

# **GChem3d manual**

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## **Abstract**

GChem3d allows you to display molecular structures.

# Introduction

The GChem3d application is a simple molecular structures visualizer.

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# Chapter 1

## Getting started

### 1.1 To Start GChem3d

You can start GChem3d in the following ways:

**Applications list** Choose “Molecules Viewer”. It might be listed either in the Education or Science category.

**Command line** Type `gchem3d`, then press **Return**.

### 1.2 When You Start GChem3d

When you start GChem3d, the following window is displayed:

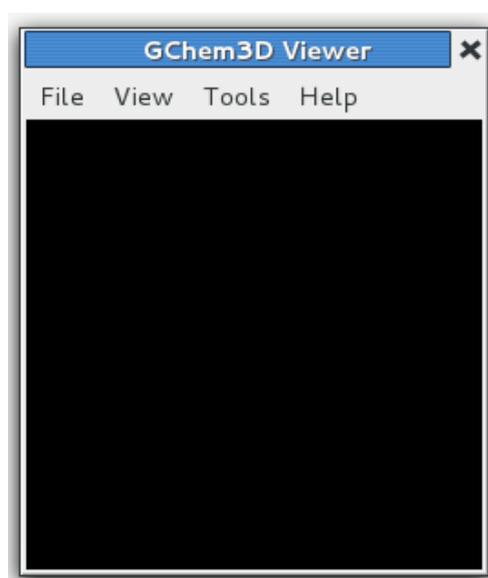


Figure 1.1: GChem3d main window

The GChem3d window contains the following elements:

**Menubar** The menus on the menubar contain all of the commands you need to work with files in GChem3d.

**Display area** The display area contains the contents of an opened file if any.

## 1.3 To Open a File

To open a file, choose File → Open to display the Open File dialog. Select the file that you want to open, then click OK. The file is displayed in the GChem3d main window.

GChem3d can open files on a distant server.

GChem3d can open several file formats. Available formats are:

- ChemML files (\*.cml)
- MDL MOL files, MDL Structure Data files (\*.mol;\*.sd;\*.sdf)
- PDB files (\*.pdb;\*.ent)
- XYZ Coordinate Format files (\*.xyz)

You can open multiple files in GChem3d. The application displays each file in its own window.

Recently opened file appear in the File+Open recent sub-menu.

A molecule can also be loaded from it's InChI or a SMILES representation as described in the [To Load a Molecule from a String](#) section.

## 1.4 To Open Multiple Files from a Command Line

You can run GChem3d from a command line and open a single file or multiple files. To open multiple files from a command line, type the following command, then press **Return**:

```
gchem3d file1 file2 file3
```

## Chapter 2

# Usage

### 2.1 To Save the View as an Image

To open a file, choose File → Save as Image... to display the Save as image dialog. Select a file name and, if wanted, a file type and a size, then click OK. Default image size is 300 pixels wide and 300 pixels high.

Supported types are VRML, Postscript, Encapsulated Postscript, PDF, and all types that GdkPixbuf can export. You'll find an exact list in the drop-down file type menu.

If no file type is specified, GChem3d tries to determine the type from the file name. If it does not succeed, the default type (VRML) will be used.

An appropriate extension will be added to the file name if none is found.

PostScript and PDF files can also be obtained with the [Print command](#).

### 2.2 To Load a molecule from an InChI or a SMILES

To import a molecule from a string, choose Tools → Import molecule... . A dialog box pops up:

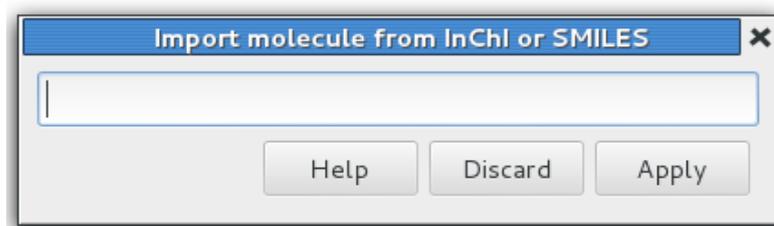


Figure 2.1: The string input dialog box.

