



Manual

Structure and Reaction Editor

Version 2.0

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1 Introduction

ICEDIT is a powerful chemical structure editor, which is available as (i) Windows application, (ii) applet for all platforms supporting Java and as (iii) enhanced Java applet for web applications.

Furthermore, the integration of ICDIT in ICREDIT allows rendering as well as editing functionalities of chemical structures and reactions in any HTML document.

- **Windows application:** The ICDIT application offers full editing functionalities (chemical as well as display functionalities). ICDIT is a registered OLE-Server and therefore, it allows the integration in MS Office (Word, Excel, Access and PowerPoint) and in any other OLE-Client.
- **Java applet:** The ICDIT Java applet is an Internet browser based query editor for the input of chemical structures and reactions. It is downloaded on the fly and therefore, it does not have to be installed on the user's computer.
- **Enhanced Java applet:** The ICDIT enhanced applet is a Java applet with extended functionalities like full superatom support, which can be used as front end in web applications managed by a Servlet container like Apache Tomcat.
- **ICREDIT:** The trusted applet ICREDIT is an Internet browser based combination of rendering and/or editing chemical structures and reactions. For edit functionalities an ICDIT application installation is required. Therefore, ICREDIT does only work on Windows based systems.

1.1 Overview

Support of	ICEDIT application	ICEDIT applet	Enhanced IEDIT applet
Drawing of structures, reactions and fragments	+	+	+
Atom query features	+	+	+
Bond query features	+	+	+
Reaction query features	+	+	+
R-group query features	+	+	+
Integration in web applications	+ ¹⁾	+	+
Superatoms	+		+
Calculation of molecule values	+		
Display features	+		
OLE functionalities (MS Office integration)	+		

1) ICREDIT offers the opportunity to integrate the IEDIT application in web applications.

1.2 ICEDIT Windows Application

1.2.1 Functionality

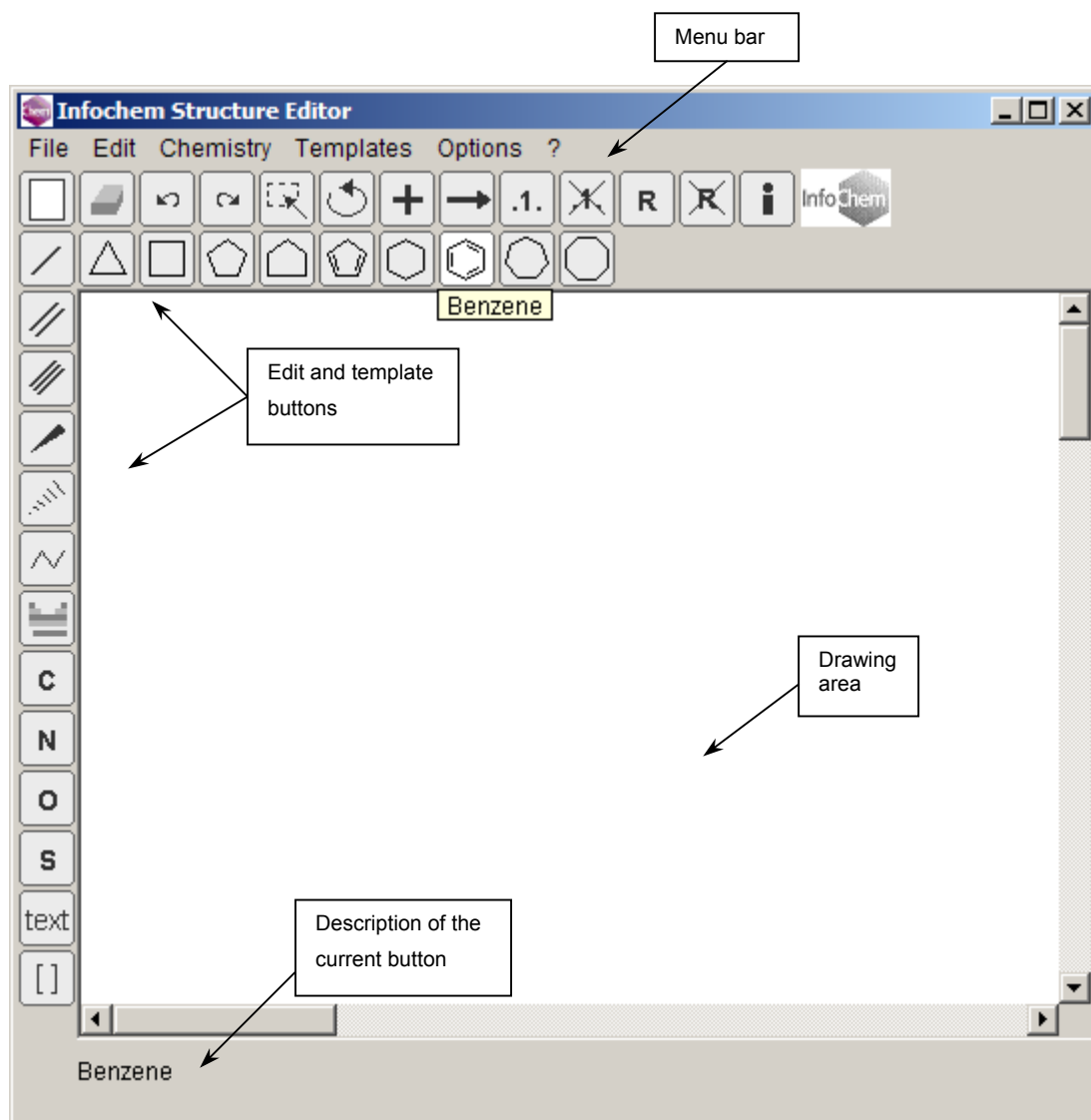


Fig. 1: The ICEDIT Windows application.

The Windows application of ICEDIT provides the following drawing features:

- Drawing of chemical structures, reactions and fragments.
- Full support of standard query features (input and interpretation).
- Drawing and support of complex R-group query specifications.
- Additional chemical features like full superatom support, the calculation of molecule values and the input and interpretation of brackets.

The Windows application of *ICEDIT* provides the following display features:

- Color.
- Bond thickness.
- Atom font type, size and style.
- Text font type, size and style.

The Windows application of *ICEDIT* provides the following additional features:

- Integration in MS Office (Word, Excel, PowerPoint and Access) and any other OLE-Client.
- Application Programming Interface (API) for Java, VB 6, VBA and .NET.

1.2.2 System Requirements

Supported Platforms:

Windows 7, Windows Vista, Windows XP, Windows 2000, Windows NT, Windows ME and Windows 98.

1.3 ICEDIT Java Applet

1.3.1 Functionality

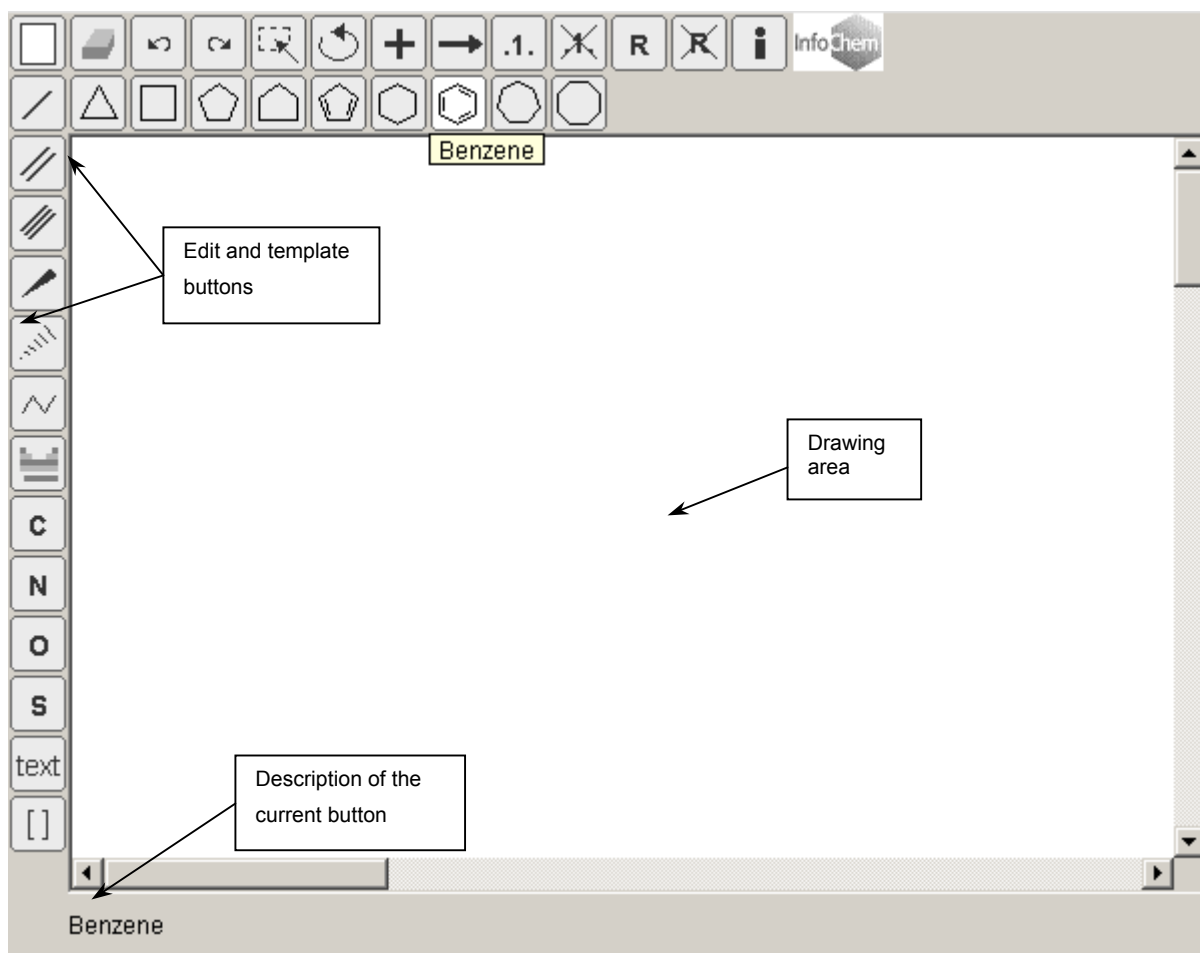


Fig. 2: The ICEDIT Java applet.

