



## **Manual**

Structure and Reaction Editor

Version 3.1

Spring 2019

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# 1 Introduction

ICEDIT is a powerful chemical structure editor, which is available as Windows application, as HTML5 based JavaScript editor and as enhanced JavaScript editor for web applications.

- **Windows application:** The IEDIT application offers full editing functionalities (chemical as well as display functionalities). IEDIT is a registered OLE-Server and therefore allows the integration in MS Office (Word, Excel, Access and PowerPoint) and in many other OLE-Clients.
- **HTML5 based JavaScript editor:** InfoChem's IEDIT JavaScript editor is an HTML5 based structure and reaction editor developed for many common browsers. Of course, the IEDIT JavaScript version supports all features needed in a chemical query editor for structures and reactions.
- **Enhanced JavaScript editor:** In addition to the classic IEDIT JavaScript version an enhanced IEDIT JavaScript editor is available based on InfoChem's ICNATIVE Webservice covering additional advanced features like resolution of alias labels to superatoms, "Convert Name to Structure" functionality, standardization of molecules etc. (please see table below).

Support of	ICEDIT application	Enhanced IEDIT JavaScript editor	ICEDIT JavaScript editor
Drawing of structures, reactions and fragments	+	+	+
Full support of standard query features	+	+	+
R-group query features	+	+	+
Integration in web applications	-	+	+
Superatoms	+	+	-
Calculation of molecule values, InChIs, InChIKeys and SMILES	+	-	-
Display features	+	+	+
OLE functionalities (MS Office integration)	+	-	-
Automap function <sup>1)</sup>	+	+	-
Standardization of molecules/reactions <sup>1)</sup>	+	+	-
Add Hydrogen(s) functionality <sup>1)</sup>	+	+	-
Convert Name to Structure <sup>1)2)</sup>	-	+	-

1) Availability is dependent on the licensed options. Please contact us for further licensing information (iceditsupport@infochem.de).

2) Name2Structure webservice and a relational database is required.

## 1.1 ICEDIT Windows Application

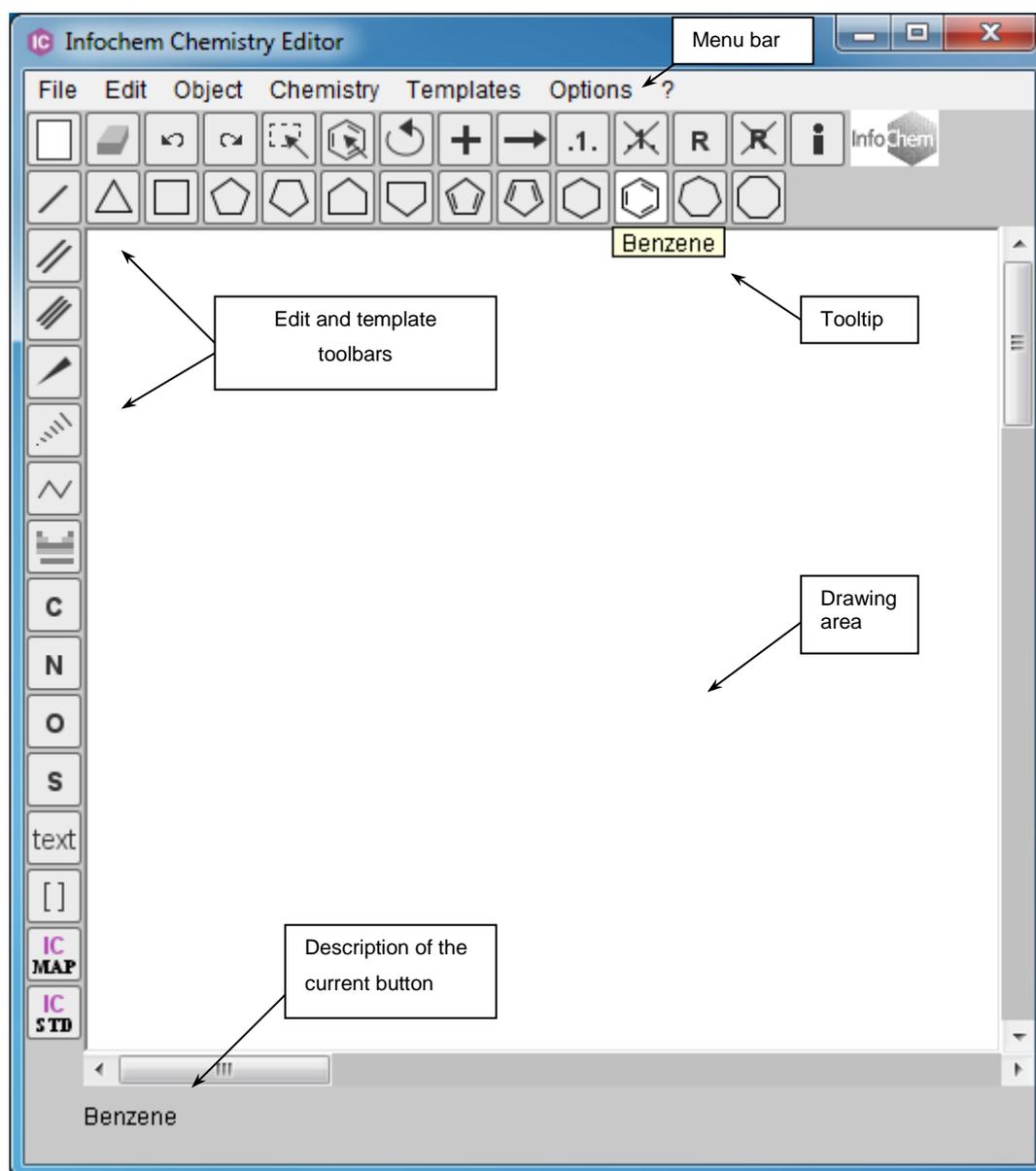


Fig. 1: ICEDIT Windows application.

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 and calculation of molecule values, InChIs, InChIKeys and SMILES.
- Standardization of structures and reactions (add-in button functionality).
- Automap function; automatically mapping of reactions (add-in button functionality).

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

- Atoms: font type, size and style as well as different display modes for implicit hydrogens.
- Bonds: length and thickness.
- Text: font type, size and style.
- Objects: alignment, size and color.

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

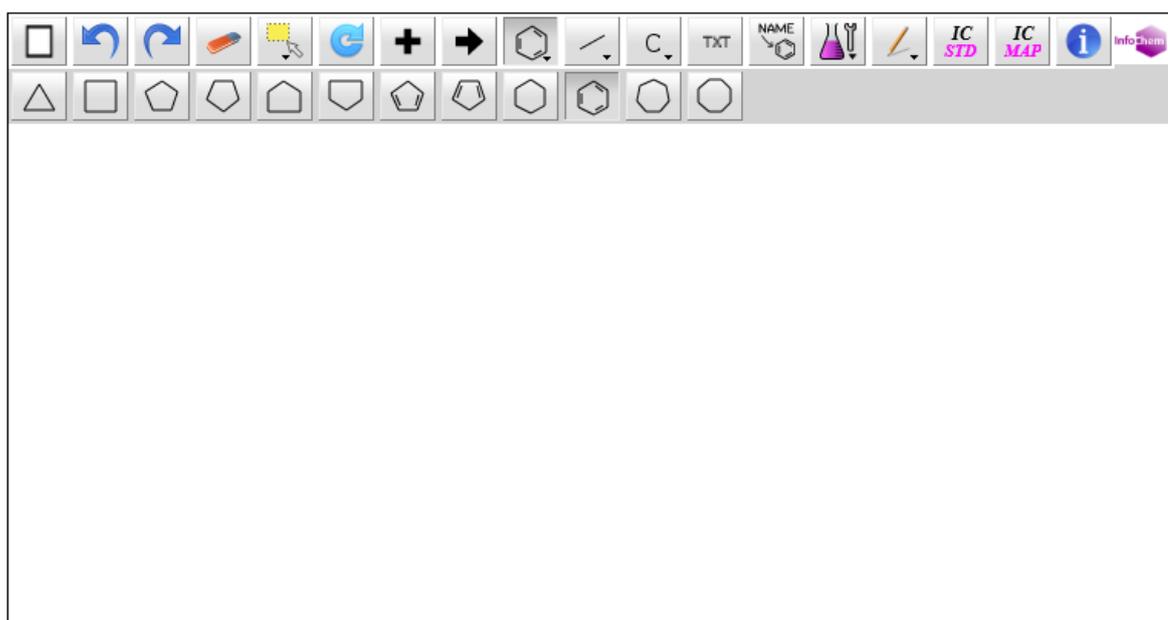
- Integration in MS Office (Word, Excel, PowerPoint and Access) and many other OLE-Clients.
- Application Programming Interface (API) for Java, VBA and .NET.

### 1.1.1 System Requirements

#### Supported Platforms:

Windows 10, Windows 8 and Windows 7

## 1.2 (Enhanced) IEDIT JavaScript Editor



**Fig. 2:** JavaScript version of IEDIT.

Since the HTML5 based JavaScript Editor is completely Java free, this version of IEDIT is the perfect query editor for modern web applications. An installation on the client computer is not necessary and the editor can be used in all common web browsers supporting HTML5. The easy integration in any desktop or web application makes IEDIT an ideal tool to create queries to searchthrough structure and reaction databases.

In addition to the classic IEDIT JavaScript version an enhanced IEDIT JavaScript editor is available based on InfoChem's ICNATIVE Webservice covering additional advanced features like resolution of alias labels to superatoms, "Convert Name to Structure" functionality and standardization of molecules.

For a detailed description of the IEDIT JavaScript editor please refer to the corresponding documentation which can be found on the InfoChem homepage.

### 1.2.1 System Requirements

#### Supported Browsers:

Mozilla Firefox, Google Chrome, Microsoft Edge, Internet Explorer, Opera and Apple Safari.

**Please note:** JavaScript must be enabled.

## 2 ICEDIT Setup

### *Windows application only*

Run **Setup.exe** if the setup does not start automatically.

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

**Please note:** For automap and standardization functionalities a valid license file is required. Please copy the “*icedit.lic*” file into the installation path of ICEDIT. Please contact us for further licensing information ([iceditsupport@infochem.de](mailto:iceditsupport@infochem.de)).

## 3 General Information

This documentation comprises the complete functionality of the IEDIT Windows application. Due to license file settings or front-end configuration your actual IEDIT editor may differ from the information given below.

### 3.1 Description of the Menu Bar

#### 3.1.1 "File" – Menu Items

##### **Transfer to client**

Transfers the current structure/reaction back to the calling application and closes IEDIT (only visible if IEDIT is called from another application) (keyboard shortcut: CTRL + B).

##### **New**

Creates a new empty document (keyboard shortcut: CTRL + N).

##### **Open**

Opens a structure or reaction from a file in ICF format (keyboard shortcut: CTRL + O).

##### **Save**

Saves a structure or reaction to a file in ICF format (keyboard shortcut: CTRL + S).

##### **Save As**

Opens the "Save as" dialog window to save a structure or reaction scheme to a 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 and drawing elements are not fully supported.

##### **Export - SMILES**

Exports a structure to SMILES file format.

**Export – Canonical SMILES**

Exports a structure to canonical SMILES file format.

**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 fully supported.

**Import - SMILES**

Imports a structure from SMILES format and generates coordinates.

**Import - Cdxfile**

Imports a structure or reaction from the CambridgeSoft CDX file format.

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

**Recent Files**

Includes a list of recently opened or imported files.

**Print**

Prints the structures or reactions drawn in the drawing area.

**Exit**

Closes the current application.

### 3.1.2 “Edit” – Menu Items

#### **Undo**

Undoes the last operation (keyboard shortcut: CTRL + Z).