You need to input a valid string such as this SMILES:

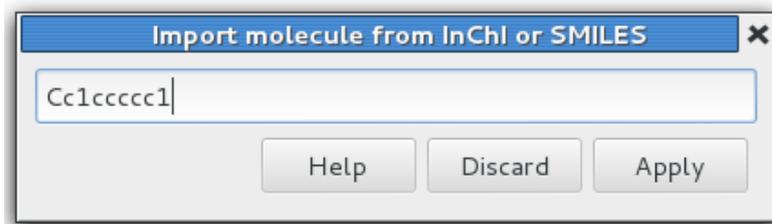


Figure 2.2: The string input dialog box with a SMILES inside.

Please note that if you use an InChI as input, you must not skip the “InChI=” prefix.

After activating the Apply button you get:

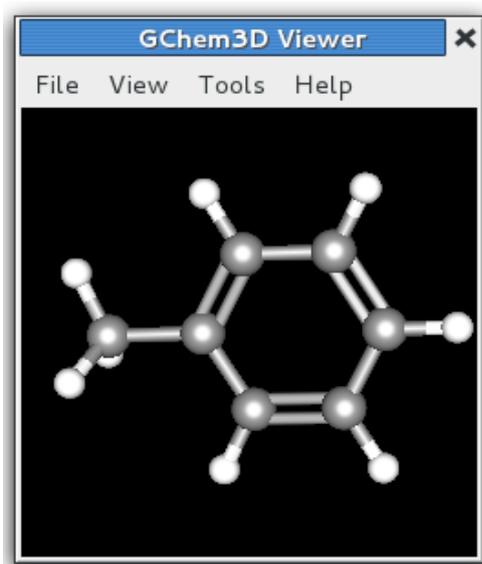


Figure 2.3: The 3D View.

## 2.3 To Use the Tools Menu with a molecule.

When a molecule is displayed, several menu items appear in the Tools menu:

**Open in GChemPaint** Opens the 2D editor **GChemPaint** with a copy of the molecule. The molecule has been converted to a 2D representation using the **OpenBabel** library.

With the *trans*-1,2-dimethylcyclohexane molecule, you get:

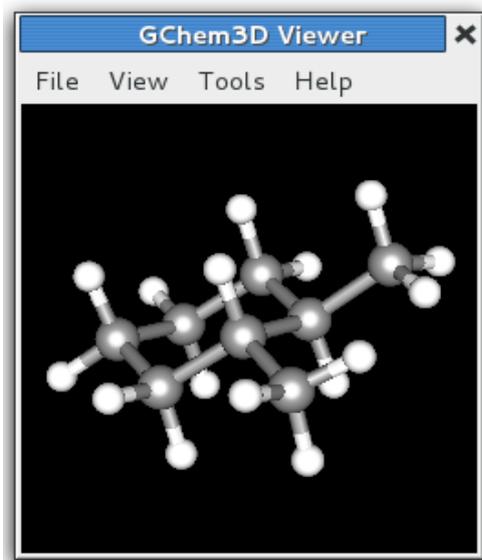


Figure 2.4: Initial view in GChem3D.

And after conversion in GChemPaint:

