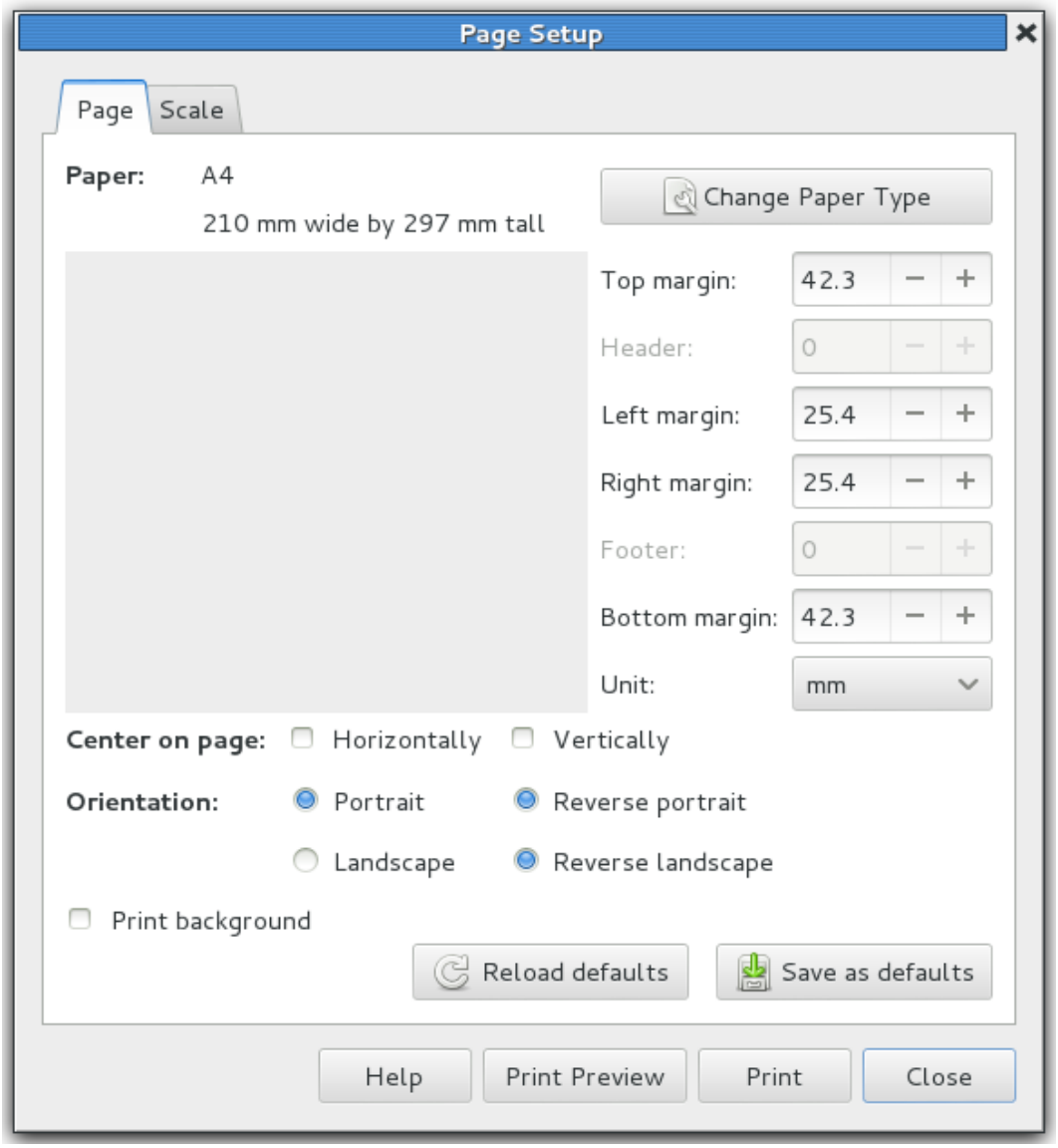

Figure 2.5: The Page Setup tab.

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 (none of the options is equivalent to no scaling).