#### **Redo**

Redoes the last undone operation (keyboard shortcut: CTRL + Y).

#### **Copy**

Copies the selected object(s) into the Windows clipboard (keyboard shortcut: CTRL + C). Transfer to Microsoft Office products, ISIS/Draw, MDLDraw and ChemDraw is supported.

#### **Paste**

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

**Please note:** Transfer from ISIS/Draw, MDLDraw and ChemDraw is not supported for complex schemes and drawing elements.

#### **Delete**

Deletes the selected object(s) (keyboard shortcut: DEL).

#### **Select all**

Selects all objects (keyboard shortcut: CTRL + A).

#### **Duplicate**

Duplicates the selected object(s) (keyboard shortcut: CTRL + D).

### 3.1.3 “Object” – Menu Items

#### Group

Merges multiple selected chemical objects into a group (keyboard shortcut: CTRL + G).

**Please note:** The menu item “Group” is only enabled if multiple chemical objects are selected.

#### Ungroup

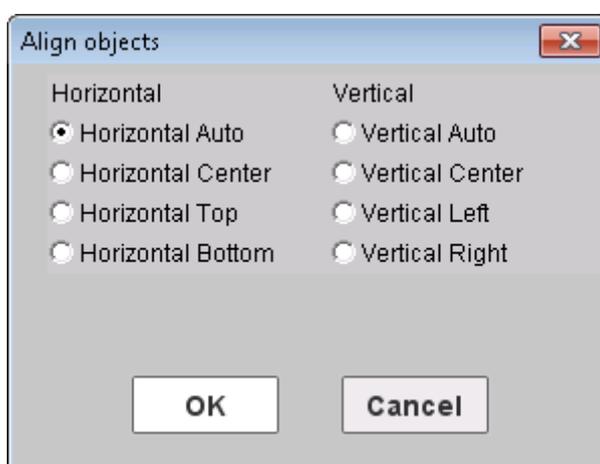
Ungroups a selected group of chemical objects (keyboard shortcut: CTRL + H).

**Please note:** The menu item “Ungroup” is only enabled if a group of chemical objects is selected.

#### Align

Opens the “Align objects” dialog window. Please choose the appropriate align option from the dialog window to align the selected objects accordingly (keyboard shortcut: CTRL + I).

**Please note:** The menu item “Align” is only enabled if multiple objects are selected.



**Fig. 3:** “Align objects” dialog window.

### 3.1.4 “Chemistry” – Menu Items

#### Superatoms - Expand all

Expands all superatoms.

#### Superatoms - Contract all

Contracts all superatoms.

#### Superatoms - Show Info

Opens a document in PDF format containing the supported alias-labels (“Supported Aliaslist”).

#### Molecule Values - Calculate

Calculates molecule values of all or the selected chemical object(s) (single molecules, multiple compounds and grouped compounds).

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**

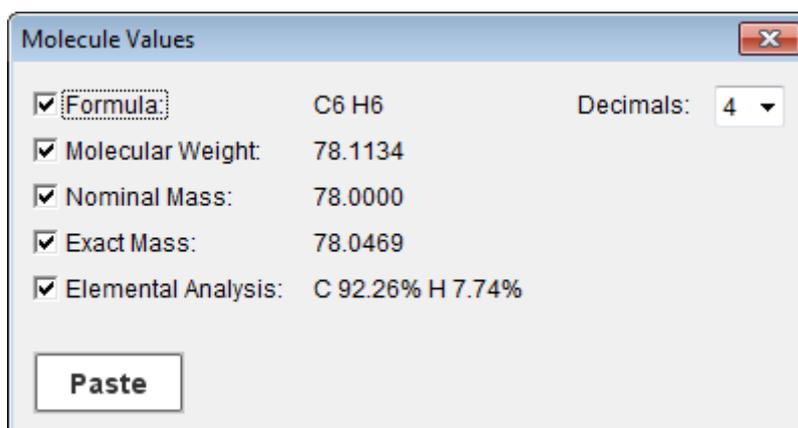


Fig. 4: “Molecule Values” dialog window.

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 unchecked and will not be transferred into the drawing area.

### InChI/InChIKey - Calculate

Calculates InChIs and InChIKeys of all or the selected chemical object(s) (single molecules, multiple compounds and grouped compounds). Additionally, any standardization of molecules during InChI calculation is mentioned in the Comment field.

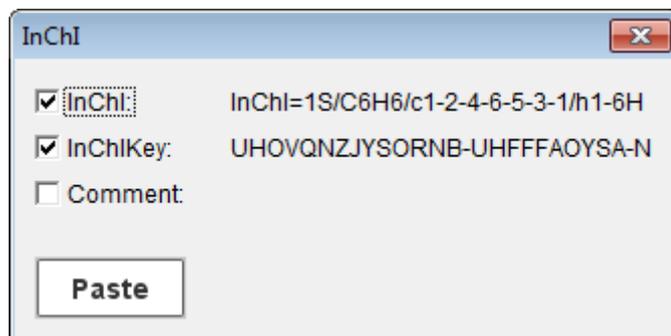


Fig. 5: “InChI” dialog window.

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

### SMILES - Calculate

Calculates SMILES and Canonical SMILES of all or the selected chemical object(s) (single molecules, multiple compounds and grouped compounds).

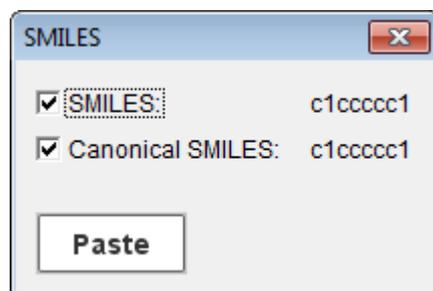


Fig. 6: “SMILES” dialog window.

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

### Create No-Structure:

Opens the “Create No-Structure” dialog window to create a No-Structure label. Please refer to chapter 10 for further details on No-Structures.

### 3.1.5 “Templates” – Menu Items

#### Open

Opens the “Templates” dialog window.

#### Insert templates:

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

It is also possible to connect a template molecule to an existing structure on the drawing area. Please click on the desired docking site (atom or bond) from the template. This selected atom or bond is highlighted in red in the template dialog window. The template will be connected by clicking on an attachment site (atom or bond) at a structure within the drawing area.

If no specific docking site is chosen the default docking site is used.

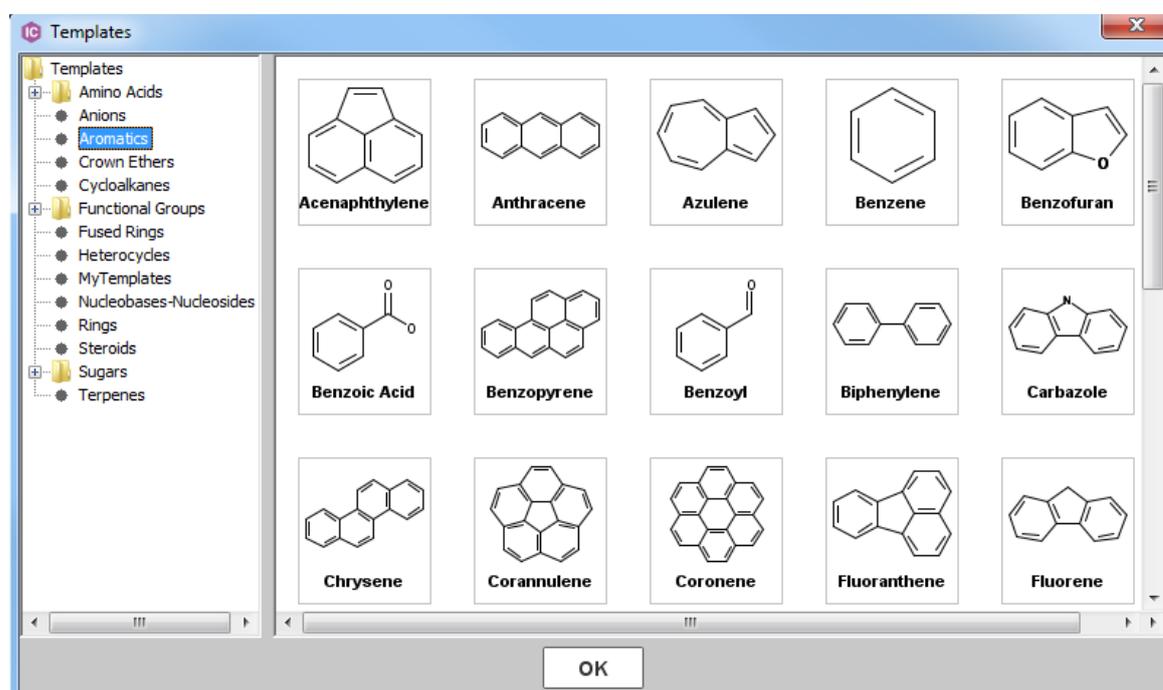


Fig. 7: “Templates” dialog window.

For creation of user-defined templates please refer to chapter 11.

**Please note:** The sugar molecules included in the folder “alpha-D-Sugars – chair conformers” do not contain stereo information that can be automatically interpreted. They are for graphical representation only.

### 3.1.6 “Options” – Menu Items

#### 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 5.6.1 for further details.

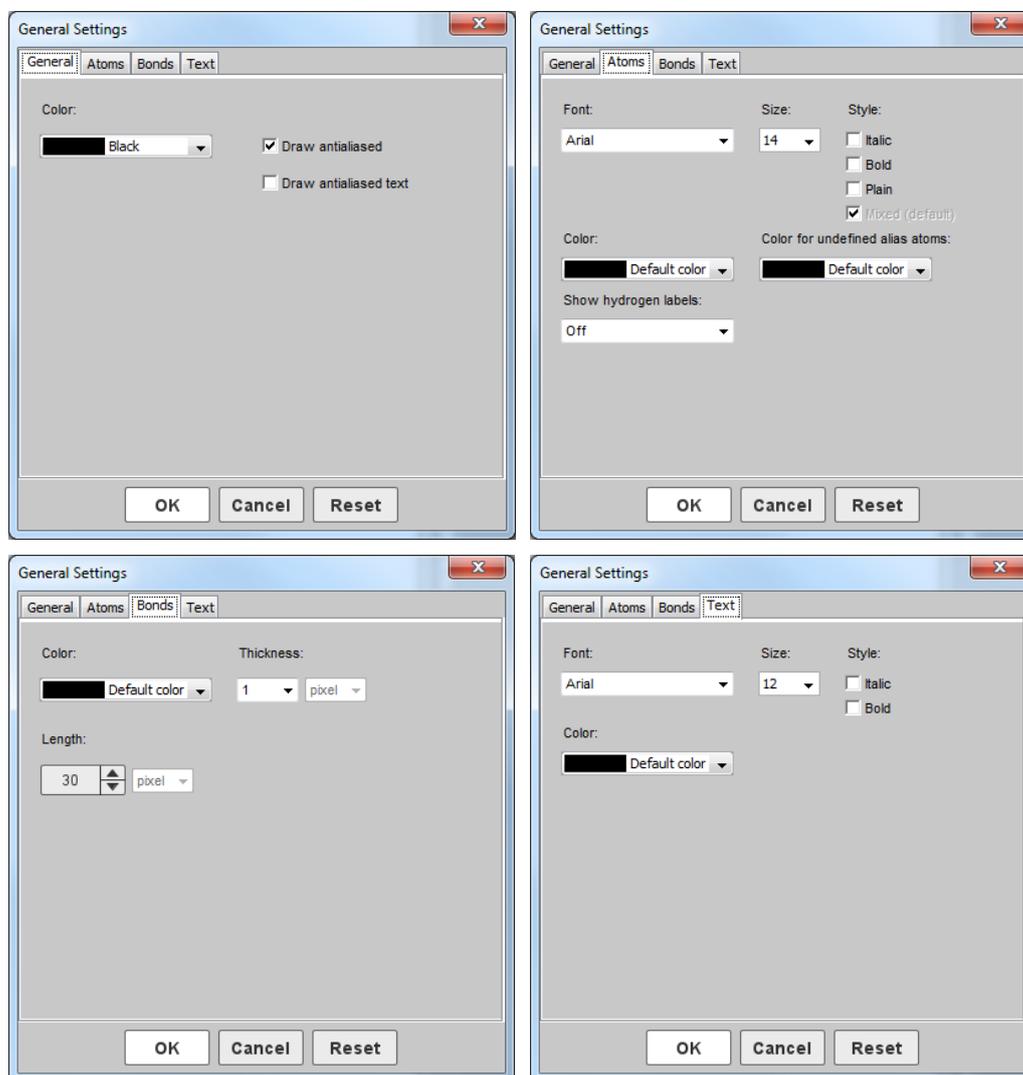
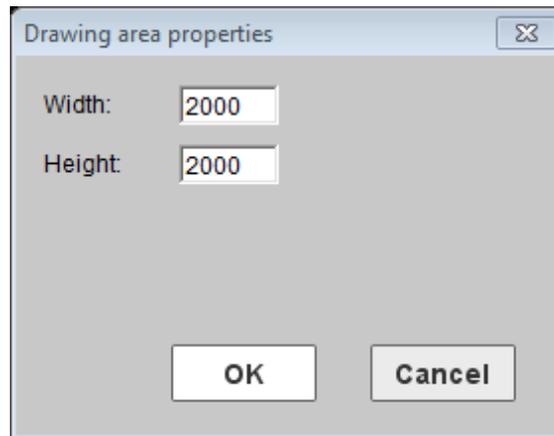