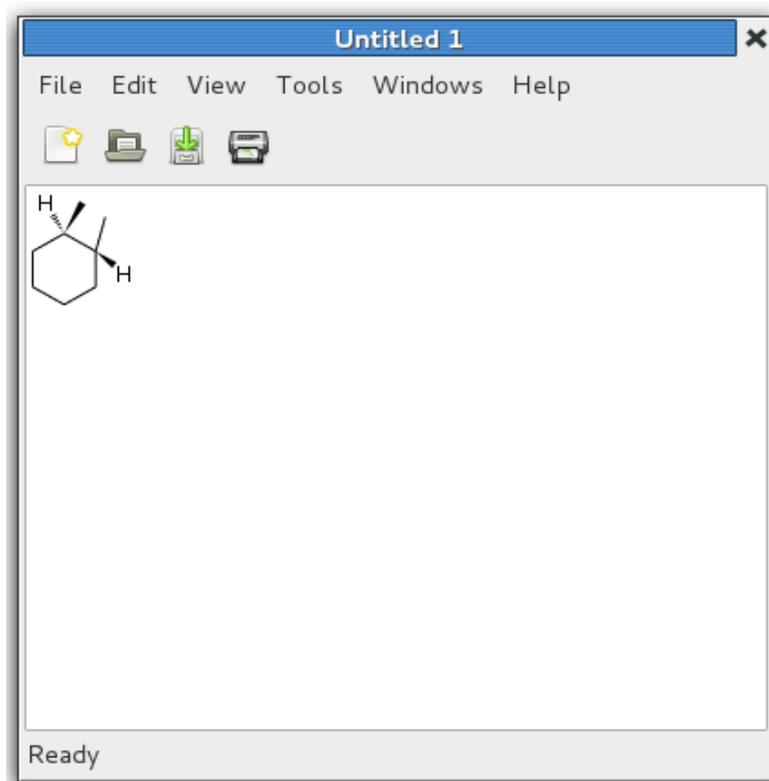


Figure 2.5: The molecule in GChemPaint.

**Open in GChemCalc** Opens the chemical calculator **GChemCalc** with a copy of the molecule formula and performs the available calculations. With the same molecule as above, you get:

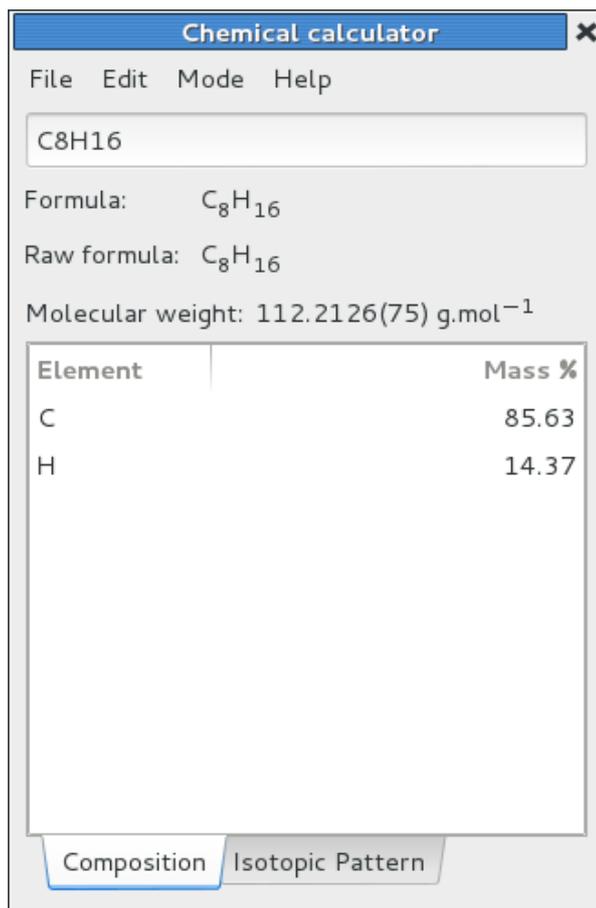


Figure 2.6: The molecule in GChemCalc.

**Generate InChI** Generates the InChI for the molecule and displays it in a popup window.

**Generate InChIKey** Generates the InChIKey for the molecule and displays it in a popup window.

**Generate SMILES** Generates the SMILES for the molecule and displays it in a popup window.

**Search in an online database** The molecule can be searched for in online databases, either predefined or user defined.

To add custom databases, you need to create an xml file listing them. The file must be named `.gchemutils/databases.xml` in your home directory.

Entries inside the file must be inside a `databases` top node, each entry being a `database` node with children `name`, `uri`, and `class`, like for the NIST webbook (which is predefined):

```
<database>
  <name>NIST webbook</name>
  <uri>http://webbook.nist.gov/cgi/cbook.cgi?Name=%K&Units=SI"</uri>
  <class>molecule</class>
</database>
```

where `%K` will be replaced by the InChIKey. You use the InChI, the code is `%I` and for the SMILES, `%S`.

The `class` node is for future usages and must contain "molecule".

## 2.4 To Print the View

To print a file, choose `File` → `Print...`

GChem3d uses a 300 dpi resolution when printing.

You might want to **change the background color** before printing.