The ICEDIT Java applet is an Internet browser based query editor for the input of chemical structures and reactions.

The easy integration in any desktop or web application makes ICEDIT an ideal tool to create queries for searching structure and reaction databases.

It is downloaded on the fly and therefore, it does not have to be installed on the user's computer. The Java applet does not have access to the clients file system and hence, it does not have the full functionality of the ICEDIT Windows application.

1.3.2 Enhanced ICEDIT Java Applet

The enhanced ICEDIT applet is an enriched version of the Java applet that offers additional functionalities like full superatom support. Due to the fact that the standard Java applet does not have access to the clients file system a system managed by a Servlet container like Apache Tomcat is necessary. Please contact us for further information.

1.3.3 System Requirements

Supported Browsers:

Internet Explorer 5.5 or higher, Firefox (Windows, Mac OS X), Opera and Safari (Mac OS X).

Software:

Java Runtime Environment JRE 1.1x or higher.

Please note: JavaScript must be enabled.

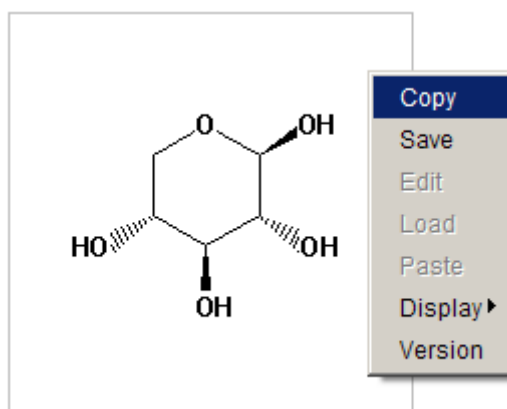
1.4 ICREDIT

1.4.1 Functionality

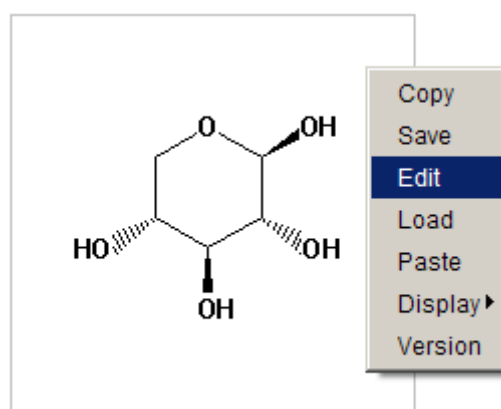
ICREDIT is a small Java applet primarily to render one or more chemical structures in an HTML document. An editing functionality is implemented by connecting to an ICEDIT installation at the client side. It is based on the full application and therefore, all ICEDIT application functionalities like the full support of superatoms, templates, general setting display features, etc. are supported.

ICREDIT can be used to integrate chemistry into a browser application either only with display-functionalities (renderer component) or with full display and editing functionalities (editor component).

Example of the renderer component: Only display, copy, save and version functionalities are supported.



Example of the editor component: All display and edit functionalities are supported.



1.4.2 System Requirements

Supported Browsers:

Internet Explorer 5.5 or higher, Firefox (Windows) and Opera.

Software:

Java Runtime Environment JRE 1.5x or higher.

Please note: JavaScript must be enabled.

Please note: ICREDIT is only supported for Windows based systems.

2 ICEDIT Setup

Windows application only

Run **Setup.exe** if the setup does not start automatically. If there is no Java Runtime Environment (JRE) installed on your system, the setup launches the Java Installer.

IMPORTANT: We strongly recommend to use “Add/Remove Programs” to uninstall ICEDIT.

2.1 Using ICEDIT in Reaxys

The installation of ICEDIT supports the integration in Elsevier’s Reaxys as additional structure editor, if Reaxys is installed.

Before using ICEDIT within Reaxys you have to download and install the “Reaxys Structure Editor Plugins” from the Reaxys homepage (http://www.info.reaxys.com/support_downloads).

After having installed the “Reaxys Structure Editor Plugins” the “ICEDIT for Reaxys” component will be installed automatically with every new setup.

Please note: If ICEDIT is already installed on your computer we recommend to uninstall and re-install the application to get the “ICEDIT for Reaxys” component.

To set ICEDIT as default drawing tool in Reaxys under “My Settings” please

1. Open “Modify Application Settings”.
2. Select “ICEDIT” and click “Save”.
3. Restart the browser.

3 General Information

3.1 Description of the Menu Bar

Windows application only

3.1.1 "File" - Menu

Transfer to client

Transfers the current structure/reaction back to the calling application and closes ICEDIT (only visible in the application when called from another application). (Keyboard shortcut CTRL + B).

New

Creates a new empty structure file. (Keyboard shortcut CTRL + N).

Open

Opens a structure file. (Keyboard shortcut CTRL + O).

Save

Saves a structure file in *.icf format. (Keyboard shortcut CTRL + S).

Save As

Saves a structure file in *.icf format with a different file name.

Export - Mol/Rxnfile

Exports a structure to MDL MOL or a reaction to MDL RXN file format.

Export - Skcfile

Exports a structure or reaction to MDL Sketch file format.

Please note: Complex schemes are not yet supported.

Import - Molfile

Imports a structure from MDL MOL file format.

Import - Rxnfile

Imports a reaction from MDL RXN file format.

Import - Skcfile

Imports a structure or reaction from MDL Sketch file format.

Please note: Complex schemes and drawing elements are not yet supported.

Import - SMILES

Imports a structure from the SMILES format and generates coordinates.

Import - Cdxfile

Imports a structure or reaction from the Cambridge Soft CDX file format.

Please note: Complex schemes and drawing elements are not yet supported.

Exit

Closes the current application. (Keyboard shortcut CTRL + E).

3.1.2 “Edit” - Menu**Undo**

Undo last operation. (Keyboard shortcut CTRL + Z).

Redo

Redo last operation. (Keyboard shortcut CTRL + Y).

Copy

Copies the current objects into the Windows clipboard. Transfer to Microsoft Office products, ISIS/Draw, MDLDraw and ChemDraw is supported. (Keyboard shortcut CTRL + C).

Paste

Pastes objects from the clipboard. Transfer from Microsoft Office products, ISIS/Draw, MDLDraw and ChemDraw is supported. (Keyboard shortcut CTRL + V).

Please note: Complex schemes and drawing elements are not yet supported.

Delete

Deletes the selected objects. (Keyboard shortcut DEL).

Select all

Selects all objects. (Keyboard shortcut CTRL + A).

Duplicate

Duplicates the current selected objects. (Keyboard shortcut CTRL + D).

3.1.3 “Chemistry” - Menu**Superatoms - Expand all**

Expands all superatoms.

Superatoms - Contract all

Contracts all superatoms.

Superatoms - Show Info

Opens a PDF document containing the supported superatoms (“Supported Aliaslist”).

Molecule Values - Calculate

Calculates molecule values of all or the selected objects (single molecules, multiple molecules and parts of structures).

The following molecule values are supported:

- **Formula**
- **Molecular Weight:** The calculation is based on the natural atomic weight of the element, unless an isotope is specified explicitly. In this case the atomic mass of the specified isotope is used.
- **Nominal Mass:** The calculation is based on the atomic mass of the most abundant isotope, unless an isotope is specified explicitly. In this case the atomic mass of the specified isotope is used. The atomic mass is the rounded exact mass of the element.
- **Exact Mass:** The calculation is based on the exact atomic mass of the most abundant isotope, unless an isotope is specified explicitly. In this case the atomic mass of the specified isotope is used.
- **Elemental Analysis**

By using the drop down list “Decimals” the number of decimal places can be adjusted (1-4).

The calculated values can be pasted in the drawing area using the “Paste” button. Not required information can be unselected and will not be transferred into the drawing area.

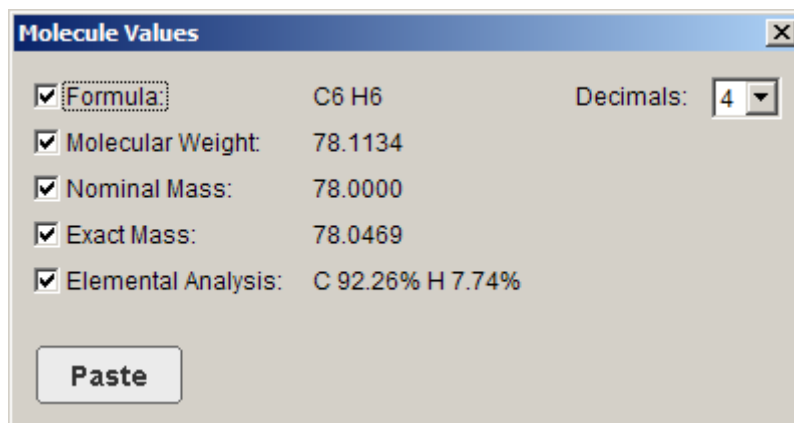


Fig. 3: “Molecule Values” dialog window.

Atom Numbers - Show

To enable automatic atom numbers select “Atom Numbers – Show”. The menu item is now enabled.

To disable automatic atom number select “Atom Numbers – Show” again. The menu item is now disabled.

3.1.4 “Templates” - Menu

Open

Opens the “Templates” dialog.

Insert templates:

To transfer a template into the drawing area, click at a template in the dialog window. The selected template will be highlighted. Then click into the drawing area.

It is possible to choose the docking point (atom or bond) from the template. This selected atom or bond is highlighted in red in the template dialog. The template will be connected by clicking at an attachment point in a structure within the drawing area.