Fig. 8: “General Settings” dialog windows.

## Drawing Area Properties

The maximum size of the drawing area (width and height in pixel) can be adjusted here.



**Fig. 9:** "Drawing area properties" dialog window.

### 3.1.7 “?” – Menu Items

#### **Help**

Opens a documentation file in PDF format (keyboard shortcut: F1).

#### **About**

Returns information about IEDIT, the used components, their version numbers and the used license file.

## 3.2 Context Menus

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

- **Edit ...:** Opens the corresponding “Edit ...” dialog window. Atoms, bonds, brackets, No-Structures and entered text can be edited using the appropriate edit entry from the context menu. Please right-click a selected bond, atom, bracket, text or No-Structure to obtain the corresponding edit entry from the context menu. The currently selected atoms, bonds, brackets, No-Structures or text entries can now be edited.
- **Delete:** Deletes the currently selected atom(s), bond(s) or object(s) (keyboard shortcut: DEL).
- **Copy Object(s):** Copies the selected object(s) (into an internal buffer).
- **Paste Object(s):** Pastes the selected object(s) (from an internal buffer).
- **Duplicate Object(s):** Duplicates the selected object(s) (keyboard shortcut: CTRL + D).
- **Copy:** Copies the selected object(s) into the Windows clipboard (keyboard shortcut: CTRL + C).
- **Paste:** Pastes the object(s) from the Windows clipboard into the drawing area (keyboard shortcut: CTRL + V).
- **Expand Superatoms:** Expands the selected superatom(s).
- **Contract Superatoms:** Contracts the selected superatom(s).
- **Create Superatom:** Creates a superatom. Please refer to chapter 7.2 for further details on self-defined superatoms.
- **Add Hydrogen(s):** Fills all atom free sites with explicit hydrogen(s), i.e. additional explicit bond(s) and H atom(s) will be created, which may result in a different hit list when used as substructure query. Please refer to chapter 10 for further details.
- **Create Chiral Flag:** Creates a chiral flag on the selected molecule(s). Please refer to chapter 8 for further details.
- **Group:** Merges multiple selected chemical objects (keyboard shortcut CTRL + G).
- **Ungroup:** Ungroups a selected group of chemical objects (keyboard shortcut CTRL + H).
- **Create No-Structure:** Opens the “Create No-Structure” dialog window to create a No-Structure label. Please refer to chapter 10 for further details on No-Structures.
- **Grid:** Enables or disables grid view of the drawing area.
- **Align...:** Allows the alignment of the selected objects. Different horizontal and vertical align modes are supported (keyboard shortcut CTRL + I).
- **Color...:** Changes the color of the selected object(s). Please refer to chapter 5.5.5 for further details.

**Please note:** The three object methods “Copy Object(s)”, “Paste Object(s)” and “Duplicate Object(s)” do only work within ICDIT.

### 3.3 Keyboard Shortcuts

The following keyboard shortcuts are supported by the IEDIT Windows application:

- **CTRL + C:** Copies the selected object(s) into the Windows clipboard.
- **CTRL + V:** Pastes the object(s) from the Windows clipboard.
- **CTRL + B:** Transfers the object(s) to the calling application (only available if IEDIT is called from another application).
- **CTRL + N:** New window.
- **CTRL + O:** Opens a file in ICF format.
- **CTRL + S:** Saves the current structure(s) or reaction to a file in ICF format.
- **CTRL + A:** Selects all objects within the drawing area.
- **CTRL + Z:** Undoes the last operation.
- **CTRL + Y:** Redoes the last undone operation.
- **CTRL + D:** Duplicates the selected object(s).
- **CTRL + G:** Merges multiple selected chemical objects.
- **CTRL + H:** Ungroups a selected group of chemical objects.
- **CTRL + I:** Opens the "Align objects" dialog window to allow specific alignment of the selected objects.
- **DEL:** Deletes the currently selected atom(s), bond(s) or object(s) from the drawing area.
- **F1:** Opens a documentation file in PDF format.

## 4 Buttons

Various edit and template buttons are provided in the toolbars of the IEDIT application. The selected 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.

Please find below a detailed description of all template and edit buttons.

### 4.1 Standard Edit Buttons



Clear screen.

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



Delete object.

The object(s) (atom(s), bond(s), molecule(s) and text) you are selecting with your mouse will be deleted. If you draw a rectangle, all objects within that area will be deleted (keyboard shortcut: DEL).



Undo last operation.

Undoes the last operation (keyboard shortcut: CTRL + Z).



Redo last operation.

Redoes the last undone operation (keyboard shortcut: CTRL + Y).



Select.

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



Select object.

Use this tool to select whole objects or grouped objects. Click on a specific object as soon as it is marked by a red frame to select the complete object. The selected object(s) can then be moved (drag with your mouse), deleted, copied or edited using the context menu, the menu bar items or the appropriate keyboard shortcuts.



Rotate selected objects.

Use this tool to rotate the selected object(s) either clockwise or anti-clockwise around the center of the selection frame.



Add reaction plus.

Adds a reaction plus to the drawing area.



Add reaction arrow.

Adds a reaction arrow to the drawing area.

**Please note:** Only one arrow per reaction is supported in reaction queries.

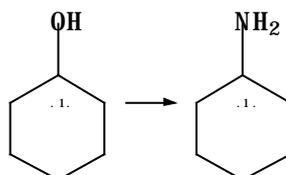


Map atoms.

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:



**Please note:** Depending on the license file settings the IEDIT application provides also automapping functionality via the „Automap the reaction“ button. Please refer to the description given below for further information.



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 for the definition of Rgroup queries. Please refer to chapter 10 for further information on Rgroup input.



Remove Rgroup Info from atom.

Click single atoms to remove the Rgroup information.



Show Info dialog.

Returns information about IEDIT, the used components, their version numbers and the used license file.



Transfer structure back to calling application.

Transfers the current structure(s) or reaction back to the calling application and closes IEDIT (only visible if IEDIT is called from another application) (keyboard shortcut: CTRL + B).



Draw text.

Activates the text input cursor within the drawing area at the selected position. Please refer to chapter 6 for further information on text input and editing options.



Draw Brackets.

Draws a pair of brackets. Please refer to chapter 9 for further details.



Automap the reaction.

Mapping numbers and reaction center information will be added automatically to a drawn reaction. Please refer to chapter 11 for further information.



Standardize the structure.

Standardizes the selected molecule or reaction in accordance with InfoChem's standardization rules. Please refer to chapter 12 for further information.

## 4.2 Template Buttons

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

### 4.2.1 Molecule Template Buttons

The following molecule template buttons are available within the IEDIT application:



Furthermore, the IEDIT Windows application provides many additional templates via the "Templates" dialog window (please refer to chapter 3.1.5). For creation of user-defined templates please refer to chapter 11.

### 4.2.2 Atom Buttons



Draw an atom.

Use the "Draw an atom" dialog window to define atom types, atom properties and atom query features. Please refer to chapter 5.3 for further information about editing atoms.



Draw carbon atoms.

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 nitrogen atoms.

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 oxygen atoms.

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 sulfur atoms.

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

### 4.2.3 Bond Buttons



Draw single bonds or change existing bonds.

Adds a single bond. Either click (i) on a free spot within the drawing area, (ii) on an existing atom or (iii) drag a bond between two atoms. With additional clicks on a single bond, you can convert it into:

- a double bond: one additional click,
- a triple bond: two additional clicks,
- a single bond again: three additional clicks.

**Please note:** It is only possible to convert a double bond into a triple bond if the valence on the connected atoms is not exceeded. If the valence is exceeded a single bond is drawn instead. In this case a triple bond can be drawn using the “Draw triple bonds” button or the “Edit Bond” dialog window.



Draw double bonds or change existing bonds to double bonds.

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



Draw triple bonds or change existing bonds to triple bonds.

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



Draw up wedges or change existing bonds to up wedges.

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

**Please note:** The orientation of up wedges is important for the automatic detection of the stereochemistry (e.g. in case of query features).



Draw down wedges or change existing bonds to down wedges.

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

**Please note:** The orientation of down wedges is important for the automatic detection of the stereochemistry (e.g. in case of query features).



Draw a chain.

Draws a chain of C-C single bonds.

## 5 Using the Editor

### 5.1 Draw Objects

To draw atoms, bonds or templates, click the corresponding button to activate the drawing mode. You can change the orientation of 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.

### 5.2 Select Objects

To select whole objects or parts of objects please choose the "Select" button and draw a rectangle covering the desired bond(s) and/or atom(s) and/or object(s).

To select a bond or an atom, please click the desired bond or atom. For the selection of multiple bonds and/or atoms, please press down the SHIFT button while clicking the atoms and/or bonds.

Choose the "Select Object" button to select whole objects or grouped objects at once.

### 5.3 Scale Objects

To scale one or more objects please select the object(s) and use the double headed arrow from one of the four corners of the selection frame to change the size of the object(s).

## 5.5 Edit Objects

### 5.5.1 Edit Atoms

You can change the atom label of a selected atom by using the keyboard. Please type an atom label and press ENTER. The input of atom types is not case sensitive.

**Please note:** After drawing a bond, the atom at the end of the bond is selected automatically. This feature facilitates the input of atom labels by simply drawing a bond, typing the atom label and pressing ENTER.

Atom charge and isotope information can be entered together with the corresponding atom label:

- 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 isotope number and the atom symbol respectively (e.g. 2H).

**Please note:** If multiple atoms are selected (or a whole molecule) and an atom symbol is entered using the keyboard all atoms within the selection will be replaced.

In addition you can change an atom symbol using the “Draw an Atom” dialog window. To open the dialog window please use either the edit button “Draw an atom”, the context menu item “Edit Atom” or double-click a specific atom.

