ChatGPT

Chemtool: Open-Source Chemical Structure Drawing Program (1998–2013)

Introduction

Chemtool is a free, lightweight 2D chemical structure editor for Unix/Linux systems (X11) using the GTK toolkit [1]. It was originally written in the late 1990s by Thomas Volk (then a chemistry/biology student at the University of Ulm, Germany) [2]. Released under the GNU General Public License (GPLv2) [3], Chemtool allows chemists to easily draw and annotate organic molecules on Linux (no native Windows or macOS support) [4]. Development of the "OG" Chemtool spanned from 1998 up to 2013, with Thomas Volk maintaining it until version 1.1.1, after which Dr. Martin Kroeker (University of Freiburg) took over as primary developer from version 1.1.2 onward [5]. The final stable release was **v1.6.14** in August 2013 [6], and no official updates have been published since. *(An experimental Windows build (v1.6.15 release-candidate) was later made available as a ZIP with a Chemtool.exe, essentially v1.6.14 plus minor fixes, but no fully new version was released [7] [8].)*

Features and Capabilities

Chemtool provides a focused set of tools for drawing structural formulas and chemical diagrams, with an emphasis on organic chemistry. Key features include:

- **Rich Bond Drawing Tools:** Chemtool supports a wide variety of bond types and styles needed for chemical structures. These include single bonds, multiple bonds (double, centered double, triple, quadruple), wedge and dashed bonds for stereochemistry, wavy lines, arrows (half-arrows, full arrows for reaction mechanisms), "wide" bonds, dotted lines, and even orbital lobe symbols [9] [10]. Bond angles can be constrained to common geometries – e.g. hexagonal (120°/60°), pentagonal (72°), 45°, etc. – to neatly draw rings and chains. In fact, rings of size 3–12 can be generated semi-automatically by drawing a single bond while holding the Ctrl key, which causes Chemtool to complete the ring in a chosen size and orientation [11]. Using modifier keys and mouse buttons, users can quickly change bond types (e.g. toggle a single bond to a double) or delete bonds, making the sketching process efficient [12] [13].

- **Text Annotations and Chemical Notation:** The program allows adding text labels (atom symbols, group labels, notes) with formatting for chemical notation. It supports subscripts and superscripts (via `_` and `^` syntax, e.g. `CH_3` for CH₃, `N^+` for N^+), italic or bold text for labels, and even Greek letters or special symbols (by switching to a symbol font mode) [14] [15]. This enables proper chemical formulas and charges (e.g. ⊕/⊖ as @+/@- in Chemtool) to be displayed. Text can be aligned left, center, or right relative to attachment points [16], and multiple font sizes and seven standard colors are available for use [17]. These capabilities let users annotate structures with chemical names, substituents, or mechanism arrows directly on the diagram.

- **Editing, Templates, and Utilities:** Chemtool provides basic editing operations and helpers to simplify creating complex drawings. It features essentially unlimited undo/redo for error recovery [18]. A "mark" tool allows selecting part of a drawing (by rubber-band box) and then moving, rotating, flipping (horizontal/vertical mirror), or scaling that fragment as a unit [19] [20]. Marked fragments can also be copied and pasted within the drawing [21], enabling reuse of common substructures. There are built-in **templates** for frequently used structures – e.g. common rings (carbocycles), sugar rings, heterocycles, and amino acid residues – which can be inserted from a template window with one click [22]. This saves time in constructing standard chemical backbones. A grid (square or hexagonal) can be toggled as a backdrop to help align atoms and bonds neatly [17]. Additionally, a companion command-line tool `cht` is included to calculate the molecular formula and exact molecular weight of the drawn molecule (or a selected fragment) [23]. This utility parses the Chemtool drawing file and outputs the sum formula (e.g. C_6H_6) and molecular mass, which can be invoked from within Chemtool or run standalone [24]. (The formula calculator was contributed by Radek Liboska [25] [26].) These features – from template libraries to on-the-fly formula calculation – illustrate Chemtool's focus on making chemical drawing fast and chemically intelligent [27].

