BKChem

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by Beda Kosata

Table of Contents

List of Tables

Foreword and Warning

I am not a programmer by training. Programming is just my hobby and I am doing it for fun. Therefor you should not expect BKChem to be perfect or even usable. The coding style is probably horrible and trying to read the code may seriously affect your mental health :)

You are however welcome to read the code, modify it and send me suggestions or patches. I'm still learning. On the other hand don't flame me about the style - you have been warned.

Any reports on bugs are also welcome (especially those with suggestions on their sources or solutions).

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I. Users Guide

Chapter 1. Introduction

BKChem is a chemical drawing program written in Python. The documentation as well as the program itself are in constant development. Therefor this manual is not meant to be complete, but rather tries to cover the very basics and the things that are not easy to find out without help. On the other hand many things are so self-evident that it would be useless to describe them. If you find that something you would like to know is not described in this manual, please email me to <beda@zirael.org>.

Chapter 2. Drawing

2.1. Introduction to the terms

Before we begin I should explain some terms that are used in the documentation and in the program itself.

Table 2-1. Used terms

Term	Definition
item	Any single undividable piece of the drawing - atom, bond, arrow point, plus. Not a molecule or arrow (see container).
container	Containers serve as a storage place for items (e.g. molecule stores atoms and bonds). Further I will use the term container also for texts and pluses even if they are also items (If it does not make sense to you don't just ignore it). As a synonym for container I will also use object or top-level object.
focus(ed)	Focused items are those that have a mouse pointer over them. The focus is usually visualized by some change of the item (e.g. circle drawn around atom, grey background of text etc.)
select(ed)	In contrast to focus, to select an item the user must take some action (usually click the mouse while the pointer is over an item (it is focused). The focus follows the mouse pointer, the selection is permanent until some action that unselects the item is performed. In contrast with focus it is possible to have more selected items.
mode	BKChem has several modes for different operations (e.g. for drawing molecules, drawing arrow, text, rotating existing objects). You select the mode by selecting one of the buttons on the top of the application window. You can find more on individual modes in the following chapters.

2.2. Simple drawing

2.2.1. Bond-by-bond drawing

The bond-by-bond drawing in BKChem is performed in the "draw mode".

The drawing is realized in a very intuitive way. You can just click on the drawing canvas and two atoms with a single bond between them will appear. By default the atoms are carbons and their symbol is not drawn. When you change the atom symbol to something else the symbol will appear. To attach more atoms to the currently drawn two, just focus one of them and click a mouse. By default the new atoms are added so that the new bond has angle of 120 deg. If you want to change that you can instead of a

click on focused atom use dragging. Press down a mouse button on a focused atom and without releasing it move the mouse. You will find out that the new bond is drawn in a direction of your mouse move and keeps moving while you keep dragging. To help you with precision of the drawing, there are several possible resolutions of the angle produced by dragging. The default is 30deg and is suitable for usual drawing (perfect for 6 membered rings). The resolution of 18deg is great for five membered rings and the others (6 and 1) are for finer work. For completely freestyle drawing use the "freestyle" submode.

To create double or triple bonds, just click on a bond in a "draw mode" and the bond order will increase by 1. After triple bond it will fall back to simple bond. This way you can also change the centering of the double bond (whether the two lines that form double bond will be centered and when not on which side the second line will appear). If you only want to change the centering of double bond you can just click it while holding "Shift" key.

By changing the bond type of drawn bonds you can create stereo-bonds.

2.2.2. Templates

BKChem comes with set of ready-to-use templates of common rings. To use them just select the "template mode" and then select a template.

The behavior of template depends on where you place it. Clicking on the canvas just creates the molecule from the template. Clicking on atoms or bonds attaches the template to the existing molecule in different ways (depending on whether you clicked bond or atom and whether the atom had one or more other bonds) - just try it to see.

2.2.3. Arrows

For drawing of arrows use "arrow mode". The way to draw arrow resembles bond-by-bond drawing of molecules. The arrow can be extended from both sides points can be even inserted inside the arrow. To draw arrows in different than horizontal position used the dragging while drawing.

You can select on which side the arrow-head will be drawn by clicking the arrow (the line, not the point) in the arrow mode. The arrow-head position will cycle in the start-end-both-none cycle (so you can use the arrow also for drawing lines).

To change the appearance of existing arrow you can move individual points (after you select them - see the following parts of this chapter.

2.2.4. Text

Most of this section applies not only to texts but also to atoms that have visible text. To create or modify the text use the "text mode". The text can be set in any mode (there is a difference between setting and modifying text - when modifying text you can just change it, when setting it you have to retype the whole sequence).

2.2.4.1. Text formatting

To give the user a simple way to alter the font properties of text (italic, bold, subscript and superscript) the text is entered as an XML fragment. You do not specify the enclosing tag (this is done automatically by the program), just the formating. For instance the text "hi, are you ready to rock?" will display "are you ready to" as italic and "rock" as bold-italic. For subscript and superscript use <sub> and <sup> respectively.

When using XML formating there is a problem with using characters as < and & because they are treated as special in XML. When you enter some text such as "a<b" that cannot be parsed as XML, the program will automatically "escape" all the special characters, thus giving you the right result. When you need only some of the special characters to be escaped (e.g. for <i>a<b</i>" you want to escape the < only in the "a<b") you must do it manually. This means entering an "escape sequence" instead of the special character. For "<" use "<" and for "&" use "&" (and "&" for "&" :). Easy, isn't it?