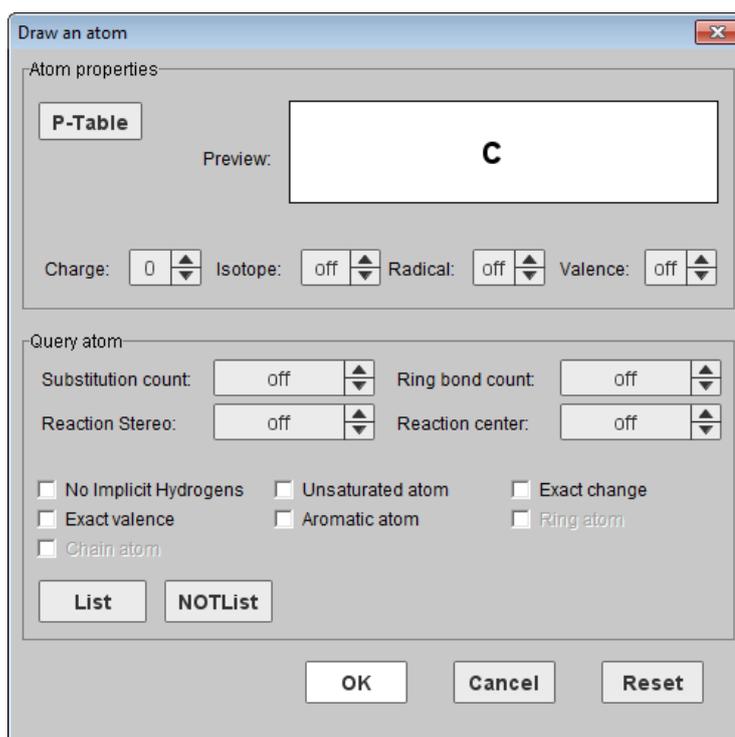
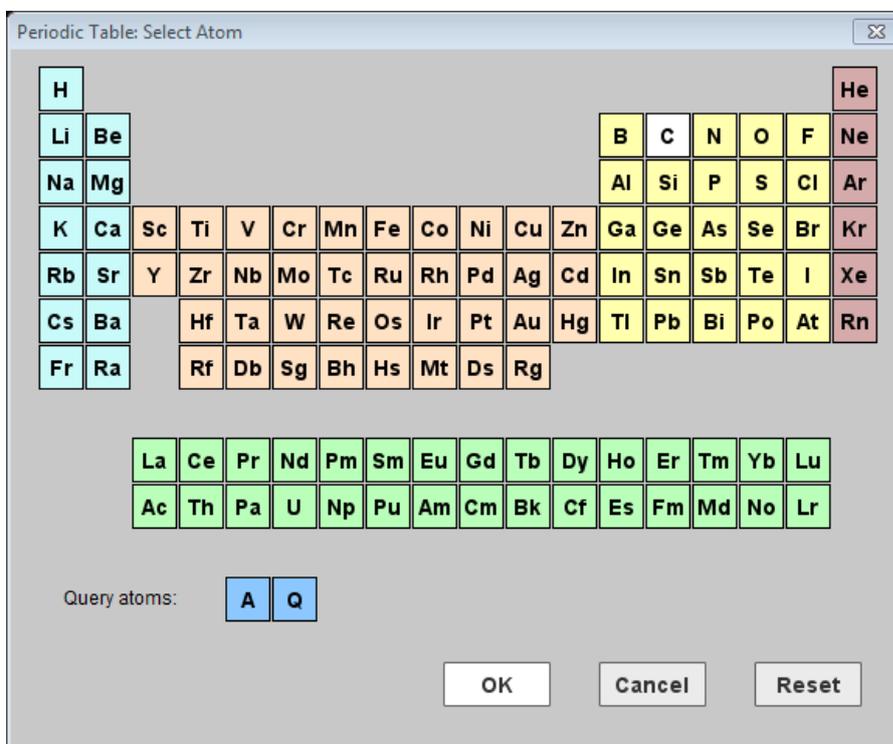


Fig. 10: “Draw an Atom” dialog window.

Use this dialog window to define atom properties and atom query features:

**Atom properties:** Use this dialog window to define charge, isotope or radical information and atom valence.

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



**Fig. 11:** "Periodic Table" dialog window.

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

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

**Query atom:** The following query features are implemented and can be adjusted:

- Substitution count (s0-s6, s\*).
- Ring bond count (r0, r2-r4, r\*).
- Reaction Stereo (retention, inversion).
- Reaction center (not center, R-center) will be supported in future.
- List: opens the "Periodic Table" dialog window where you can create an atom list for a query.
- NOT List: opens the "Periodic Table" dialog window 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.

Please refer to the document ICFSE\_Tutorial.pdf in the "Documentation" folder in the IEDIT installation path for further information on the input and use of query features.

## 5.5.2 Edit Bonds

Select one or several bond(s) and click on the right mouse button. Select “Edit Bond(s)” from the context menu to open the “Edit Bond” dialog window or double-click a specific bond.

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.

**Please note:** If multiple bonds are selected (or a whole molecule) and the bond characteristics are changed using the “Edit Bond” dialog window all selected bonds will be edited. This is especially useful when query features or delocalized double bonds are added to a molecule.

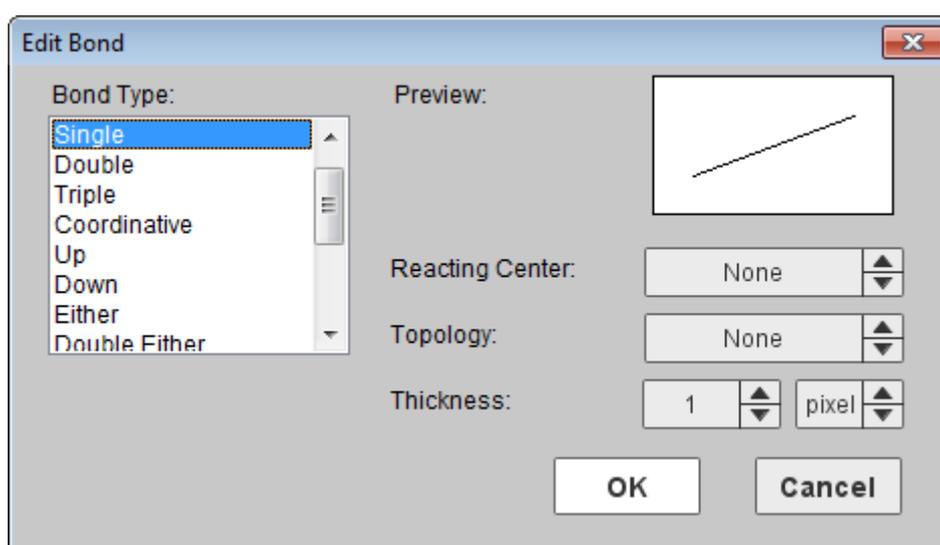


Fig. 12: “Edit Bond” dialog window.

The following bond types are supported:

—	Single	=====	Aromatic
==	Double	----	Any
≡	Triple	= =	Single/Double
▲	Up	==	Single/Aromatic
▼	Down	==	Double/Aromatic
⚡	Either	-----	Coordinative (display only)
✂	Double Either		

The following reaction query features are supported:

### Reacting Center

- |                                   |                          |
|-----------------------------------|--------------------------|
| <del>✕</del> Not Center           | <del>  </del> Make/Break |
| <del>  </del> Make/Break & Change | <del>#</del> Center      |
| <del>+</del> Change               |                          |

### Topology

- |                     |                    |
|---------------------|--------------------|
| <del>Ch</del> Chain | <del>Rn</del> Ring |
|---------------------|--------------------|

### 5.5.3 Group or Ungroup Chemical Objects

#### Group

To group multiple chemical objects please select the desired objects and use either the context menu item "Group", the keyboard shortcut CTRL + G or the item "Object - Group" from the main menu.

The selected objects are now grouped and will be treated as a single object, as you can see from the single selection frame which is covering all objects belonging to the created group.

#### Ungroup

To ungroup a group of multiple chemical objects please select the desired group and use either the context menu option "Ungroup", the keyboard shortcut CTRL + H or the item "Object - Ungroup" from the main menu.

**Please note:** Multiple objects that are grouped act as one single object.

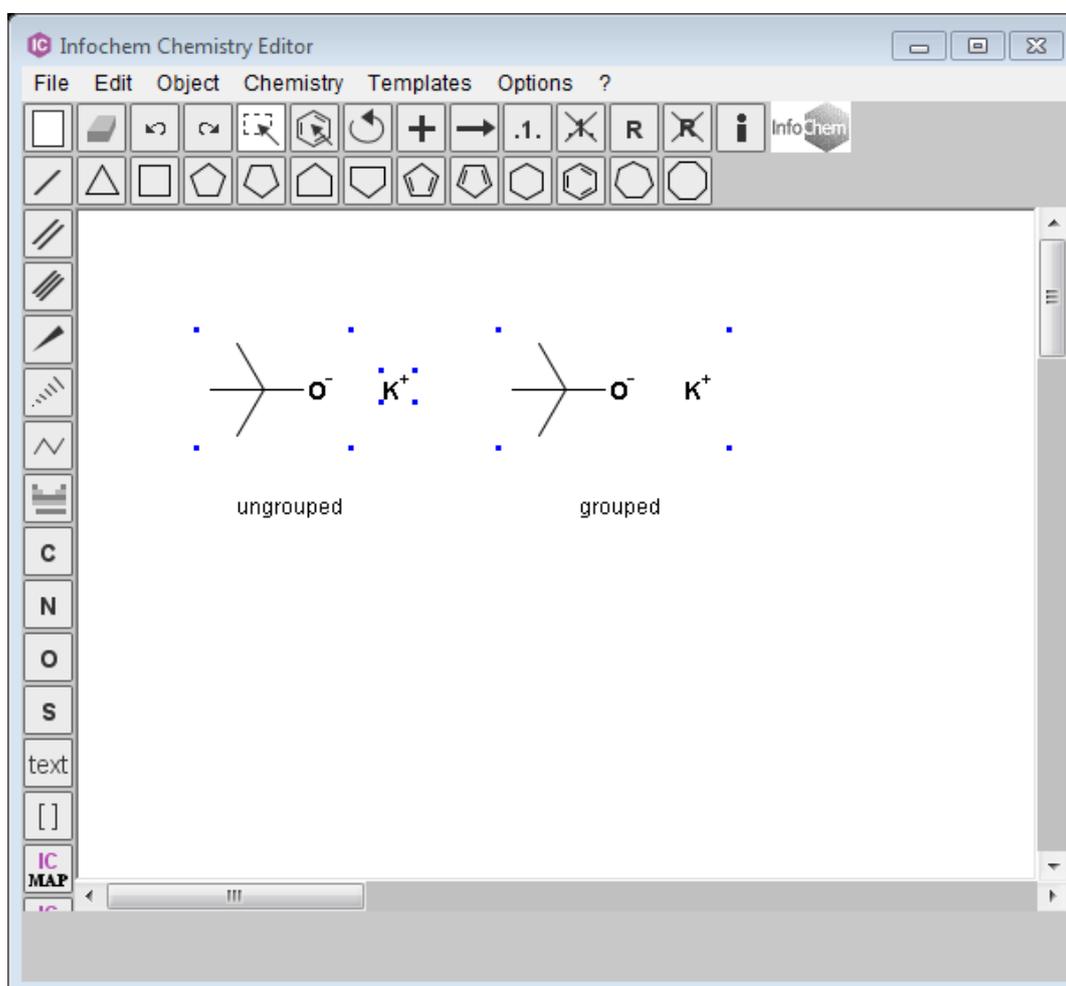


Fig. 13: Example for different selection frames of ungrouped and grouped objects.

## 5.5.4 Create a Chiral flag

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

To add a chiral flag, please select the molecule you want to label as chiral and use the context menu item "Create Chiral Flag".