- **Import/Export and Integration:** Drawings made in Chemtool can be exported to numerous file formats for further use in publications or modeling. Natively, it can save as **X bitmap** images and (with the help of external tools) export to **PNG** or **EMF** image files, **SVG** vector graphics, **XFig** `.fig` files, **EPS** (encapsulated PostScript), **PiCTeX** (LaTeX picture environment code), and MDL **MOL** files [28] [29]. It can also output to **PDB** format (Protein Data Bank file) for compatibility with molecular modeling software [23]. Many of the export functions leverage Brian Smith's **Transfig/fig2dev** utility behind the scenes [30]. For example, Chemtool's "Export" menu will call `fig2dev` to produce EPS, PDF, PNG, or PiCTeX output, meaning that having the `transfig` package installed extends Chemtool's output capabilities. If **OpenBabel** (an open-source chemistry file conversion toolkit) is available, Chemtool adds an option to export or import **any format** supported by OpenBabel, greatly expanding the program's interoperability [31] [32]. Chemtool can directly **import** structures from PDB or MOL files as well – when a 3D structure is loaded, it appears as a rotatable preview (in a temporary blue overlay) which the user can orient in 3D before Chemtool "flattens" it into a 2D sketch [33]. This is useful for taking 3D models and generating a 2D structural diagram. (Chemtool discards certain labels like explicit carbons on import to clean up the diagram [34].) The program also supports direct printing of drawings to PostScript printers or print queues. Since version 1.6, it can embed a TIFF preview image into EPS files for compatibility with office suites that cannot render raw PostScript on screen [35] [36] – a helpful feature for using Chemtool graphics in word processors or presentation software.

- **User Interface:** The Chemtool interface is simple and purpose-built for chemical drawing. The toolbar provides buttons to select bond angle modes (e.g. hexagon, pentagon orientations), bond types, text alignment and style (normal/bold), bond color, and various editing tools [16] [37]. For instance, one can choose an initial bond angle mode (e.g. 120° hexagon mode) and draw a chain of bonds at fixed angles, then switch to another mode or freeform as needed. Other toolbar buttons activate the selection/mark tool, move/rotate/flip tools, copy, scale, bracket-addition (to add parentheses or brackets around a group), and a "clean-up" tool (depicted as a broom) that automatically deletes any overlapping bonds and tidies near-straight lines to perfect horizontal/vertical. A text entry box is provided to input custom labels or formulas to place on the diagram. Overall, the UI is optimized for quick sketching: one typically selects the bond tool or text tool, clicks

to draw or label, and uses keyboard shortcuts for common atoms (e.g. pressing "C" places a carbon label, "O" for oxygen, etc.) [38]. The learning curve is modest, and a detailed **user manual** (`using_chemtool.html`) has been provided with examples of all features. Chemtool's interface may appear basic by modern standards, but it is effective for creating clear structural formulas for reports and publications [22] [39].

Screenshot of the Chemtool application interface drawing a chemical structure (example from Softpedia)

(Image: Chemtool running on Linux – note the toolbar with bond types and tools, and a sample molecule drawn on the canvas.) [40] [41]

Usage and Workflow

In practice, Chemtool is often used in combination with other tools to prepare publication-quality figures. For drawing tasks specific to chemical structures (bonds, rings, stereochemistry), Chemtool provides all necessary functionality. For more general diagram elements (shapes, arbitrary arrows, text annotations not tied to atoms), the author recommends exporting the Chemtool drawing to **XFig** format and then using the XFig program to add further embellishments [42] [43]. This is because XFig is a general-purpose vector drawing tool, while Chemtool focuses on chemical drawing conventions (e.g. fixed bond angles and "chemical" line styles). The Chemtool manual explicitly notes that features like free-form lines or complex drawing shapes are better handled in XFig, which complements Chemtool's niche [43]. Similarly, one can export a Chemtool diagram to SVG for refinement in Inkscape or to LaTeX (PiCTeX code) for inclusion in TeX documents. Chemtool's output options give flexibility depending on the user's workflow – whether the end goal is a printed paper, a presentation slide, or a figure in a word processor, the structure can be drawn in Chemtool and then converted to the appropriate format.