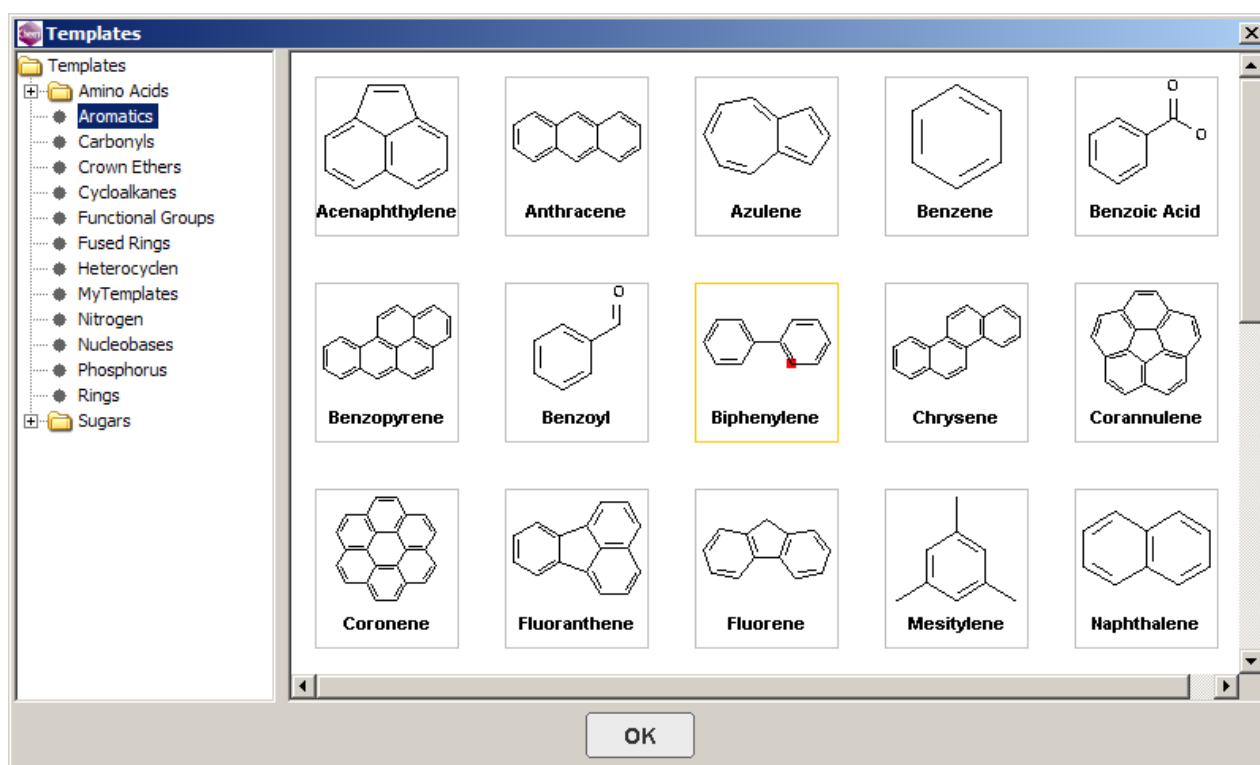
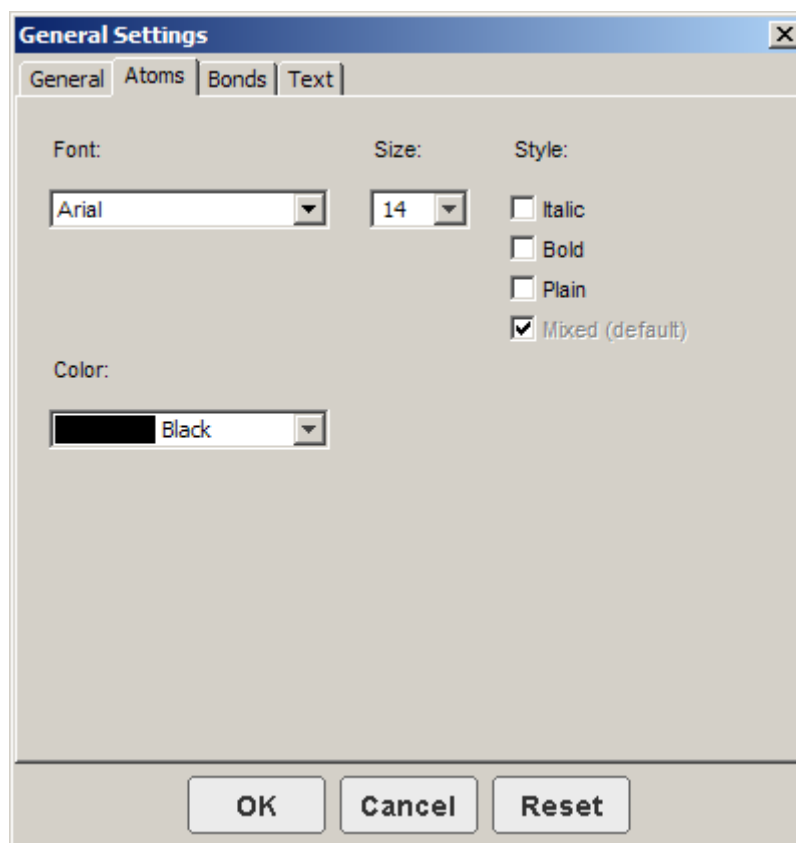


Fig. 4: The “Templates” dialog window.

3.1.5 “Options” - Menu

Settings

Opens the “General Settings” dialog window and allows the adjustment of settings (i) in general, (ii) for atoms, (iii) for bonds and (iv) for text objects. Please refer to chapter 5.4.1 for further details about the “General Settings” dialog.



3.1.6 “?” - Menu

Help

Opens the PDF-documentation file.

About

Returns information about IEDIT and its version number.

3.2 Context Menus

Context menus are available by right clicking (i) on the drawing surface, (ii) on specific bonds, (iii) on specific atoms or (iv) on selected objects. The following features are available within the context menu:

- **Edit:** Edits the currently selected atoms or bonds.
- **Copy Object(s):** Copies the selected object (into an internal buffer).
- **Paste Object(s):** Pastes the selected object (from an internal buffer).
- **Duplicate Object(s):** Duplicates the selected object.
- **Copy:** Copies the selected objects (into the Windows clipboard). (Keyboard shortcut CTRL + C).
- **Paste:** Pastes the objects (from the Windows clipboard) into your drawing area. (Keyboard shortcut CTRL + V).
- **Delete:** Deletes the currently selected atom or bond. (Keyboard shortcut DEL).
- **Expand Superatom:** Expands a selected superatom.
- **Contract Superatom:** Contracts a selected superatom.
- **Create Superatom:** Creates a self-defined superatom.
- **Create Chiral Flag:** Creates a chiral flag on the selected molecule(s).
- **Color:** Provides the opportunity to change the color of the selected object(s).

Please note: The three object methods (“Copy Object(s)”, “Paste Object(s)” and “Duplicate Object(s)”) do only work within IEDIT. Therefore, they cannot be merged with the Windows methods (“Copy” and “Paste”).

3.3 Keyboard Shortcuts

The following keyboard shortcuts are available in IEDIT::

- **Ctrl+C:** Copies the current object into the Windows clipboard.
- **Ctrl+V:** Pastes an object from the clipboard.
- **Ctrl+B:** Transfers objects to calling application.
- **Ctrl+N:** New window (clear screen).
- **Ctrl+O:** Opens a file.
- **Ctrl+S:** Saves structure/reaction as *.icf file (default file name and default directory).
- **Ctrl+A:** Selects all objects within the drawing area.
- **Ctrl+E:** Closes IEDIT.
- **Ctrl+Z:** Undo last operation.
- **Ctrl+Y:** Redo last operation.
- **Ctrl+D:** Duplicates the selected object.

4 Description of Standard Edit Buttons

Standard buttons are provided by the applet and the Windows application. Various edit and template buttons are provided in the button bar. The chosen edit or template button is highlighted.

Selected molecule, atom or bond templates can be used to draw the particular object into the drawing area by mouse click.

Selected edit buttons can be used to carry out the particular operation.

4.1 Standard Edit Buttons



Clear screen.

Deletes all objects from the drawing area. (Keyboard shortcut CTRL + N).



Delete object.

Deletes the object (atom, bond, molecule, text) you select with your mouse. If you draw a rectangle, all objects within that area will be deleted. (Keyboard shortcut DEL).



Undo last operation.

Undo last operation. (Keyboard shortcut CTRL + Z).



Redo last operation.

Redo last operation. (Keyboard shortcut CTRL + Y).



Select object.

Use this tool either to select a single object or a group of objects in a rectangle. The selected objects can then be moved (drag with your mouse), deleted or copied using either the context menu, the menu bar or the appropriate keyboard shortcuts.



Rotate selected objects.

Use this tool to rotate the selected objects either clockwise or anti-clockwise.



Add reaction plus.

Adds a reaction plus to the drawing area.



Add reaction arrow.

Please note: Only one arrow per reaction is supported. Complex schemes will be supported in future.

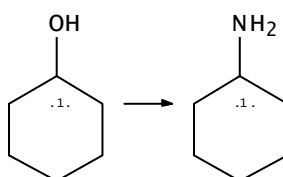


Map atoms.

Adds mapping numbers to the atoms you select. In order to do so, please click on the two atoms you want to map at the reactant and product side of the reaction.

Please note: Only mappings of reactant atoms with product atoms are supported. Furthermore, only atoms of the same atom type can be mapped.

Example:



Remove mappings from atoms and reaction center information from bonds.

Click single atoms/bonds or draw a rectangle to remove mappings or reaction center information from multiple atoms/bonds.

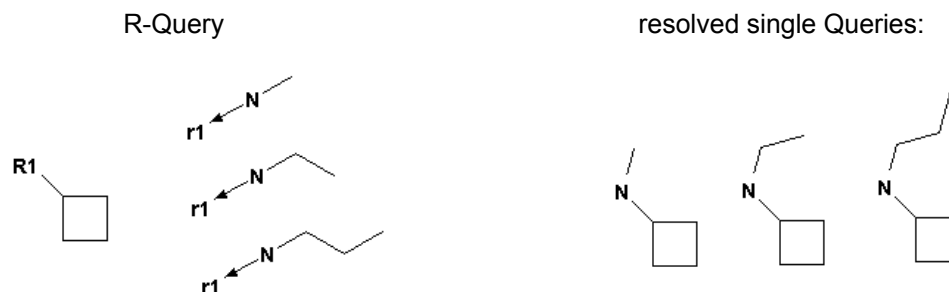


Define Rgroups.

Draw a core structure and several Rgroups.

First click on the position of the core structure, where you want to have the Rgroup attached. Then click on the connection position of the Rgroups.