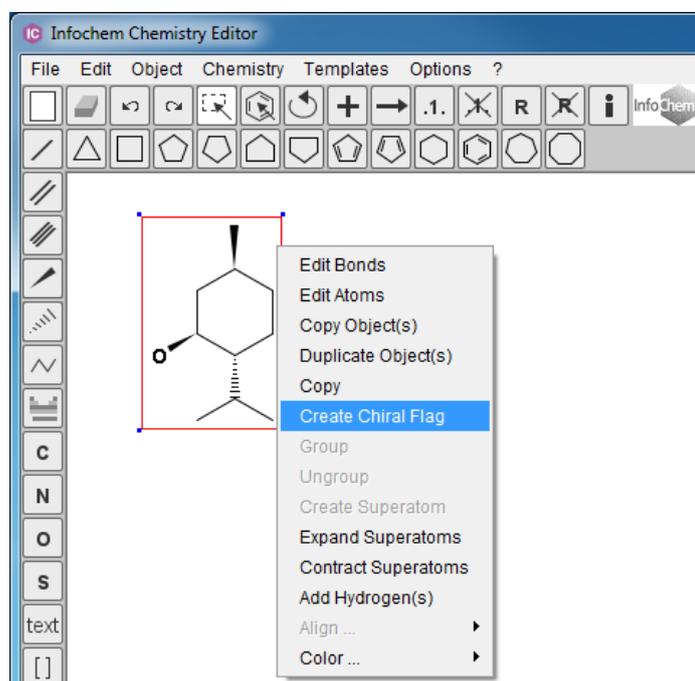


Fig. 14: Create a chiral flag.

The labeled molecule is now marked with the text box "chiral".

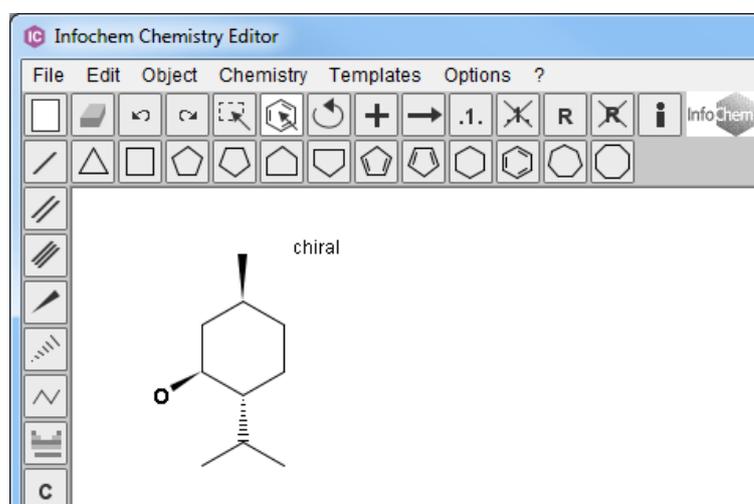


Fig. 15: Create a chiral flag - Result.

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

## 5.6 Display Features

The following display features are supported:

- **Implicit hydrogen labels:** Per default all implicit hydrogen labels are hidden. You can change the “show hydrogen labels” option via the “Atoms” tab in the “General Settings” dialog window to show implicit hydrogen labels “On All”, “On Hetero or Terminal” or “On Hetero” atoms.
- **Color (for atoms, bonds and text):** You can change the color either by using the “General Settings” dialog or by using the context menu item “Color...”. See also chapter 5.6.2.
- **Font type, size and style (for atoms and text):** You can change the font settings by using the “General Settings” dialog window. Additionally any text object can be edited using the “Edit Text” dialog window.
- **Bond thickness:** You can change the bond thickness either by using the “Bonds” tab in the “General Settings” dialog window or by using the “Edit Bond” dialog window (chapter 5.4).
- **Grid:** Please use the context menu item “Grid” to obtain grid view of the drawing area.

## 5.6.1 General Settings

### General Settings – “General” tab

The “General” tab of the “General Settings” dialog window enables changing the color of all objects. The changed settings will be used for all new objects including atom, bond and text objects.

**Please note:** Starting from ICEDIT version 3.0 atoms and bonds are drawn with antialiasing by default. To get the previous behavior please disable the “Draw antialiased” option.

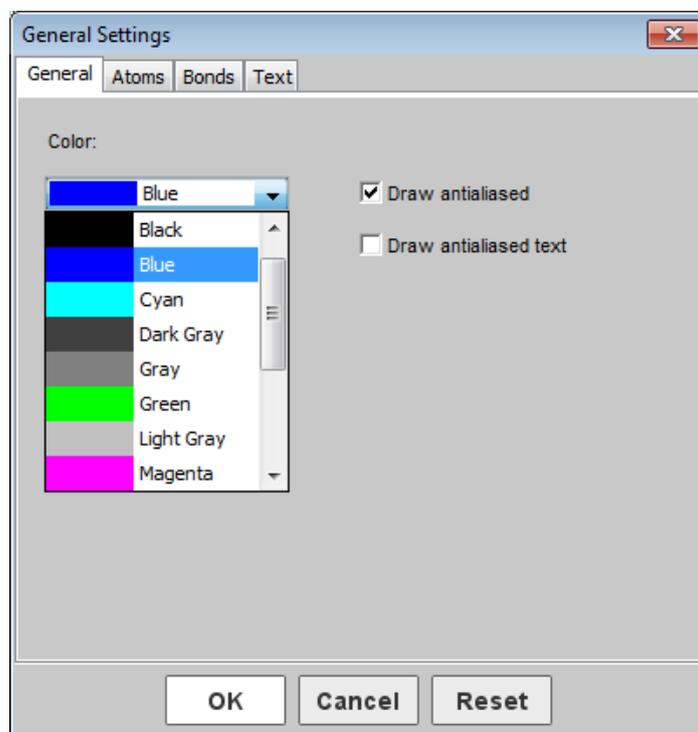


Fig. 16: “General Settings” dialog window – “General” tab.

You can activate the selected settings by clicking “OK”.

With the “Reset” button the default settings of ICEDIT are restored.

**Please note:** If you are changing any settings from the “General settings” dialog window you will be asked whether you would like to apply the changed settings to already existing objects, too. If you click “Yes” all already drawn objects will be adjusted as well. If you click “No” the already existing objects will remain unchanged.

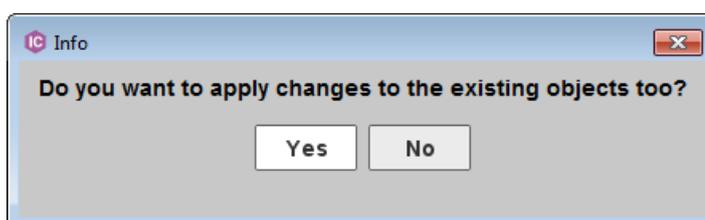


Fig. 17: “General Settings” dialog window – “Info” box.

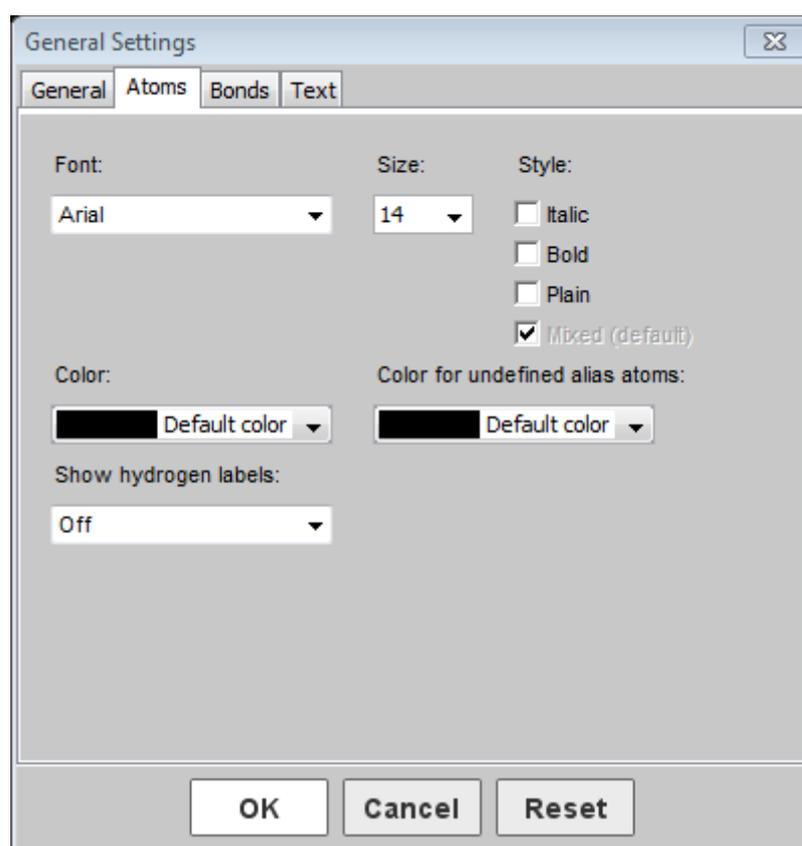
### General Settings – “Atoms” tab

In the “Atoms” tab of the “General Settings” dialog window you can adjust (i) the atom font type, (ii) the atom font size, (iii) the atom font style as well as (iv) the color of atoms and of undefined alias atoms.

In addition, you can adjust the display of implicit hydrogen labels.

You may switch the display of hydrogen labels to

- Off: No implicit hydrogen labels will be displayed.
- On Hetero: Implicit hydrogen labels will be displayed on heteroatoms.
- On Hetero or Terminal: Implicit hydrogen labels will be displayed on heteroatoms and on terminal carbon atoms.
- On All: Implicit hydrogen labels will be displayed on all atoms.



**Fig. 18:** “General Settings” dialog window – “Atoms” tab.

**Please note:** An implicit hydrogen is a hydrogen that is either assumed to be present (invisible) or attached to an atom without an explicit bond. Implicit hydrogens are not considered in a search query. If you want to create a search query that allows solely hydrogen atoms at specific positions in the structures retrieved, you must draw explicit hydrogens (hydrogen atoms connected via a single bond). You may also use the function “Add Hydrogen(s)” to add explicit hydrogens to all open sites of the selected molecule (see chapter 10).

### General Settings – “Bonds” tab

In the “Bonds” tab of the “General Settings” dialog window you can adjust (i) the thickness of the bonds, (ii) the length of the bonds as well as (iii) the color of the bonds.

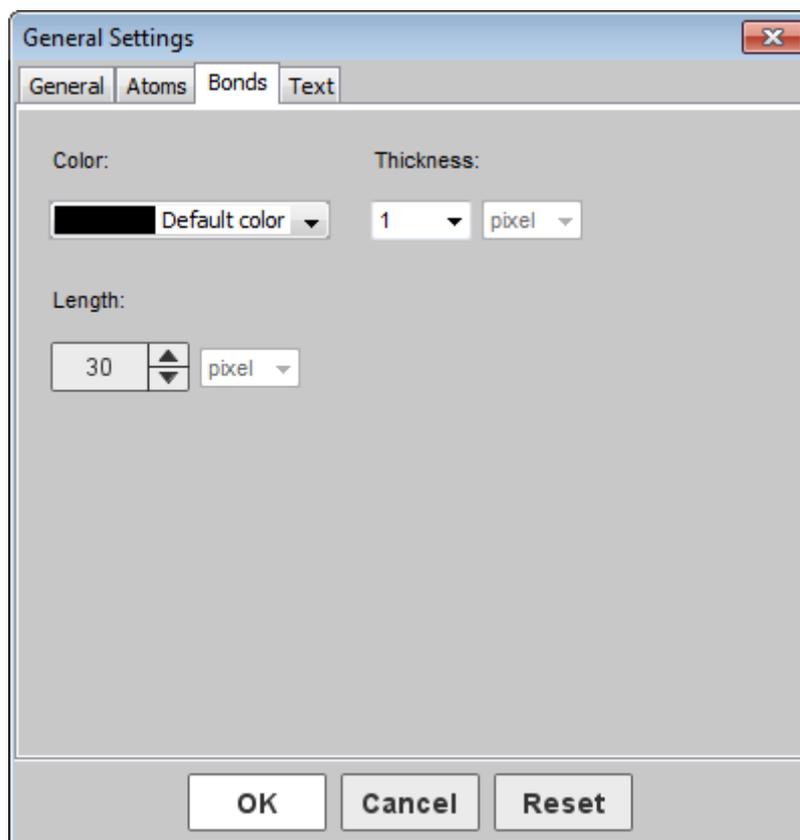


Fig. 19: “General Settings” dialog window – “Bonds” tab.