2.2.4.2. Setting and modifying text

When you hit a "Space" button with some atoms or texts selected or when you click an atom or text in "text mode" or click the canvas in "text mode", the "edit pool" will be activated letting you enter your text. To apply the entered text hit "Enter" or press one of the buttons on side of "edit pool". To cancel the action hit "Escape". The three buttons are used for setting text in different modes. The "Set" button serves for applying the text just as it was entered, "Set & Interpret" will search the inner database of BKChem to find if the entered text has some known interpretation. The "Sub-numbers" is used to turn all numbers in subscript and is useful for molecular formulas that are not known to BKChem.

2.3. Modifying the drawing

To manipulate the items use the "edit mode". This mode is used for moving items or containers, selecting items etc.

2.3.1. Selection

To select an item just click it in the "edit mode". By default selecting an item unselects all previously selected items. To change this, hold the "Shift" key while clicking the items.

By dragging a mouse with button-1 down and nothing focused you can select all items in a rectangle. The "Shift" key works in the same way as in individual selections.

2.3.2. Moving objects or items

There are two different ways of moving objects or items. The first is used for moving of arbitrary number of items. Just select them and then catch one of them with mouse and drag them.

For moving of one object (container - molecule) (which is very usual situation) you don't need to select it. Just catch some *unselected* item from this object and drag it. (Note: You can see that behavior of dragging items with mouse depends on whether the item was or wasn't selected.) (Tip: The moving of a molecule in this way performs much better, so use it. When moving a huge number of individually selected items the dragging can be horribly slow.)

2.3.3. Deleting items

You can delete selected items in any mode by simply pressing "Delete" key. Atoms are deleted with their bonds and all orphan atoms (atoms with no bonds) are also deleted. When necessary the molecule is after deletion of some atoms split to two or more separate molecules.

> **Tip:** Newly created atoms or other items are automatically selected. Thus if you want to delete atom just drawn, simply press the "Delete" key.

2.3.4. Aligning

To align containers, select them and then use either the "align menu" or key-binding (C-a 'x'; where 'x' is one of 'tblrhv' - 't' stands for 'top', 'b' for 'bottom', 'l' for 'left', 'r' for 'right', 'v' for 'vertical center' and 'h' for 'horizontal center'). E.g. - "C-a b" moves all selected container (containers with at least one item selected) down so that their bottoms are in line.

2.3.5. Modifying item properties

You can change various properties of selected items by right-clicking any of them. A dialog window will appear that will let you do that.

2.4. Key bindings

In the menu there are accelerator keys displayed on the right side of some of the commands. You can use these key sequences as shorcuts to trigger the respective actions without having to go to the menu.

The style of key bindings is very similar to that of Emacs. So if you are familiar with this concept (you know what "C-x C-f" means and how does it differ from "C-x f") you can skip this chapter. If you know nothing about "C-x C-f" then here is a short intro.

Each key-sequence can be composed from any number of individual keystrokes. Each keystroke than consists of optional modifier(s) and a key. The modifiers are "C" for "Control", "M" for "Meta", "A" for "Alt" and "S" for "Shift". For example "C-x C-f" is composed of two keystrokes. The first part tells you that you should press "x" while holding "Control" ("C"). Then, to finish the sequence, you have press "f" together with "Control" again. On contrary the sequence "C-x f" has the same first keystroke but before you press the "f" you must release the "Control" (otherwise you will end up with "C-x C-f"). It is also possible to have more modifiers in one keystroke - e.g. "C-M-S-k" means that you have to press "k" while holding simultaneously "Control", "Meta" and "Shift" keys. The best way to get used to this concept is by practice. So try it inside of BKChem or get Emacs.

Chapter 3. Saving files

3.1. Native formats

Native format of BKChem is based on XML and is called CDML (chemical drawing markup language). This format is, on contrary to CML (chemical markup language) which is designed to describe the chemistry from the semantic point of view, designed to describe the chemical drawing from the perspective of representation.

CDML is however just internal format of BKChem and does not have any broad acceptance. To use the graphical output of BKChem it was necessary to export the data into some standard graphical format, preferentially SVG. This approach has however disadvantage that it forces users to maintain two versions of each document, one with data for BKChem and one with their graphical representation. Fortunately it is possible to embed foreign data into SVG and because SVG is ideal format for vector graphics I have embedded CDML into it. This way we have format (available from version 0.1.1) that can be immediately viewed in SVG enabled programs and still has the data necessary for right interpretation by BKChem. To distinguish this new format from normal SVG I use the term CD-SVG.

This means that you can store the drawings you create in BKChem in two formats - CDML and CD-SVG. Both these formats are also available in their gzipped form (compression by gzip is almost standard way to make XML files smaller) which needs usually only 10-25% of the space needed by the unzipped form. Preferred file format is CD-SVG or if you need smaller file size its gzipped form. If you don't need the SVG representation you can also use the pure CDML. (Export to pure SVG is also available).

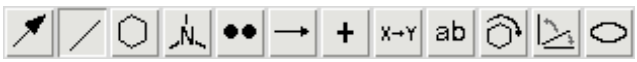
3.2. Export formats

In time of writing of this paragraph BKChem supports export only to SVG (see the section above for more information on BKChem and SVG). There are other exports available which are only experimental and incomplete. These are PNG (cannot export text), PostScript (problems with right postscript font selection) and PovRay (just a funny export not intended for something serious (the rendered scenes can however be very nice)) - see http://www.povray.org for more information about PovRay.

Chapter 4. Modes

Central part of the functionality of BKChem is provided by the so called modes. There is always one active mode, which determines how the objects respond to user actions. You can choose the mode on the Figure 4-1.

Figure 4-1. Mode selection panel



II. Programmers Guide

Chapter 5. Intro

Well, sure there will be some info on BKChem structure somewhere in the future. But for now I am too busy with other more interesting and important things.

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