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

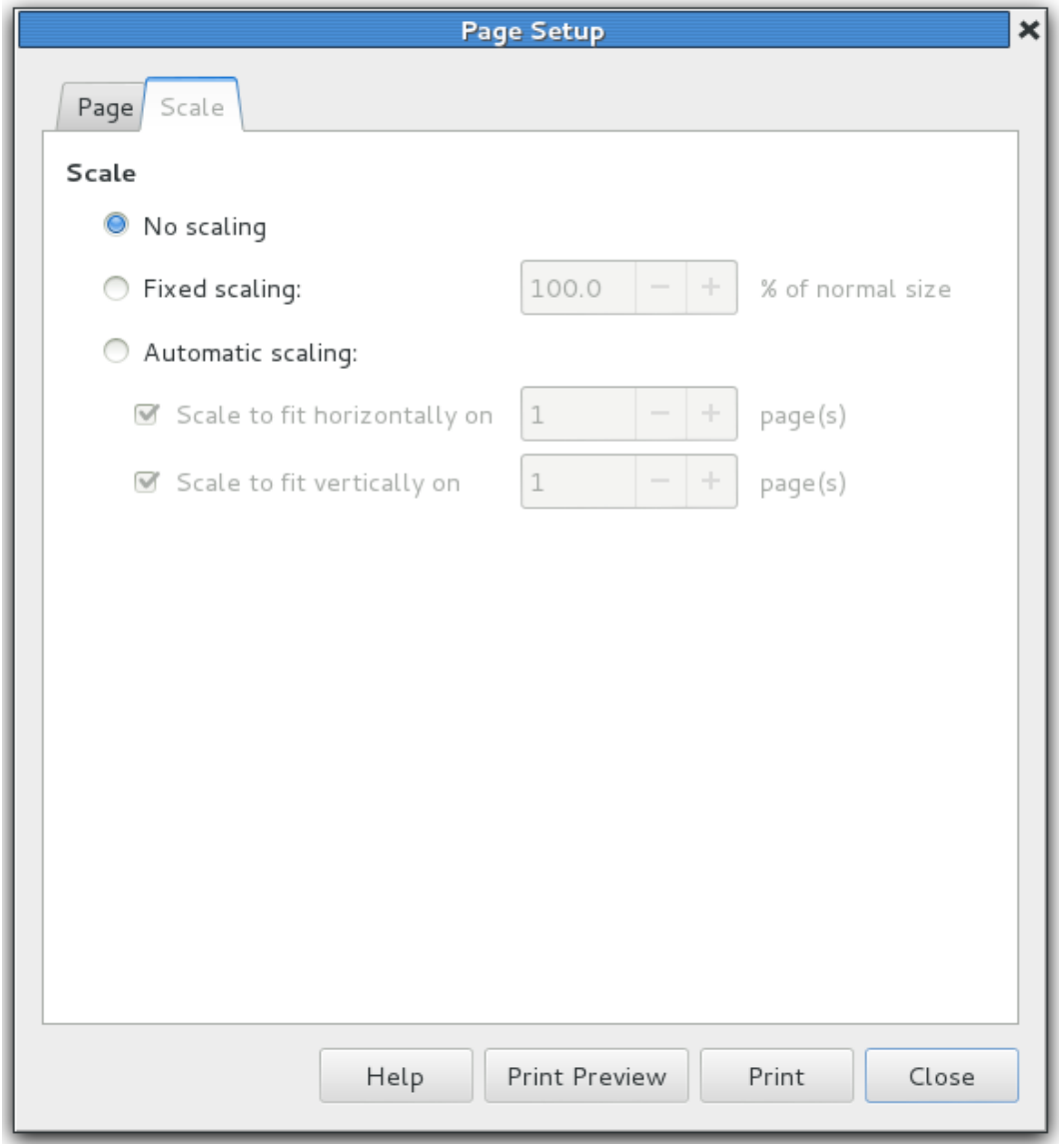

Figure 2.6: The Print Scale tab.

2.4 Export the Isotopic Pattern as an Image.

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

Available formats are SVG, EPS, PS, PDF, and the formats with write support in GdkPixbuf.

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

2.5 Copying the Isotopic Pattern Graph.

To copy the isotopic pattern graph, choose Edit → Copy and paste in the target application. Graphs will be copied as native graphs to Abiword and as svg or png data to other applications which support such formats.

Chapter 3

Support.

3.1 To Ask a Question

If you choose Help → Ask a question, your mail agent 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 channel at irc.gimp.net and ask your question there (if you are not alone on the channel).

3.2 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 Chemsitry Utils.

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

3.3 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 once to report).

You can also type the bug report page address directly in the browser. The bug repository is at https://savannah.nongnu.org/-bugs/?group=gchemutils

Chapter 4

License

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