### General Settings – “Text” tab

In the “Text” tab of the “General Settings” dialog window you can adjust (i) the text font type, (ii) the text font size, (iii) the text font style as well as (iv) the color of the text. Please use the “Edit Text” functionality as described in chapter 6 for individual adjustments to text objects and the input of Symbols or specific characters.

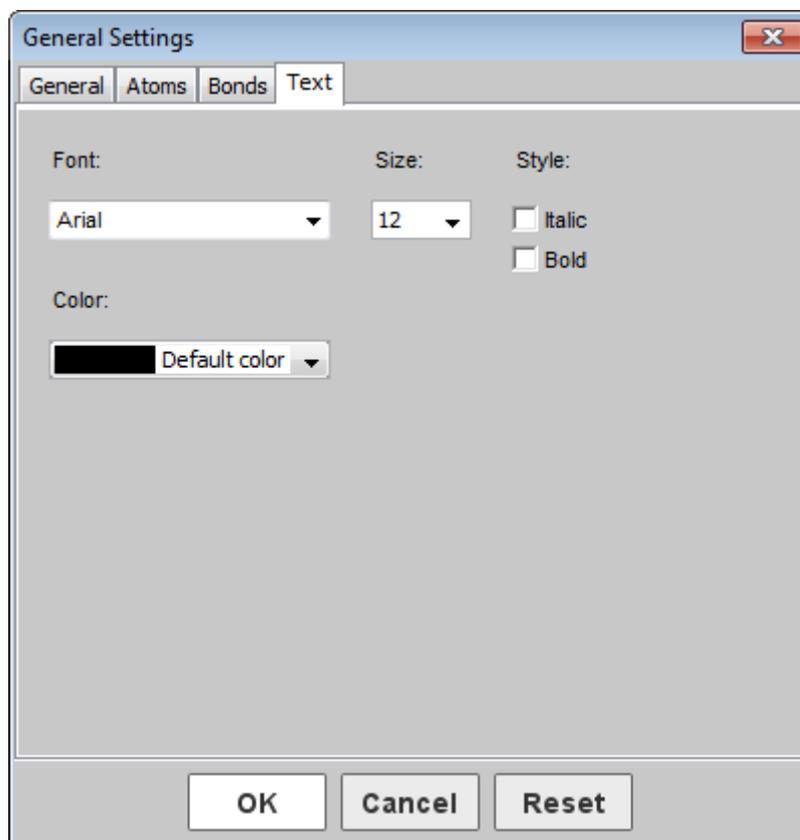


Fig. 20: “General Settings” dialog window – “Text” tab.

## 5.6.2 Color

It is possible to change the color of any selected object. Besides whole molecules and reactions also single bonds and atoms can be colored. 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.

The color of single text objects can additionally be adjusted in the “Edit Text” dialog window (please refer to chapter 6).

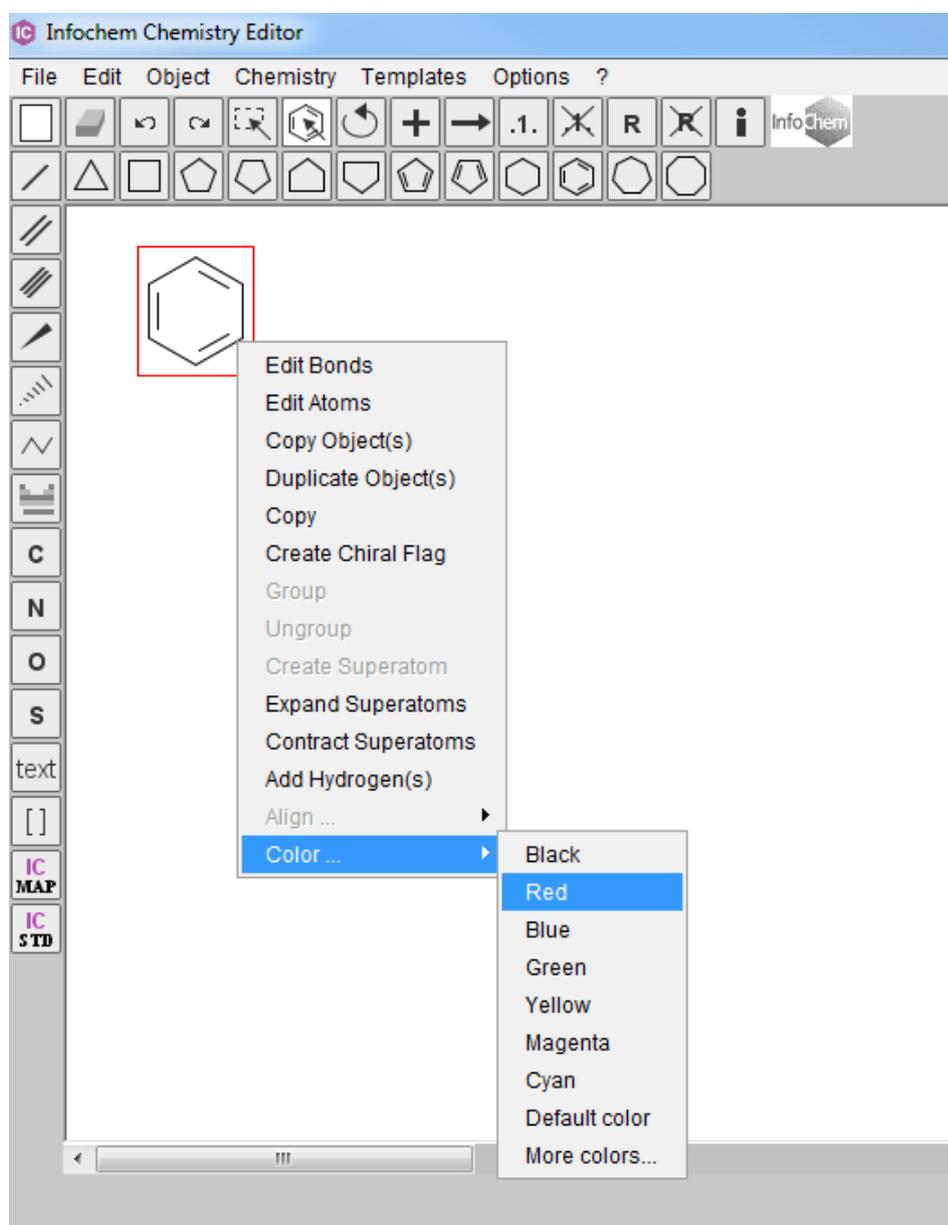
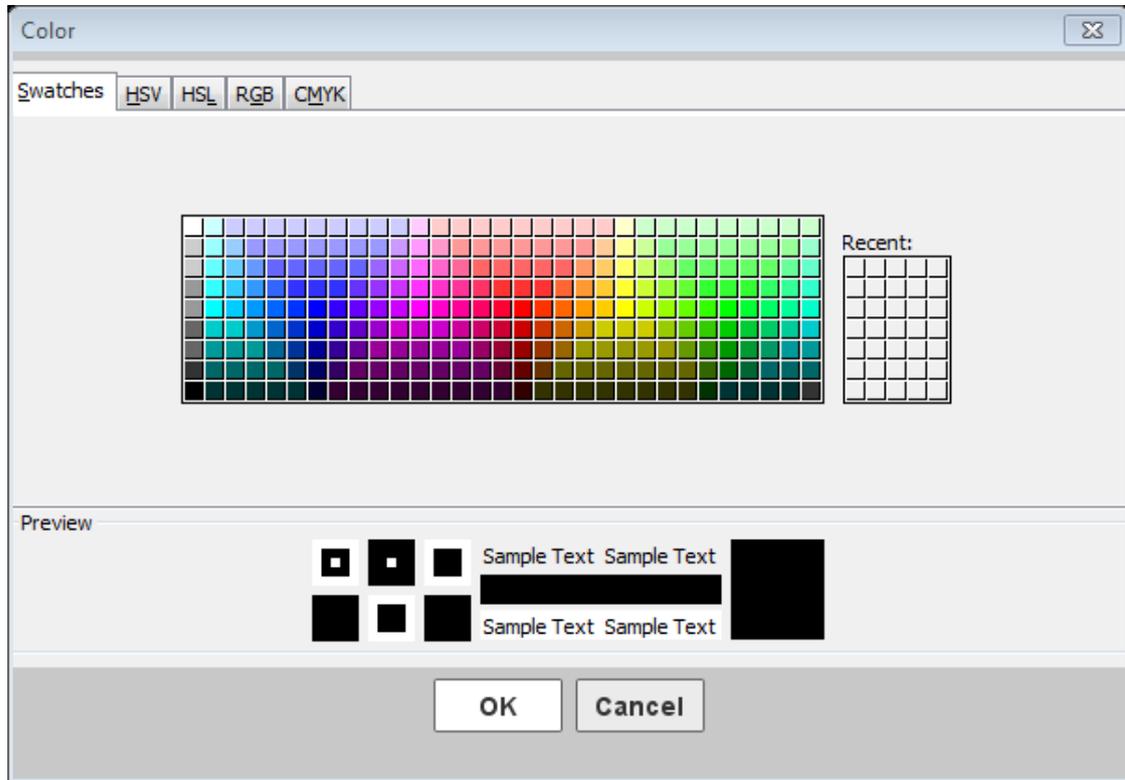


Fig. 21: “Color...” context menu.

**Please note:** The *default color* dyes all atoms and bonds black while expanded superatoms will be highlighted in dark gray (see also chapter 7). In contrast, the color *black* dyes everything black: bonds, atoms and expanded superatoms.

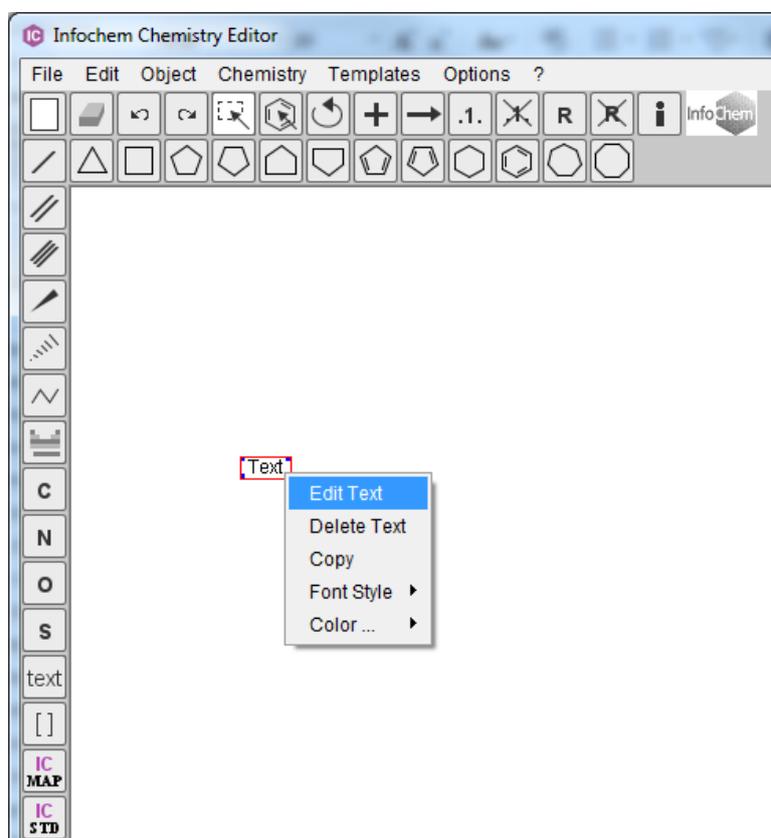
In addition to the predefined standard colors any desired color can be selected by using the “Color” dialog window. You can open the “Color” dialog window by choosing “More colors” from the color drop-down box from the “General Settings” dialog window or by choosing “More colors...” from the “Color...” context menu item.