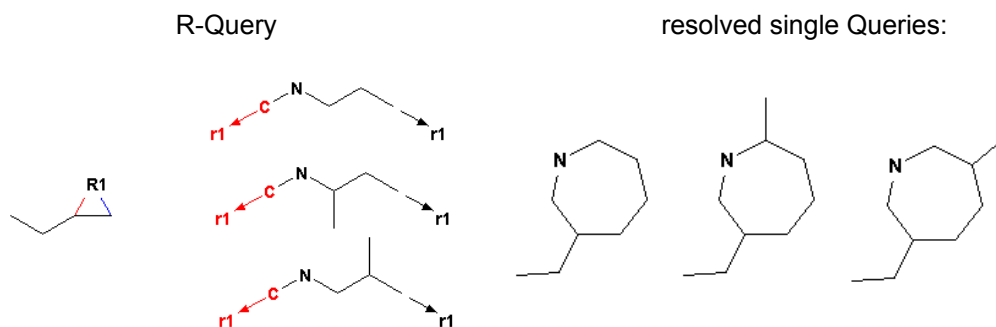
Example:



Please note: To specify two different attachments in one Rgroup, first define the attachment referring to the blue bond in the core structure, then define the attachment referring to the red bond in the core structure.

To change the Rgroup numbering, please click at the object you want to edit and enter the new number with your keyboard. To do this the “Define Rgroups” button must be selected!

Example:



Remove Rgroup Info from atom.

Click single atoms or draw a rectangle to remove Rgroup information.



Show info dialog.

Shows information about ICEDIT and its version number.



Transfer structure back to calling application.

Transfers the current structure/reaction back to the calling application and closes ICEDIT (only visible in the application when called from another application).

4.2 Standard Templates

Click in the drawing area to transfer the selected template. By clicking at an attachment point in the structure within the drawing area, the template will be connected with the chosen attachment point.

4.2.1 Standard Molecule Templates



The Windows application provides a large number of additional templates via menu selection (Templates – open).

4.2.2 Standard Bond Buttons



Draw single bonds or change an existing bond.

Adds a single bond. Either click on a free spot within the drawing area or drag a bond between two atoms. With additional clicks on a bond, you can convert it into:

- (i) a double: one additional click.
- (ii) a triple bond: two additional clicks.
- (iii) a single bond again: three additional clicks.



Draw double bonds or change an existing bond to a double bond.

Draws a new double bond or converts an existing bond into a double bond.



Draw triple bonds or change an existing bond to a triple bond.

Draws a new triple bond or converts an existing bond into a triple bond.



Draw up wedges or change an existing bond to up a wedge.

Draws a new up stereo bond or changes an existing bond into an up stereo bond. An additional click on it changes its direction.

Please note: The orientation of up wedges is important (e.g. in case of query features).



Draw down wedges or change an existing bonds to a down wedge.

Draws a new down stereo bond or changes an existing bond into a down stereo bond. An additional click on it changes its direction.

Please note: The orientation of down wedges is important (e.g. in case of query features).



Draw chain.

Draws a chain of C-C single bonds.

4.2.3 Standard Atom Buttons



Draw atom.

Use the dialog to define atom properties and atom query features. After having done the selection please click in the drawing area to place the atom.

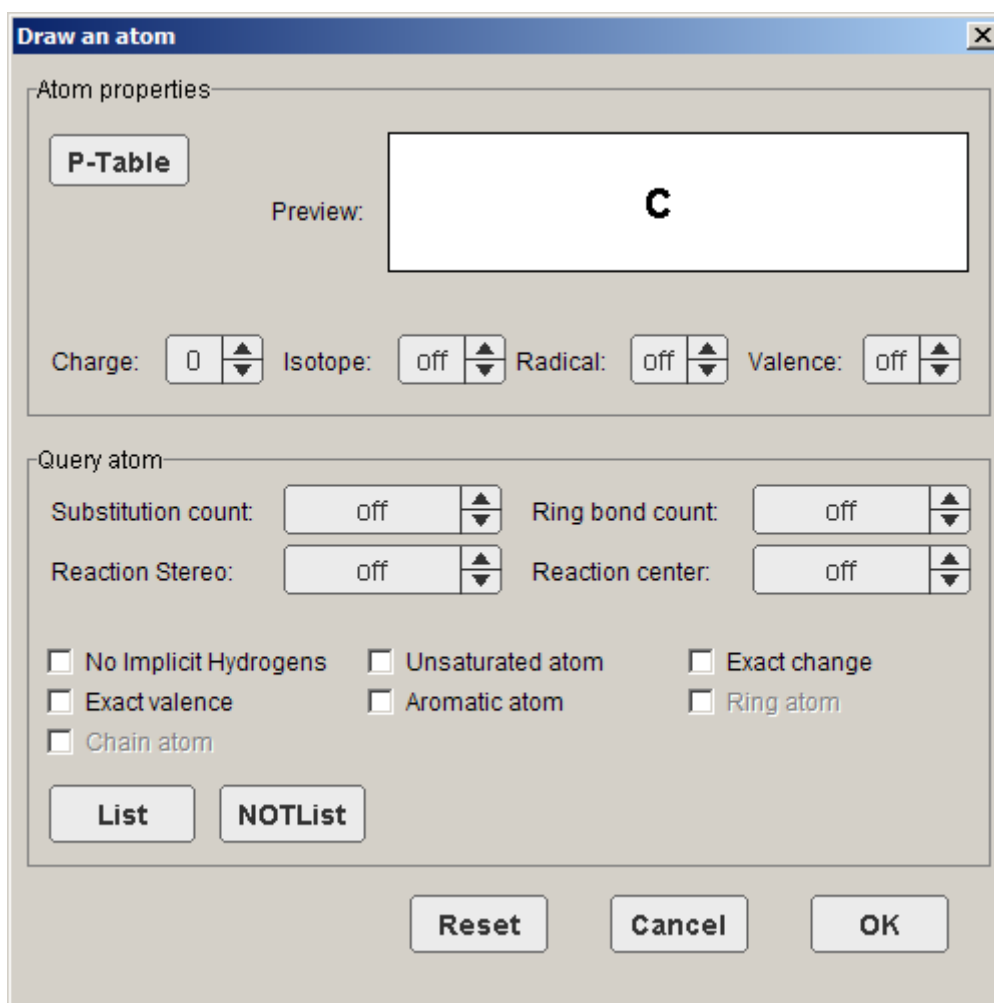


Fig. 5: "Draw an Atom" dialog window.

Atom properties:

Use this dialog to define charge, isotope information, radical information and atom valence.

P-Table Opens a dialog containing the Periodic Table of the Elements to select any element. Furthermore, this dialog contains additional buttons for non-standard and query atoms:

A: Draws an A query atom: any atom excluding H.

Q: Draws a Q query atom: any atom excluding H and C.

X: Draws a X atom; atom type used for halogens (no valid query feature).

R: Draws a R atom (no valid query feature).

Query atom:

The following query features are implemented and can be adjusted

- Substitution count (s0-s6, s*).
- Ring bond count (r0-r4, r*).
- Reaction Stereo (retention, inversion).
- Reaction center (not center, R-center) will be supported in future.
- List: opens a dialog with the Periodic Table of the Elements where you can create an atom list for a query.
- NOT List: opens a dialog with the Periodic Table of the Elements where you can create a NOT-atom list for a query.

In addition the following query settings can be adjusted

- No Implicit Hydrogens (H0).
- Unsaturated atom (u).
- Exact change (ext.).
- Exact valence (ev.) will be supported in future.
- Aromatic atom (aa.) will be supported in future.



Draw atom C.

Draws a carbon atom or converts an existing atom into a carbon atom. After selection click in the drawing area to place the atom.



Draw atom N.

Draws a nitrogen atom or converts an existing atom into a nitrogen atom. After selection click in the drawing area to place the atom.



Draw atom O.

Draws an oxygen atom or converts an existing atom into an oxygen atom. After selection click in the drawing area to place the atom.



Draw atom S.

Draws a sulfur atom or converts an existing atom into a sulfur atom. After selection click in the drawing area to place the atom.

4.2.4 Others



Draw text.

Activates the text input cursor within the drawing area at the selected position.



Draw Bracket.

Draws a pair of brackets.

5 Drawings

To draw atoms or bonds, click the corresponding button to activate the drawing mode. You can change the alignment of atoms, bonds or templates by dragging the object into the desired direction before releasing the mouse button.

Select the corresponding template button to draw rings and click once into the drawing area for one ring. To fuse rings, click on an existing ring bond. To connect rings as spiro molecules click on a ring atom and drag the object into the desired direction before releasing the mouse button. Otherwise the two rings will be automatically separated by a single bond.

Please note: Rings and bonds will be fused automatically, if the distance between two rings or bonds falls below a certain threshold.

5.1 Select Objects

To select a whole object or parts of it please choose the select button and draw a rectangle covering the desired bonds and/or atoms and/or objects. To select one or multiple bonds and/or atoms please click on all desired atoms and/or bonds while the shift button is pressed down.

5.2 Edit Atoms

You can change the atom symbol of a selected atom by using the keyboard (e.g. after drawing a bond, the atom at the end of the bond is selected automatically). Furthermore the keyboard input of charge and isotopes is also supported:

- For a charged atom please insert an atom symbol, the amount of charge and the charge type respectively (e.g. S²⁻).
- For isotopic information please insert the isotop number and the atom symbol respectively (e.g. ²H).

In addition you can change an atom symbol by the use of the “Edit Atom” dialog window. To open the dialog window please click on either the template button “Draw an atom” or the context menu “Edit Atom”. For details of the “Edit Atom” dialog please see chapter 4.2.3.

5.3 Edit Bonds

Select one or several bond(s) and click on the right mouse button. Select “Edit Bond(s)” from the context menu. The “Edit bond” dialog window opens.

It is possible to change the bond type and to add reaction query features like reacting centers or the topology of the selected bond(s). In addition the thickness of the selected bond(s) is adjustable in a range of 1 to 10 pixels.