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

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

### 2.4.1 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 GChem3d

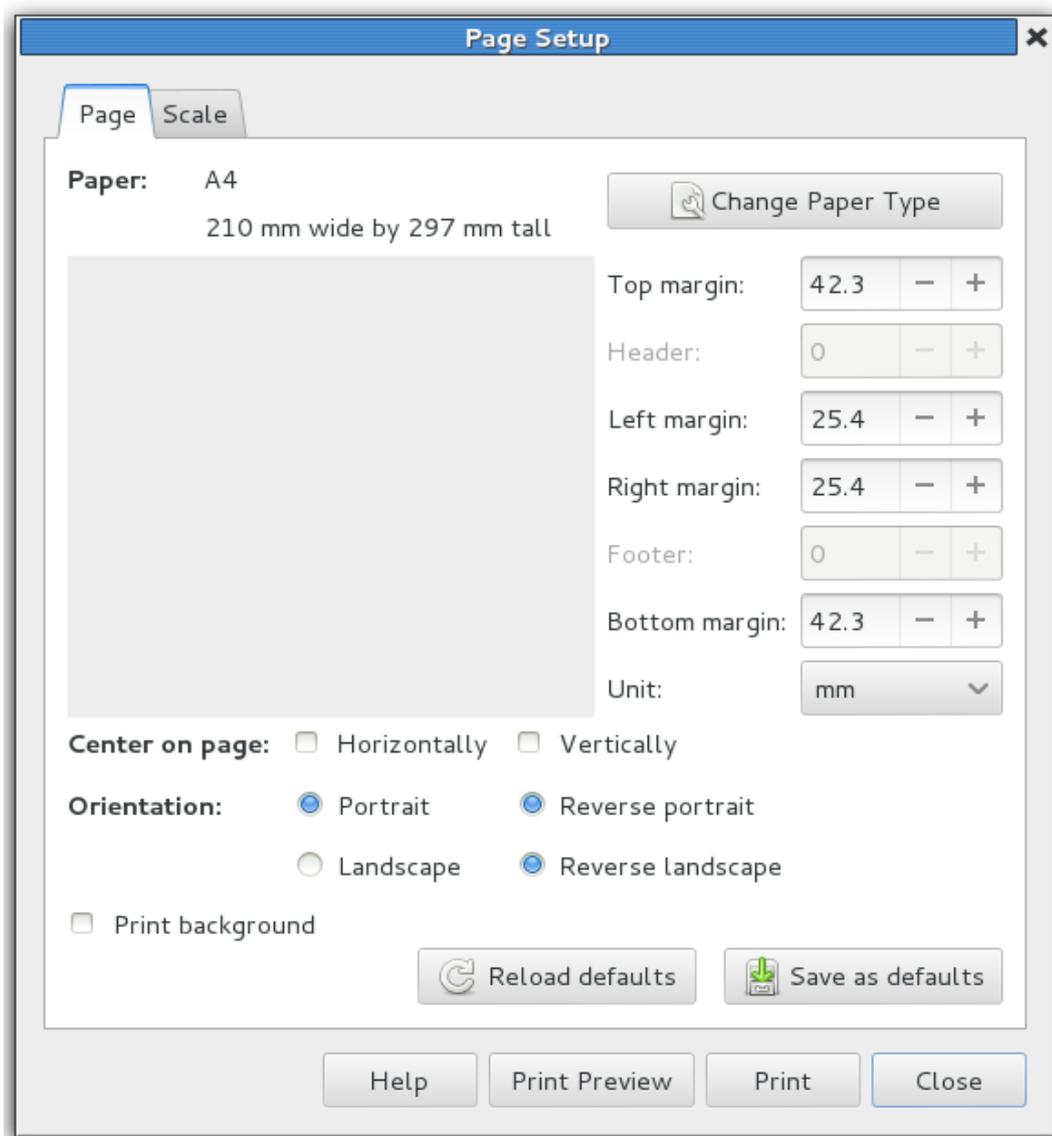


Figure 2.7: The Page Setup tab.