**Fig. 22:** “Color” dialog window.

## 6 Text

Please use the text button  from the ICEDIT application toolbar to enter a text string.



**Fig. 23:** “Text” context menu.

You can edit, delete or copy a text label using the “Text” context menu. Furthermore, the “Text” context menu allows fast adjustment of selected font styles and colors.

To edit any text either directly double-click the text label or right-click the text label and choose “Edit Text” from the context menu. The “Edit Text” dialog windows opens.

You can adjust the font type, the size, the style, the style effects and the color of the text label. For this purpose please select any text fragment from the displayed text and select the desired property. Click “OK” to leave the “Edit Text” dialog window.

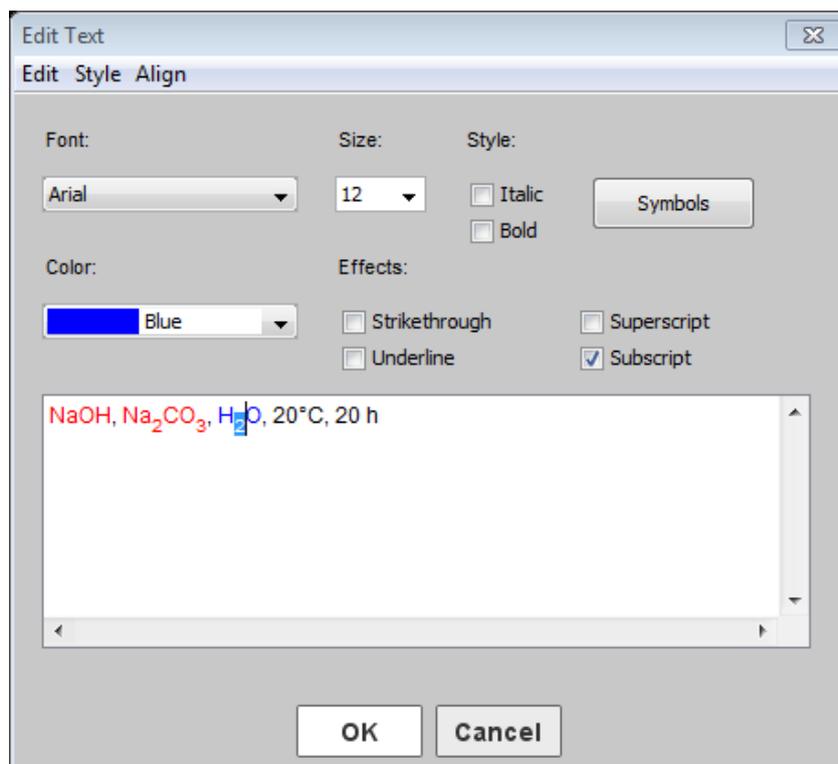


Fig. 24: “Edit Text” dialog window.

You can add particular symbols to the text label via the “Symbols” dialog window. Click the “Symbols” button to open the “Symbols” dialog window. The following characters are supported:



Fig. 25: “Symbols” dialog window.

**Please note:** General text settings like font type, size, style and color that are applied to all text fields during one ICEDIT session can be adjusted using the “General Settings” dialog window (“Options – Settings...” from the main menu, see chapter 5.6.1).

## 7 Superatoms

### 7.1 Support of Superatoms

The input and recognition of common superatom labels like COOH, OMe, Cbz, NO<sub>2</sub> is supported by the IEDIT application.

The superatom labels 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 label 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.

#### 7.1.1 Input of Superatoms

The input of superatom labels is case sensitive.

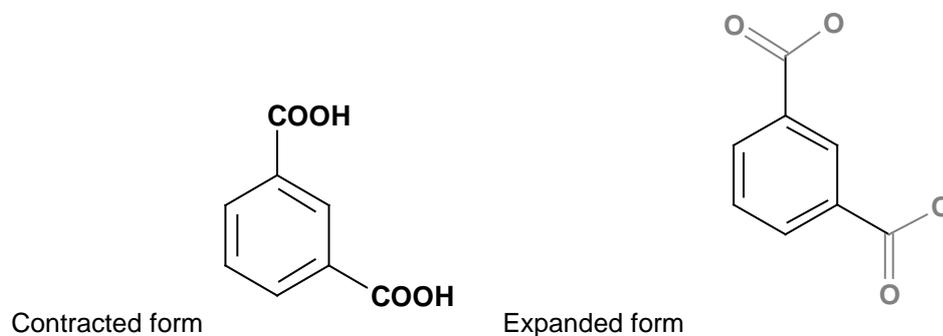
- All atom symbols in superatom labels must be drawn as represented in the Periodic Table of the Elements (e.g. **COOH**, **OMe**, **SiMe<sub>3</sub>**).
- Abbreviations are case sensitive as well. They are supported in the most common notation (e.g. Me is supported, me or ME is not supported). The standard typing of these common 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

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 label and use the right mouse button to open the context menu. Choose "Expand Superatom".
- **Contract a single superatom:** To contract a single superatom select any atom of the specific expanded structure and use the right mouse button to open the context menu. Choose "Contract Superatom".

- **Expand all superatoms:** To expand all superatoms choose “Chemistry - Superatoms - Expand all” from the menu bar. Alternatively, select all (CTRL + A) and use “Expand superatoms” from the context menu.
- **Contract all superatoms:** To contract all superatoms chose “Chemistry - Superatoms - Contract all” from the menu bar. Alternatively, select all (CTRL + A) and use “Contract superatoms” from the context menu.

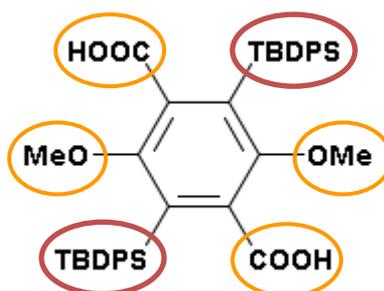
Example:



### 7.1.2 Display of Superatom Labels

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

Example:



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

**Please note:** Most abbreviations do not change their order.

Examples:

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

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. For example, 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 Info” from the main menu of the IEDIT application to find a full list of supported superatom labels.

## 7.2 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.

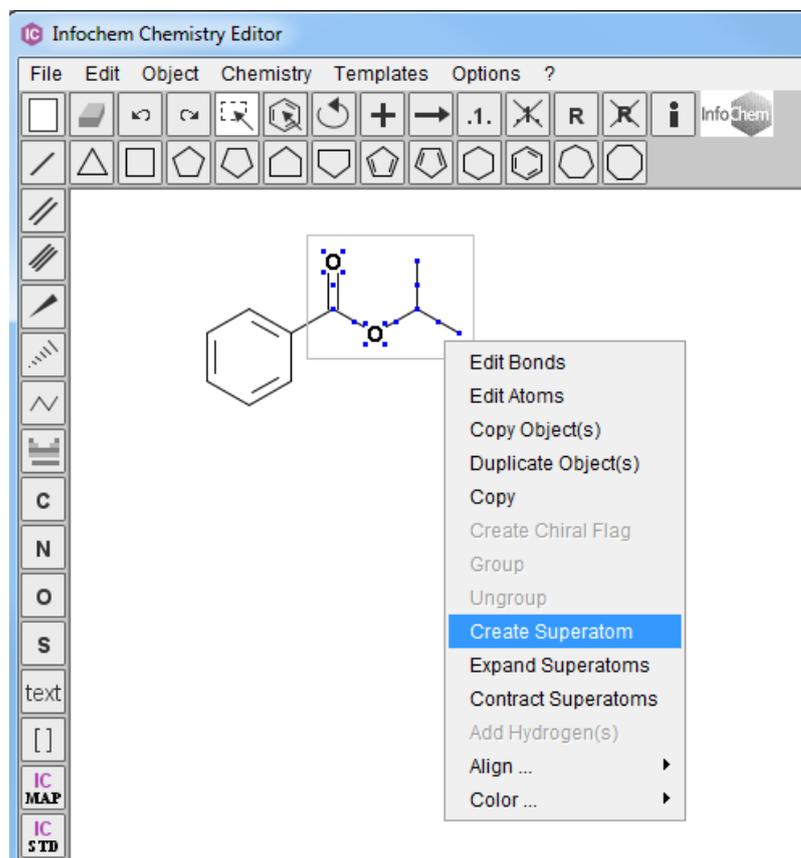
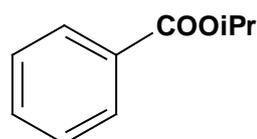


Fig. 26: Create a self-defined superatom.



Fig. 27: “Create Superatom” dialog window.



The superatom is now shown as defined alias label:

**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 in a new molecule.

Currently, the storage of self-defined superatoms as user-defined templates is not yet supported.

## 8 Brackets

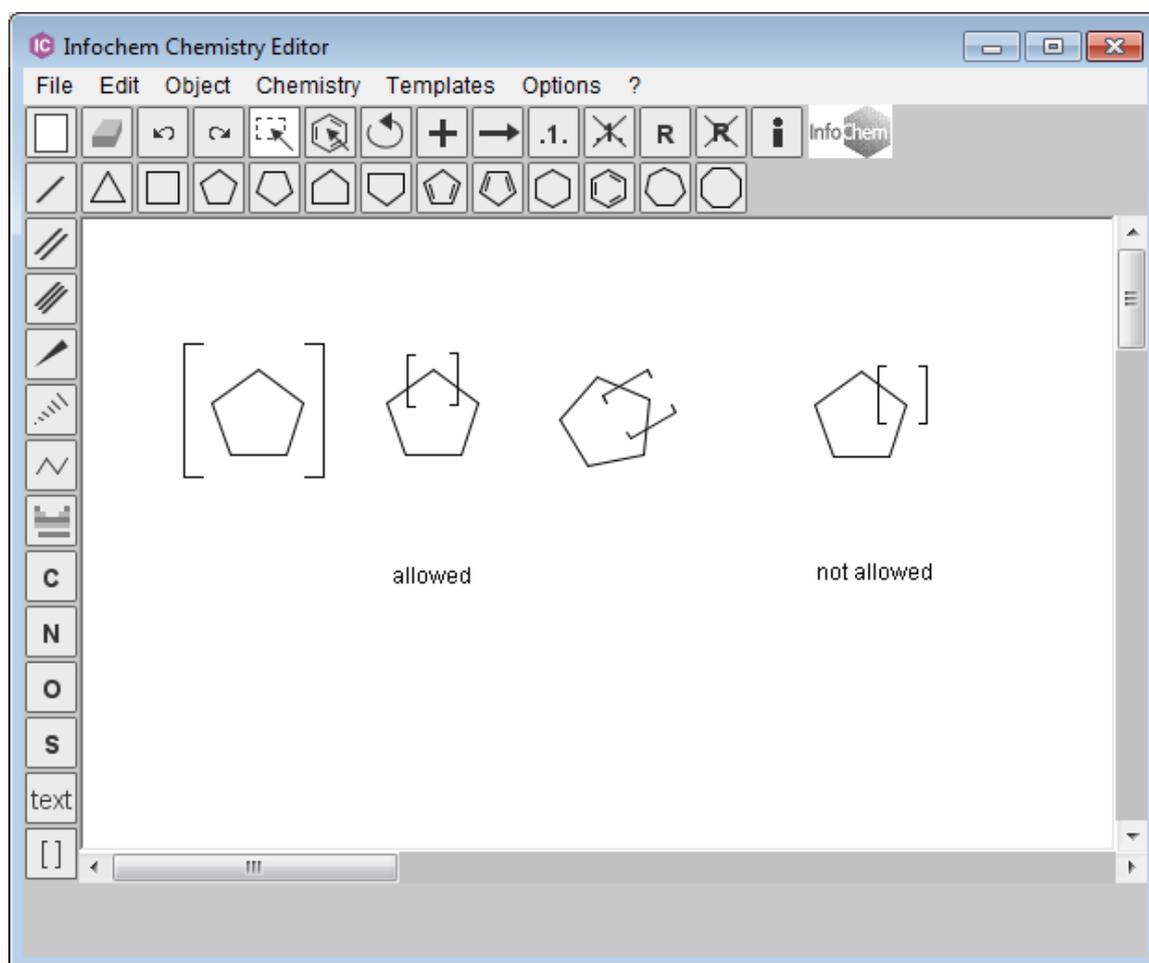
To draw a bracket, please select the bracket  button from the toolbar and draw a pair of brackets into the drawing surface using the mouse cursor.