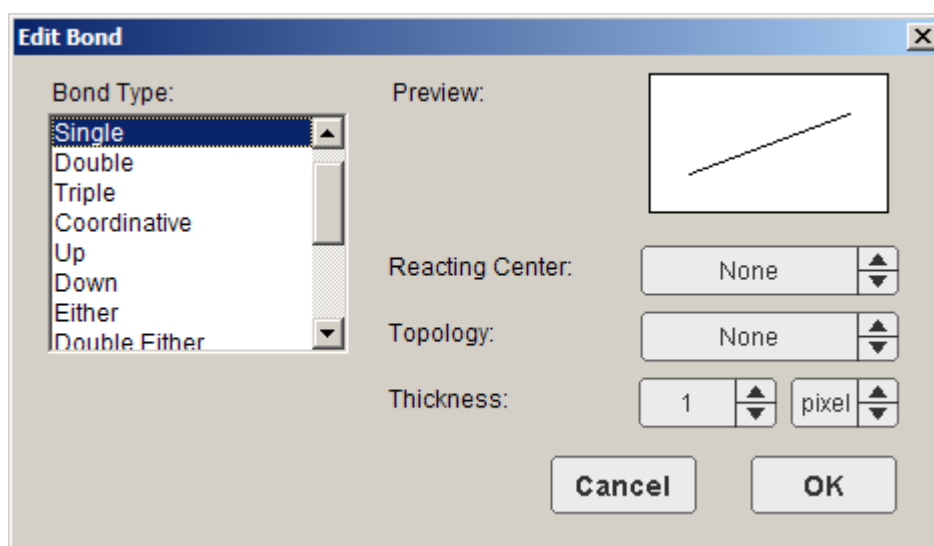


Fig. 6: “Edit Bond” dialog window.

The following bond types are supported:

—	Single	≡	Double Either
==	Double	⋯	Aromatic
≡	Triple	⋯	Any
▶	Up	= =	Single/Double
◀	Down	==	Single/Aromatic
⚡	Either	==	Double/Aromatic

In addition reaction query features can be adjusted:

Reacting Center

—X	Not Center	—	Make/Break
—	Make & Change	—#	Center
—+	Change		

Topology

—Ch	Chain	—Rn	Ring
-----	-------	-----	------

5.4 Display Features

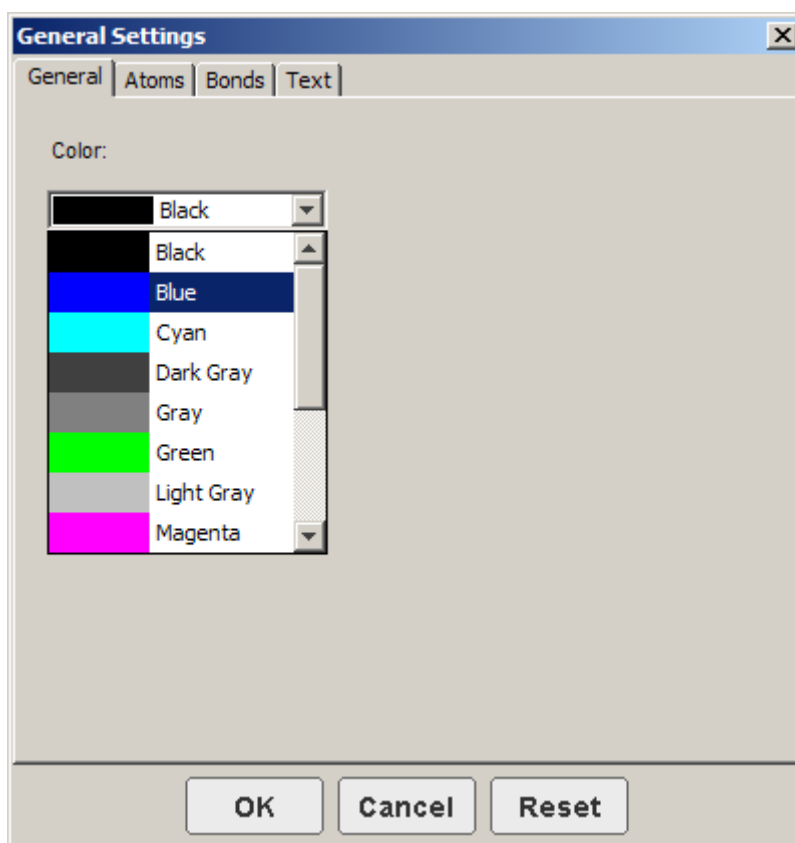
The following display features are supported:

- **Color (for atoms, bonds and text):** You can change the color either by using the “General Settings” dialog or by using the context menu. See also chapter 5.4.2.
- **Font type, size and style (for atoms and text):** You can change the font settings by using the “General Settings” dialog window.
- **Bond thickness:** You can change the bond thickness either by using the “General Settings” dialog or by using the “Edit Bonds” dialog window (chapter 5.3).

5.4.1 General Settings

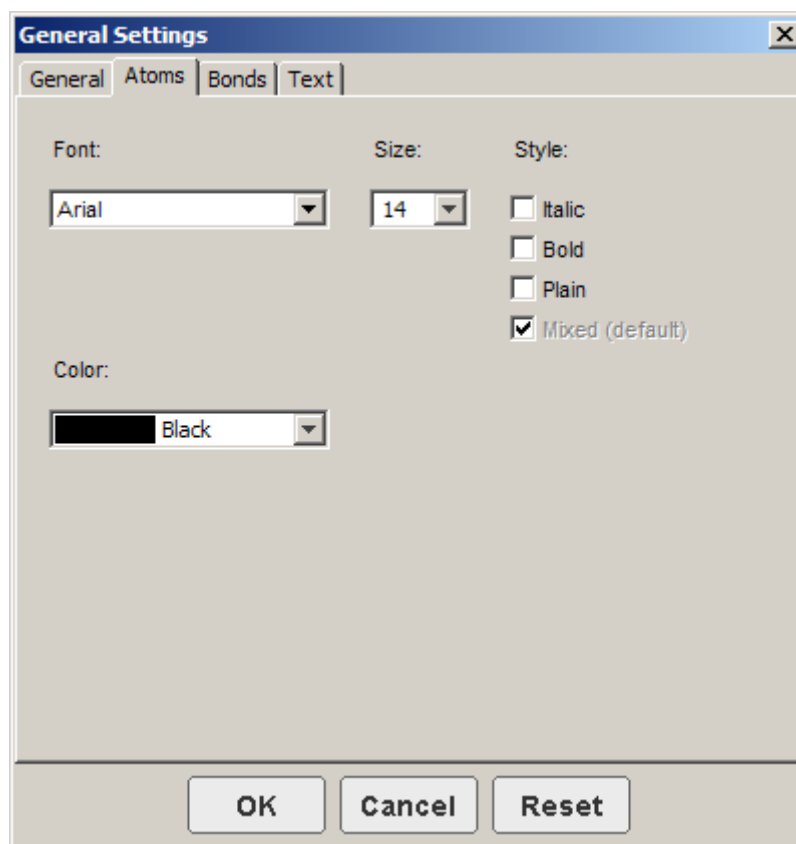
General Settings – General tab

The general tab of the “General Settings” dialog window opens the opportunity to change the color of all objects. The changed settings will be used for all new objects including atom, bond and text objects. You can activate the chosen settings by clicking “OK”.



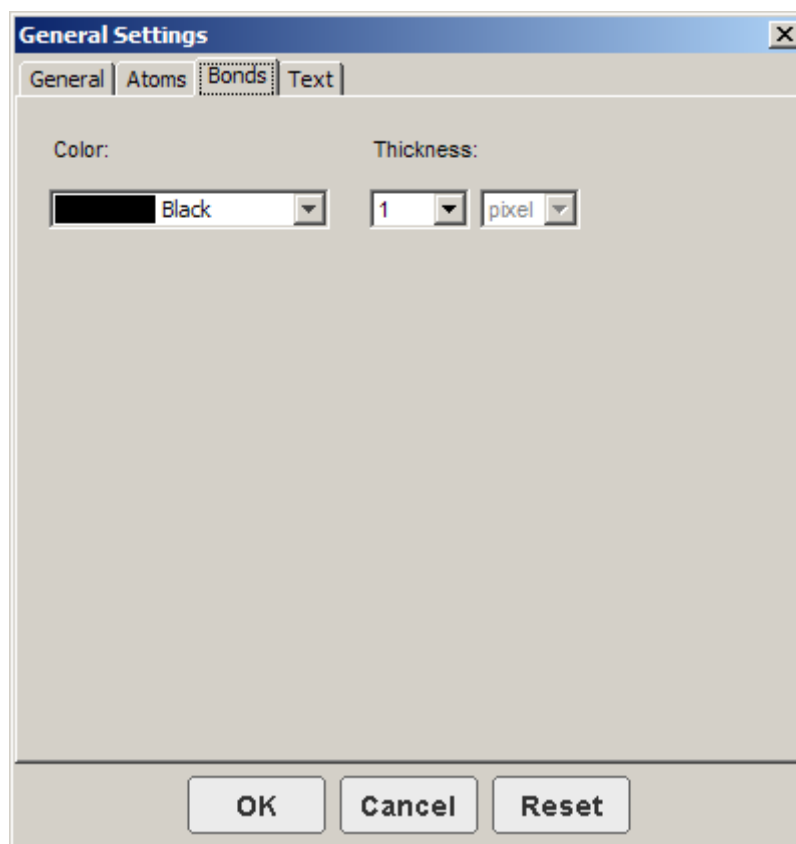
General Settings – Atoms tab

The atom tab of the “General Settings” dialog window opens the opportunity to adjust (i) the atom font, (ii) the atom font size, (iii) the atom font style as well as (iv) the color of atoms.



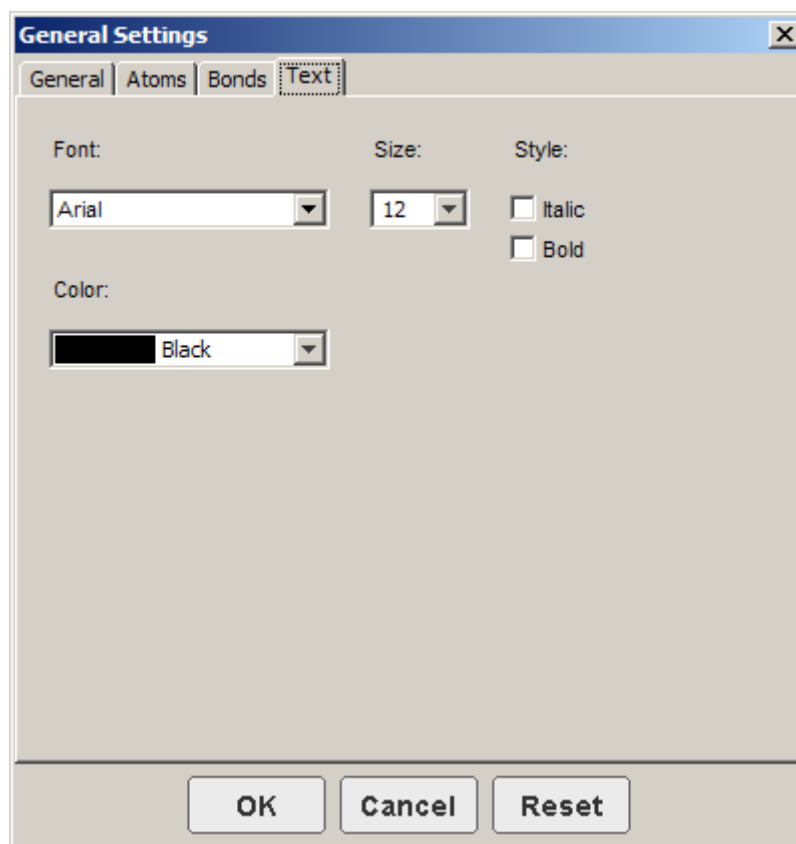
General Settings – Bonds tab

The bond tab of the “General Settings” dialog window opens the opportunity to adjust (i) the thickness of the bonds as well as (ii) the color of the bonds.