To use Chemtool, one typically sketches the molecule by clicking to draw bonds and rings, adds any necessary labels (using the text tool or keyboard shortcuts), and then saves or exports the figure. The program's simplicity means that drawing even complex organic molecules (with rings, substituents, stereochemistry, etc.) is relatively quick. For instance, to draw a cyclohexane ring, you could select the hexagon mode and draw one bond – Chemtool will auto-complete a six-membered ring [11]. You might then switch to the wedge bond tool to add a wedge bond indicating a substituent pointing out of plane. After labeling atoms or groups (e.g. adding "OH" on a certain carbon by typing it), you could mark a portion of the structure and copy-paste it to duplicate a common subunit. Chemtool's template menu further streamlines adding standard components (like a benzene ring template or a sugar). Once the structure is complete, you can calculate its formula/mass with **Tools → Sum Formula**, or directly export it. The entire process is optimized for speed and clarity, making Chemtool a handy tool for chemistry students and researchers preparing figures. Notably, Chemtool's files can also be saved in its native format and reopened for editing later, or combined (you can "Add" a previously saved molecule into the current canvas to build larger assemblies).

Development History and Status

Chemtool has its roots in the late 1990s free-software chemistry community. The first version was released around 1998 by Thomas Volk, addressing the need for a free X11 chemical drawing tool on Linux. Volk maintained and improved the program through the early versions. In the early 2000s, responsibility

transitioned to Martin Kroeker, who continued development from version 1.1.2 onward [44]. Under Kroeker's maintainership (with contributions from others like Radek Liboska and Michael Banck [26]), Chemtool saw numerous feature additions – such as support for more bond types, better text/symbol handling, template molecules, OpenBabel integration, and expanded export formats – as well as translation of the interface (Chemtool has been localized to multiple languages, including German, French, Czech, Polish, etc., as evidenced by included `.mo` files [45]). The version numbers progressed through the 1.5.x series and into 1.6.x by the 2010s. The **last official release was 1.6.14**, dated August 13, 2013 [6], which was an interim update fixing a crash in the fig2dev-based output functions. Around that time, a **Windows port** was experimentally compiled – an official development page referenced a *Chemtool 1.6.15 release candidate* as a test build for Microsoft Windows, essentially the same code with minor tweaks for portability. This Windows test version (packaged as a zip) allowed Chemtool to run on Windows, albeit not as polished as on Linux [7] [8]. However, after 2013 there have been no new releases or major code commits from the original authors. The Chemtool project is thus considered **dormant**; its website at the University of Freiburg still hosts the source and documentation, but no further development has occurred beyond minor packaging updates by Linux distributors.

Chemtool **continues to be available** via Linux distribution repositories (Debian, Fedora, etc. still carry the 1.6.14 version in their science/chemistry package collections [46] [47]). Enthusiasts have also mirrored the source on platforms like Codeberg and GitHub for preservation, but these are not "new" projects – just the original Chemtool codebase [48]. No fork has emerged that surpasses Chemtool or significantly modernizes it; instead, other independent chemistry drawing programs (such as BKChem, XDrawChem, GChemPaint, etc.) have filled the niche in subsequent years. For those specifically seeking *"Chemtool"*, the **original Chemtool (1998–2013)** remains the reference point. It is the program authored by Volk and Kroeker, as opposed to unrelated software of similar name (e.g. similarly named student projects or libraries on GitHub, which are not derived from this Chemtool). In summary, Chemtool is remembered as a nimble, no-frills chemical drawing tool from the turn of the century – one that served a generation of Linux-using chemists and still accomplishes basic structural drawing tasks today, even though its development story effectively concluded in 2013.

Sources

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