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

Printing to more than one page is not supported in this version of GChem3d

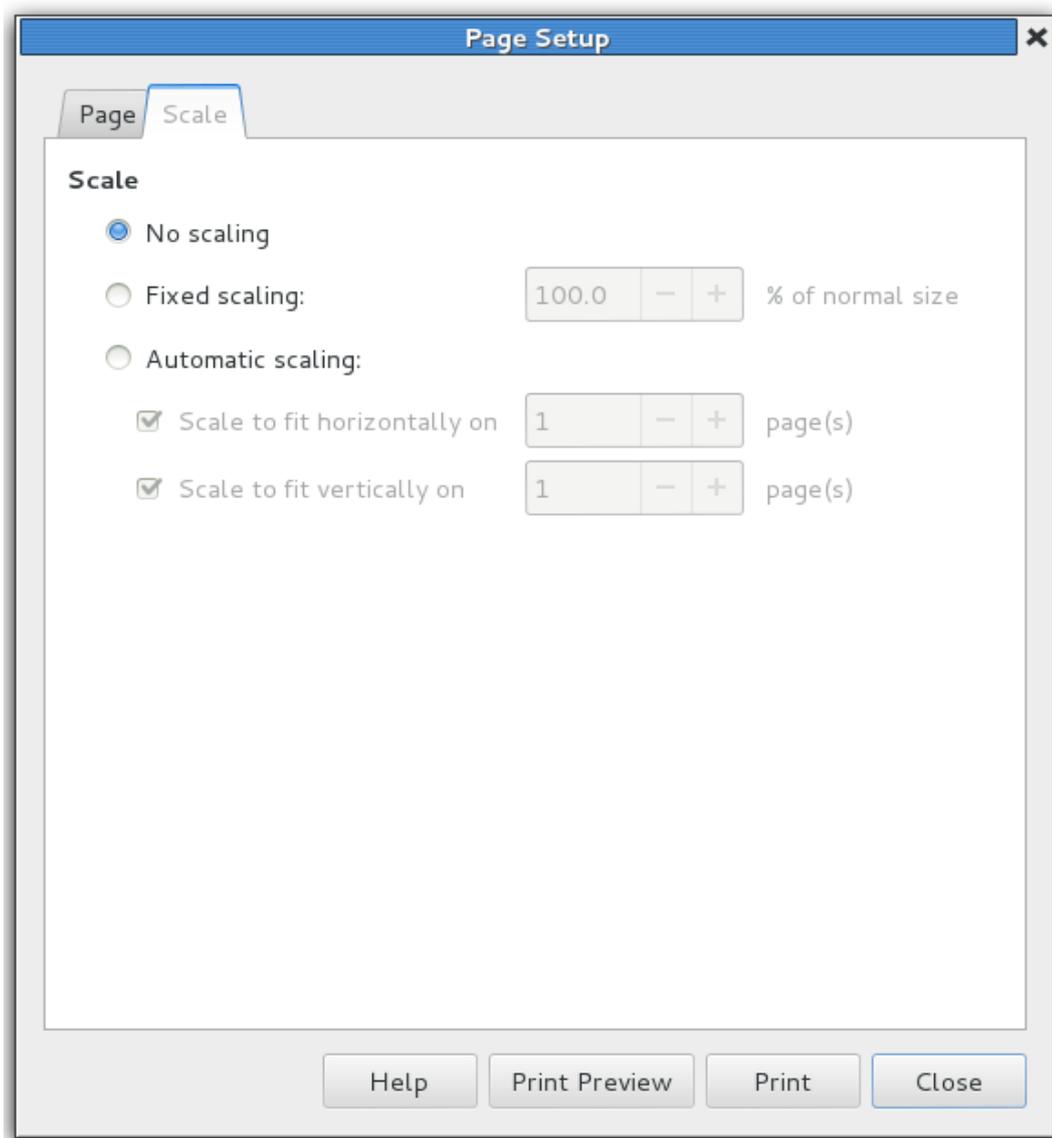


Figure 2.8: The Print Scale tab.

## 2.5 To Change the Model Options

GChem3d is able to display a molecule using four model types: the ball and stick model, the compact model, the cylinders model, and the wireframe model. The first one is the default. Multiple bonds are displayed as such in the ball and stick model.

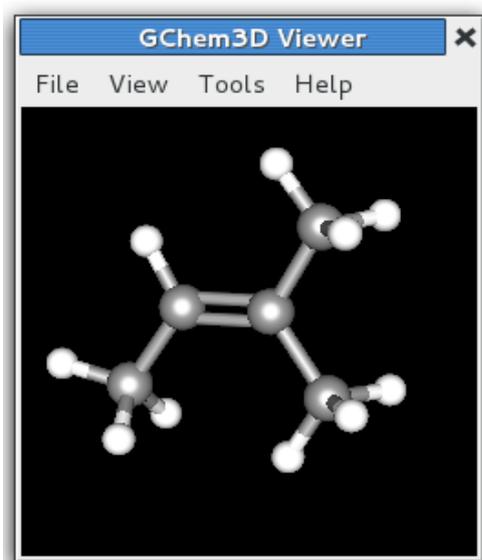


Figure 2.9: The Balls and Sticks model.