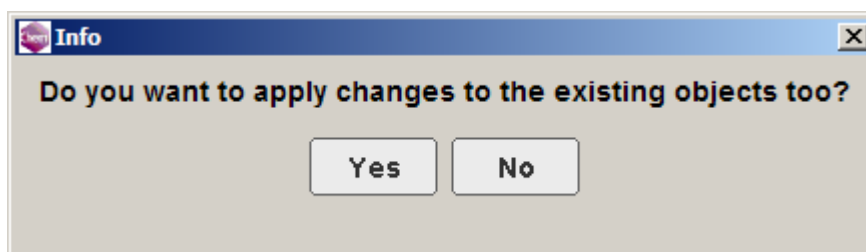


General Settings – Text tab

The text tab of the “General Settings” dialog window opens the opportunity to adjust (i) the text font, (ii) the text font size, (iii) the text font style as well as (iv) the color of the text.



Please note: If you are changing any settings from the “General settings” dialog window you will be asked if you would like to use the changed settings also for already existing objects. If you click “Yes” all already drawn objects will be adjusted as well. If you click “No” the already existing objects will remain as drawn.



5.4.2 Color

It is possible to change the color of selected objects. Besides whole molecules and reactions also single bonds and atoms can be colored. The color of text objects can be adjusted too. You can change the color of object(s) either by using the context menu or by changing the color from the “General Settings” dialog window.

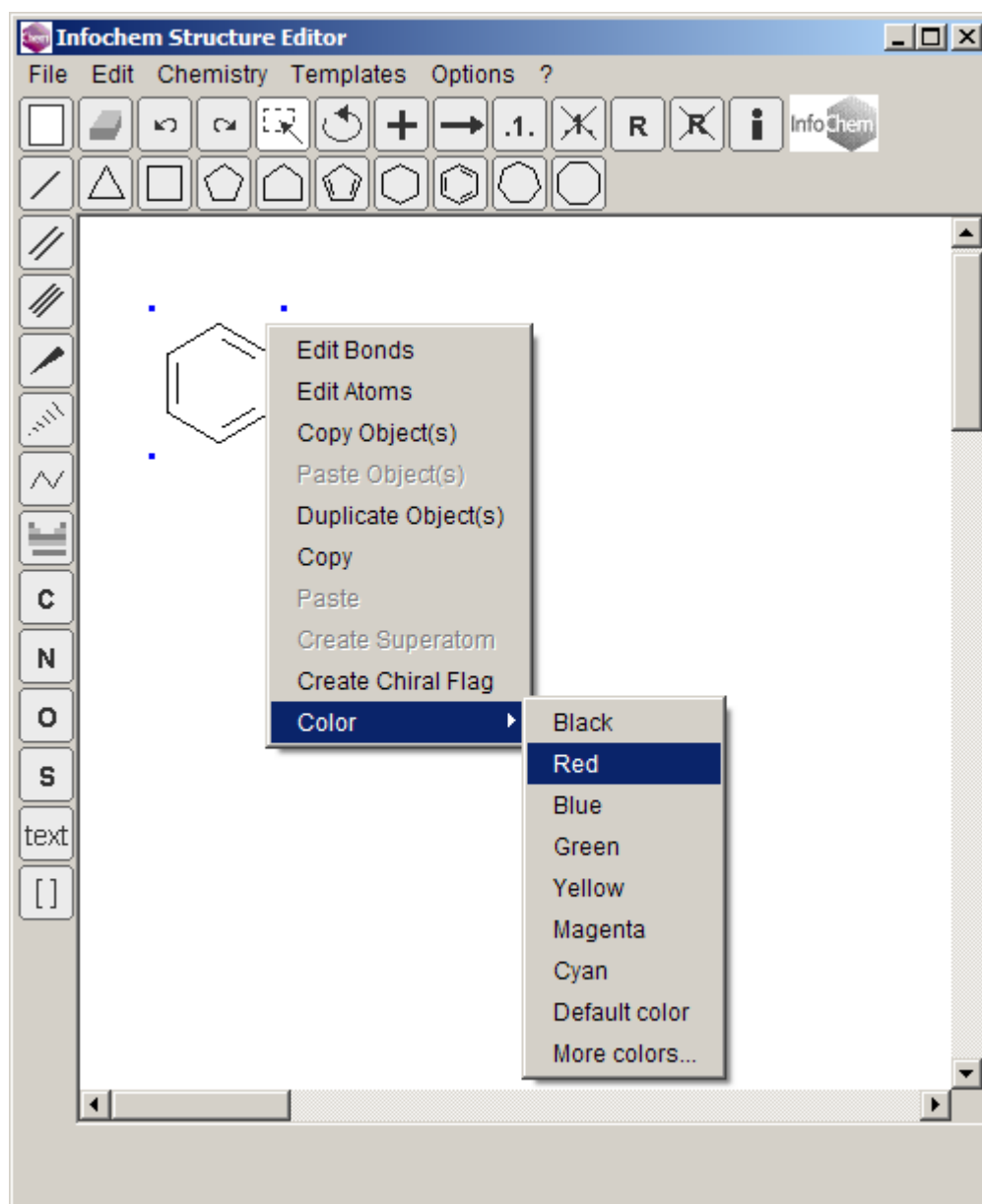
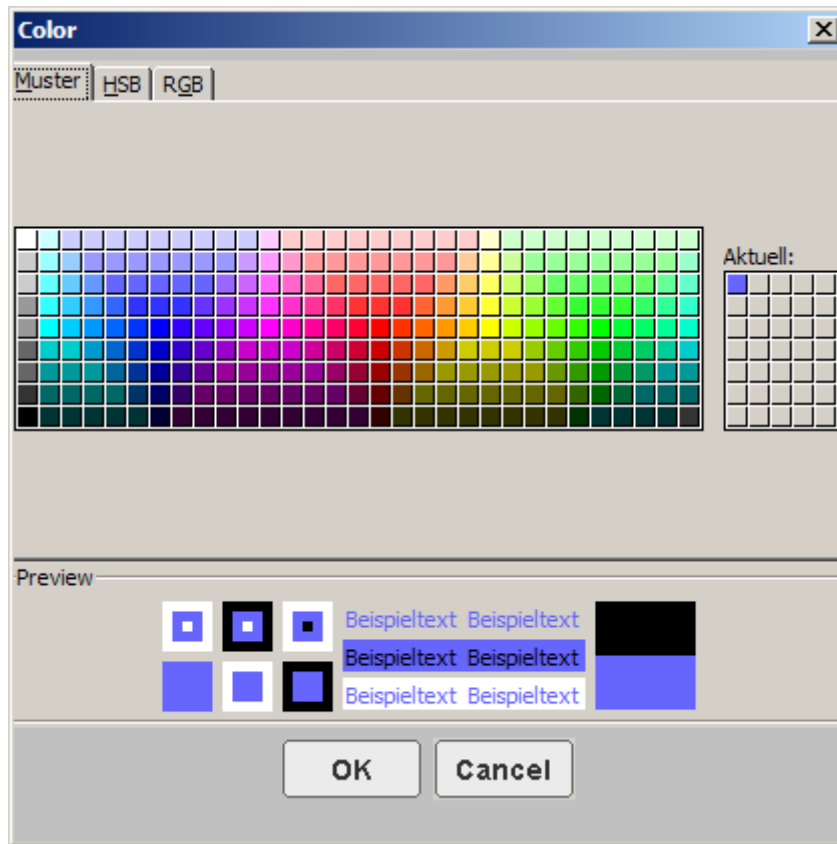


Fig. 7: “Color” context menu.

Please note: The *default color* dyes all atoms and bonds black. However expanded superatoms will be highlighted in dark gray (see also chapter 6). Whereas the color *black* dyes everything - bonds, atoms and expanded superatoms - black.

Beside the predefined standard colors any desired color can be selected by using the “Color” dialog window. You can open the “Color” dialog window by choosing “More colors” form the color drop-down box.



6 Superatoms

6.1 Preface

The input and recognition of superatoms is supported by the IEDIT application.

The superatom can either consist of (i) a standard abbreviation (Me), (ii) a sequence of elements (COOH), or (iii) a mixture of both (OMe).

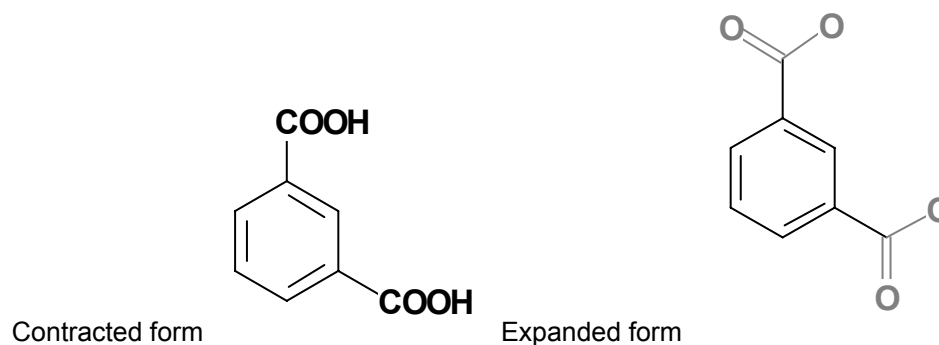
If a superatom is recognized the label is shown in default font format (plain style).

Please note: If the label is shown in italic style it is not recognized as superatom.

Every valid recognized superatom can be expanded. I.e. the label of the superatom can be replaced with the corresponding structure of the superatom. The expanded structure of the superatom is highlighted in gray. The expanded structure parts can be contracted again.

- **Expand a single superatom:** To expand a single superatom select the specific group and use the right mouse button to open the context menu. Choose “Expand Superatom”.
- **Contract a single superatom:** To contract a single superatom select the specific group and use the right mouse button to open the context menu. Choose “Contract Superatom”.
- **Expand all superatoms:** To expand all superatoms use the context menu “Chemistry - Superatoms – Expand all”.
- **Contract all superatoms:** To contract all superatoms use the context menu “Chemistry - Superatoms – Contract all”.

Example:



Input of superatoms:

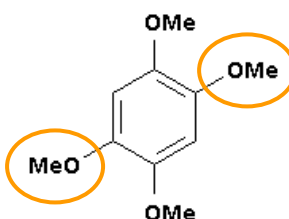
The input of superatoms is case sensitive.

- All atom symbols from superatoms have to be drawn as represented in the Periodic Table of the Elements (e.g. COOH, OMe, SiMe₃).
- Abbreviations are case sensitive as well. They are supported in the most common notation (e.g. Me is supported, me or ME is not supported). The standard typing of abbreviations is as follows:

- Bn, Boc, Bt, Bu, Bz
- Cbz, Cy
- EE, Et
- Fmoc
- Me, MEM, Mes, MOM, MPM, Ms
- Naph, NPhth
- Ph, Piv, PMB, PNB, Pr
- SEM, Su
- TBDMS, TBDPS, TBS, TES, Tf, THP, TIPS, TMS, Tol, Tr, Ts

Display of superatom labels:

The display of superatom labels is sensitive regarding the direction of the connection of the superatom to the target molecule.



On the top, the bottom and the right side of the target molecule the input of the superatom occurs in a standard way. The output of the superatom on the left side, however, is in reversed order.

Please note: Abbreviations do not change their order.

Examples:

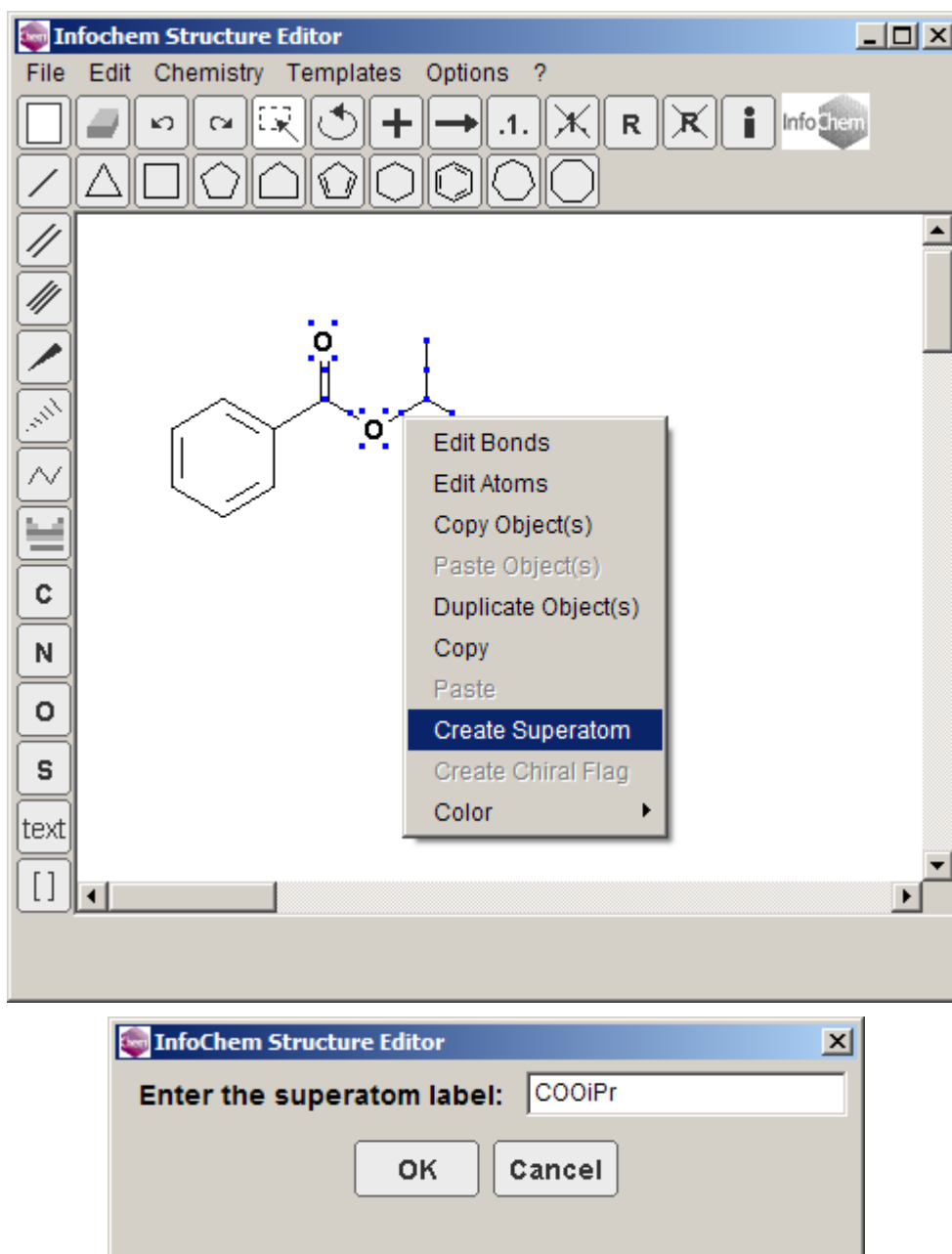
Left side superatom label	Right side superatom label
MeO	OMe
MeHN	NHMe
HOOC	COOH
TMS	TMS
H ₃ C(H ₂ C) ₅	(CH ₂) ₅ CH ₃

The label of the superatom is changed automatically according to the direction of the connection to the target molecule in order to represent the connecting atom of the superatom group correctly. E.g. the superatom label input on the left side of a molecule can be COOH and the output changes automatically to HOOC.

Please note: Please refer to “Chemistry-Superatoms-Show all” from the main menu of the ICDIT application to find a full list of supported superatoms and superatom labels.

6.2 Self-defined Superatoms

Select the desired part of a molecule and choose “Create Superatom” from the context menu to create a self-defined superatom. Enter the desired superatom label into the dialog window and click “OK” to create the superatom.



Please note: A molecule containing a self-defined superatom can be copied, saved or exported like any other usual molecule. However, the self-defined superatom is not added to the internal list of superatoms. Therefore it is not stored for future use and must be newly-created each time it is used.

Currently, the storage of self-defined superatoms as user-defined templates is not yet supported but will be supported in a future version.

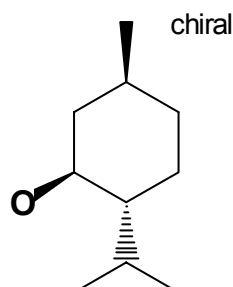
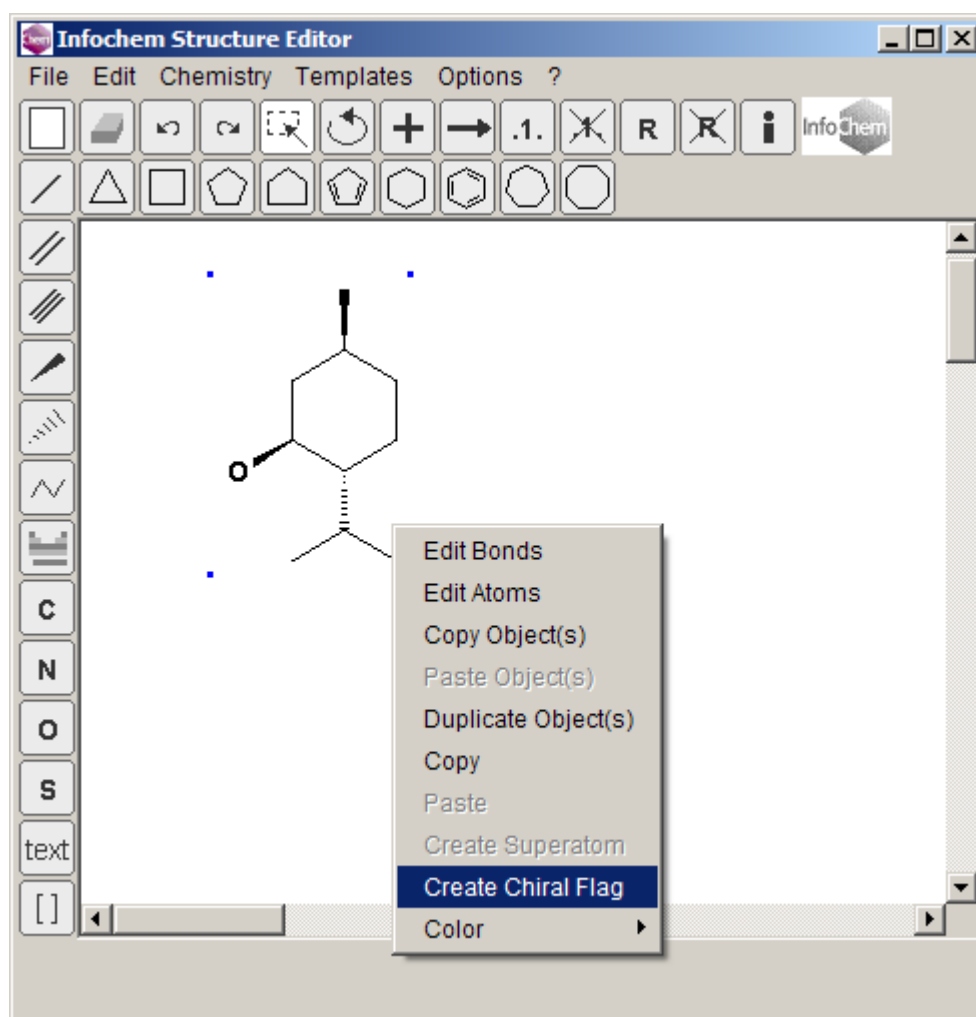
7 Chiral flag

A chiral flag is used to mark the stereochemistry of the labeled molecule as **absolute**.