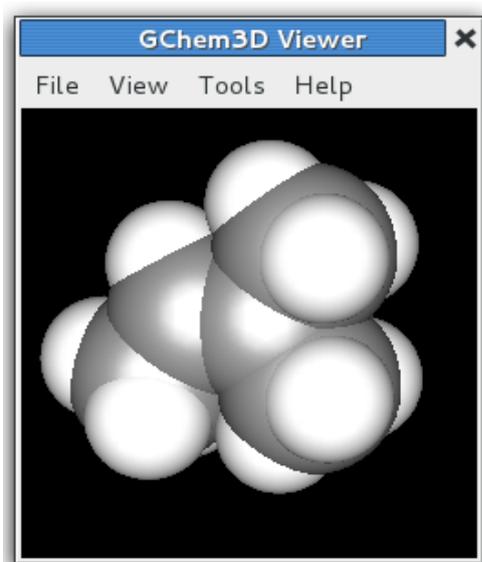


Figure 2.10: The Spacefill model.

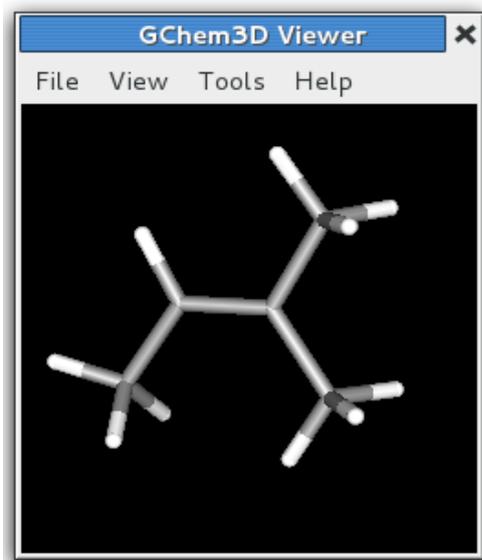


Figure 2.11: The Cylinders model.

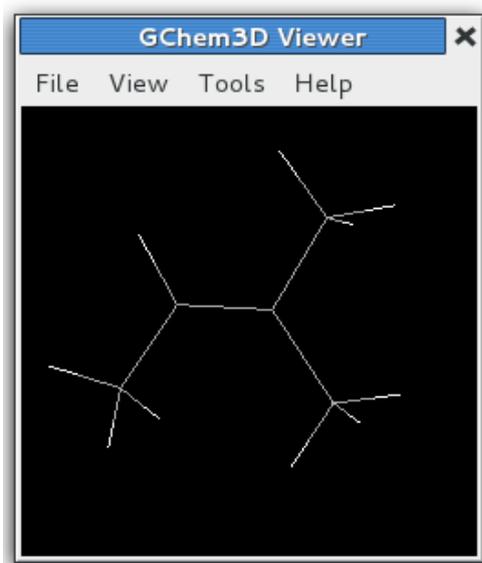


Figure 2.12: The Wireframe model.

To change the mode, choose either View → Balls and sticks, View → Space filling, View → Cylinders, or View → Wireframe.

The model can also be selected from the command line: `gchem3d --display3d=cylinders` or `gchem3d -d cylinders` will open GChem3d with the cylinders model active. The other models are entered as ball&stick, spacefill, and wireframe.

You can also change the orientation. Just click somewhere in the view and drag the mouse until you get the wanted orientation.

## 2.6 To Change the Background Color

To change the background color, choose View → Background color and select the appropriate color in the palette, or choose a custom color.

The background color can also be selected from the command line: **gchem3d --bgcolor=white** or **gchem3d -b white** will open GChem3d with a white background in windows. Recognized strings are black (the default), white, and #rrggbb where r, g, and b are hexadecimal digits.

## 2.7 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).

## 2.8 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>.

## 2.9 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>

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## Chapter 3

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