To add the chiral flag, please select the molecule you want to label as chiral and use the context menu "Create Chiral Flag". The labeled molecule is now marked with the text box "chiral".

To remove the chiral flag, please delete the text box "chiral". The stereochemistry is no longer marked as absolute.

Example:

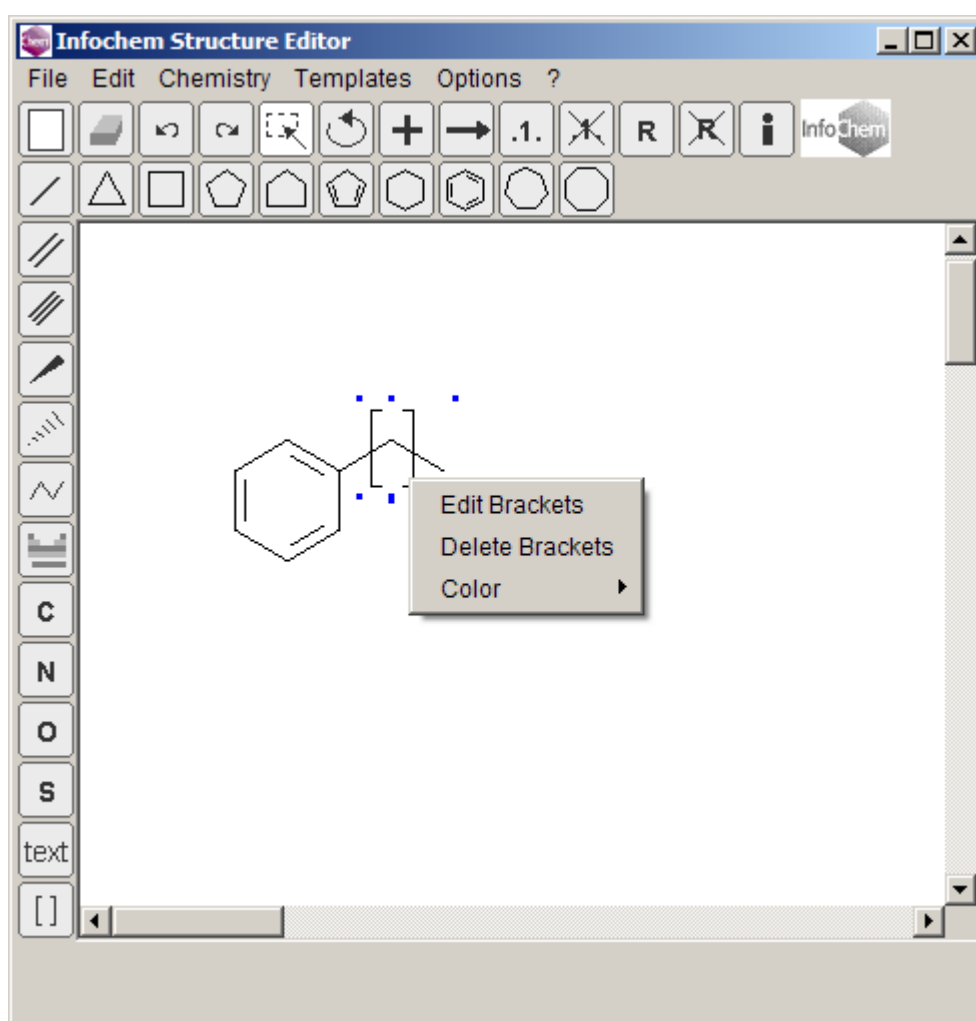


8 Brackets

To draw a bracket, please select the bracket  button from the left hand side of the template menu and draw a pair of brackets into the drawing surface by using the mouse cursor.

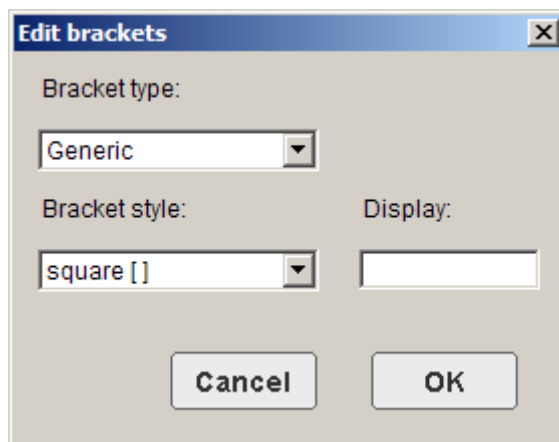
Please note: The distance between the pair of brackets can be adjusted later on by selecting and moving a single bracket. However, the height of the brackets cannot be adjusted later on. This feature will be supported in future.

You can edit, delete or color a bracket by using the “Brackets” context menu. To open the “Brackets” context menu, please move the mouse cursor above one bracket until a red frame appears. You can now open the “Brackets” context menu by right-clicking.



Edit Brackets:

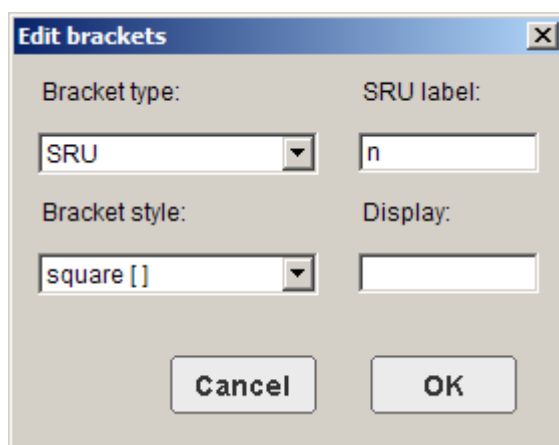
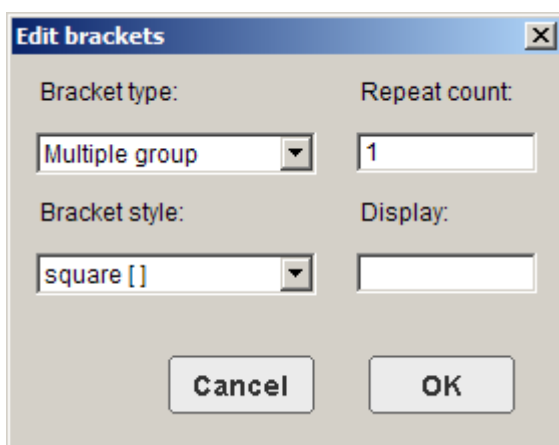
To edit a pair of brackets, choose “Edit Brackets” from the “Brackets” context menu. You can edit (i) the bracket type, (ii) the bracket style or (iii) add display features to the brackets:

Edit the Bracket Type:

The default bracket type is “Generic”. You can change the bracket type from “Generic” to “Multiple group” and “SRU”.

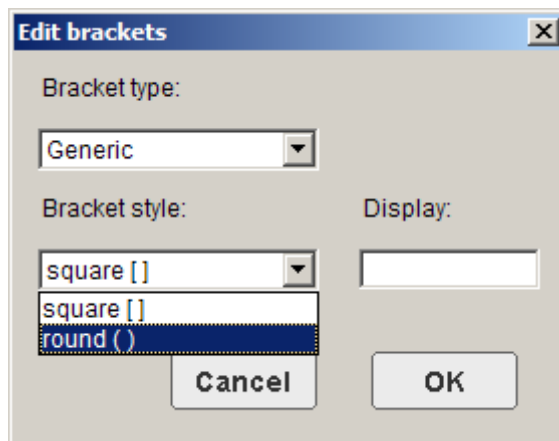
- **Bracket type - Generic:** A pair of brackets is graphically drawn. No repeating factor is displayed and no repeating factor will be interpreted chemically.
- **Bracket type - Multiple Group:** You can enter any integer beginning with 1. The multiple group information will be interpreted chemically.
- **Bracket type - SRU:** You can enter any value, number, range or free text. The SRU information is displayed, but will not be interpreted chemically.

For example: The clamped part is not multiplied, if the “SRU” value is set to 2. However, if the “Multiple group” value is set to 2 the clamped part is multiplied.



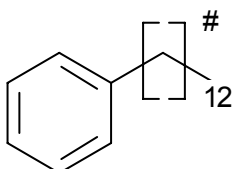
Edit the Bracket Style:

The two bracket styles “square” and “round” are supported by the IEDIT application.



Enter a Bracket Display:

You can enter any additional display information in the “Display” field. The entered display information is shown on the upper right-hand side of the right bracket pair.



Delete Brackets:

To delete a bracket, please choose “Delete Brackets” from the “Brackets” context menu to remove the whole pair of brackets.

9 User-defined Templates

Windows application only

Draw the structure you want to use as template in IEDIT and save it to the subdirectory "Templates" of your IEDIT installation directory (e.g. "My Templates" in the "Templates" folder of the IEDIT installation path). To group the templates choose an existing subdirectory or create a new subdirectory (multiple levels of subdirectories are supported).

Please note: Currently, user-defined templates containing superatoms and/or brackets are not supported.

10 OLE-Server Functionalities

Windows application only

10.1 Integration in MS Office

ICEDIT objects can be used in Microsoft Office (Word, Excel, PowerPoint and Access):

- 1) To start IEDIT in MS Word, MS Excel, etc. choose the item "ICEDIT Document" from menu "Insert – Object". Draw an object. Click the button "Back" to transfer the object from IEDIT back to MS Office. Double-clicking the image starts IEDIT again.
- 2) Draw an object in IEDIT. Choose "Copy" from IEDIT menu "Edit" to copy the object in the Windows clipboard. Choose "Paste" to insert the object in MS Office. Double-clicking the image starts IEDIT again.

The structure display format in MS Word, Excel, PowerPoint and Access is Windows Metafile, which provides a high resolution for print out.

11 Technical Documentation

In addition to this IEDIT user manual a detailed technical documentation is available. Please find the document IEdit_Technical_Documentation.pdf in the “Documentation” folder in the IEDIT installation path.

In this technical documentation you will find detailed descriptions on:

- The configuration of standard edit and drawing buttons (toolbars).
- OLE-Server functionalities: Integration in MSOffice and other OLE interfaces.
- General Programming Interfaces (API's).
- Additional clipboard formats.
- ICRENDIT.
- Add-in for MSEXcel.
- IEDIT as ActiveX Control (ICEDITOCX).

11.1 Copyright

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