**Please note:** The distance between the pair of brackets and the height can be adjusted later by selecting and moving a single bracket.

Molecules can only be interpreted correctly if the brackets are drawn properly. The following types of brackets are supported:

- A pair of brackets covering a complete molecule.
- A pair of brackets covering a section in-between a molecule.

**Please note:** Both brackets of a pair must cross a bond of the molecule in this case.



**Fig. 28:** Examples for brackets.

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.

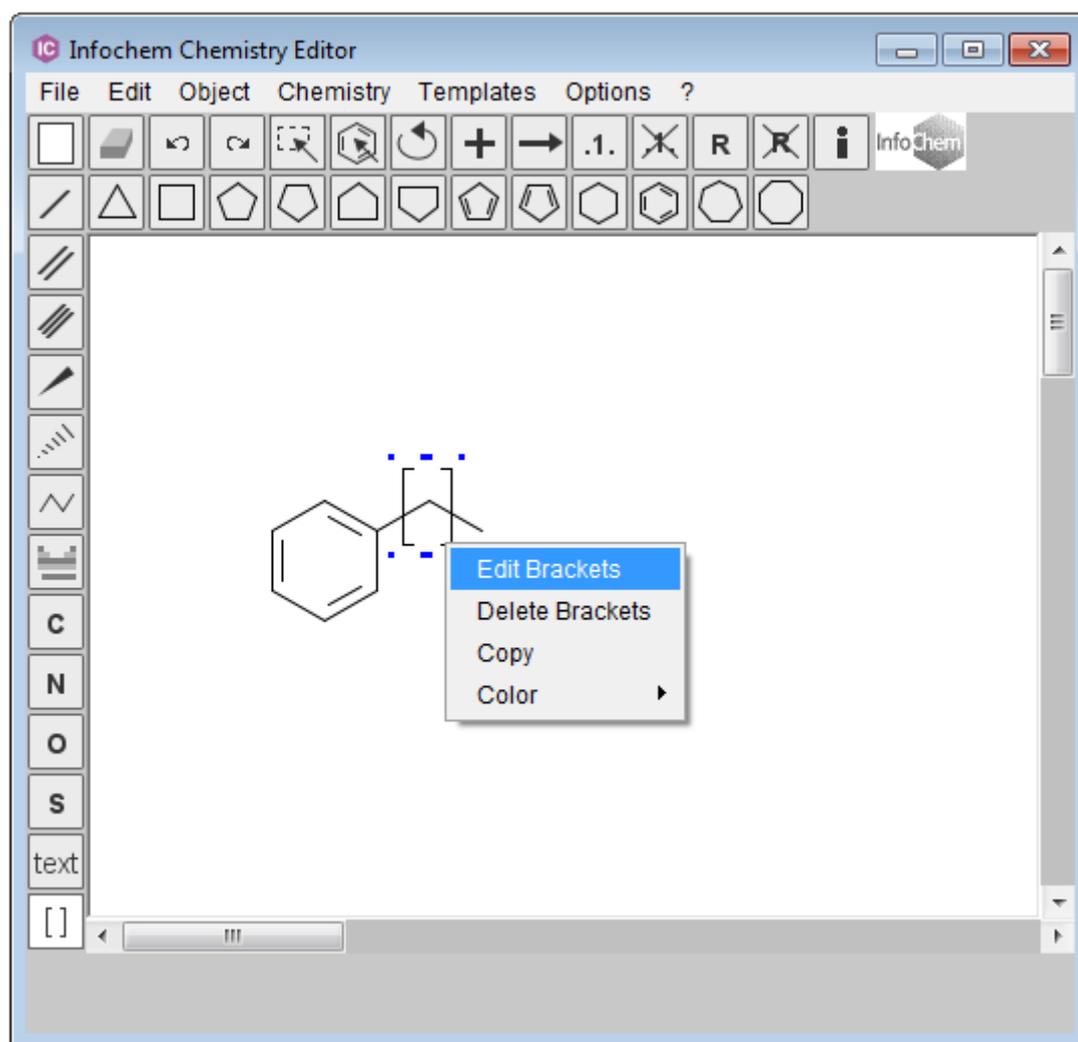
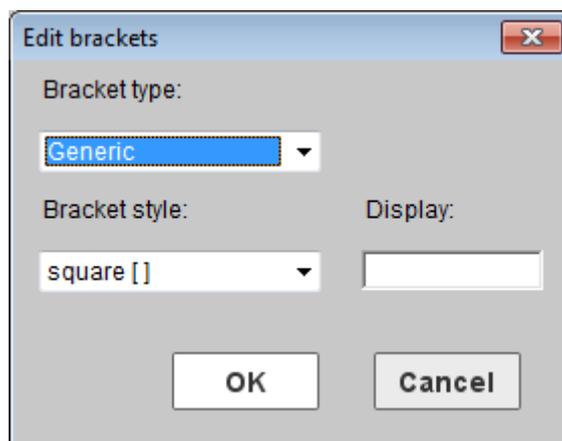


Fig. 29: "Brackets" context menu.

**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:



**Fig. 30:** “Edit brackets” dialog window.

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 starting 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 structure part inside the bracket is not multiplied, if the “SRU” value is set to 2. However, if the “Multiple group” value is set to 2 the structure part inside the bracket is multiplied.

Edit the Bracket Style:

The two bracket styles “square” and “round” are supported by the IEDIT application. However, this is only a display feature, therefore both styles are treated chemically in the same way.

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 No-Structure

### Definition:

No-Structures are used to enter non-structural components into structure or reaction databases. Some molecules cannot be represented by a drawn structure but do play significant roles in reactions, e.g. enzymes or microorganisms like baker's yeast. In these cases No-Structure labels can be used to insert the molecules into the database. This means the molecule is represented by a No-Structure label (recognized as valid database input) and not by a structure.

### Create a No-Structure:

Please use either the context menu item "Create No-Structure" or the main menu item "Chemistry>Create No-Structure" to open the "Create No-Structure" dialog window.

Please enter a desired caption or use the default caption "No-Structure" for your No-Structure. The No-Structure label will be added to the drawing area by clicking "OK".



**Fig. 31:** "Create No-Structure" dialog window.

### Edit a No-Structure:

You can edit, delete or color a No-Structure by using the "No-Structure" context menu. To open the "No-Structure" context menu, please move the mouse cursor above the No-Structure until a red frame appears. You can now open the "No-Structure" context menu by right-clicking the No-Structure label.

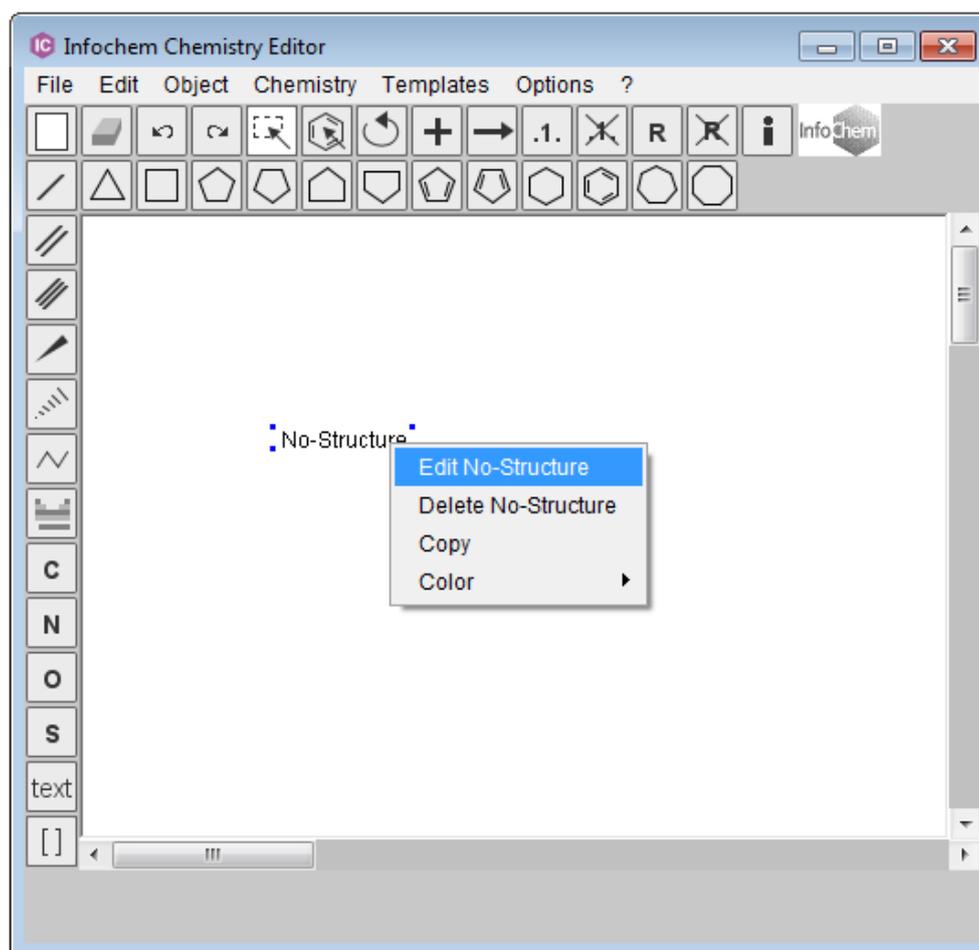


Fig. 32: "No-Structure" context menu.

**Please note:** A reaction or molecule containing a self-defined No-Structure can be copied, saved or exported like any other usual molecule. However, the No-Structure together with its self-defined No-Structure label can only be exported into ICF format. The label and the position of the self-defined No-Structure cannot be transported by any other format and will be lost.

## 10 Add Hydrogen(s)

The “Add Hydrogen(s)” functionality generates explicit hydrogens to a drawn query structure to generate closed sites.

To add the hydrogen atoms please select a structure and choose “Add Hydrogen(s)” from the object context menu.

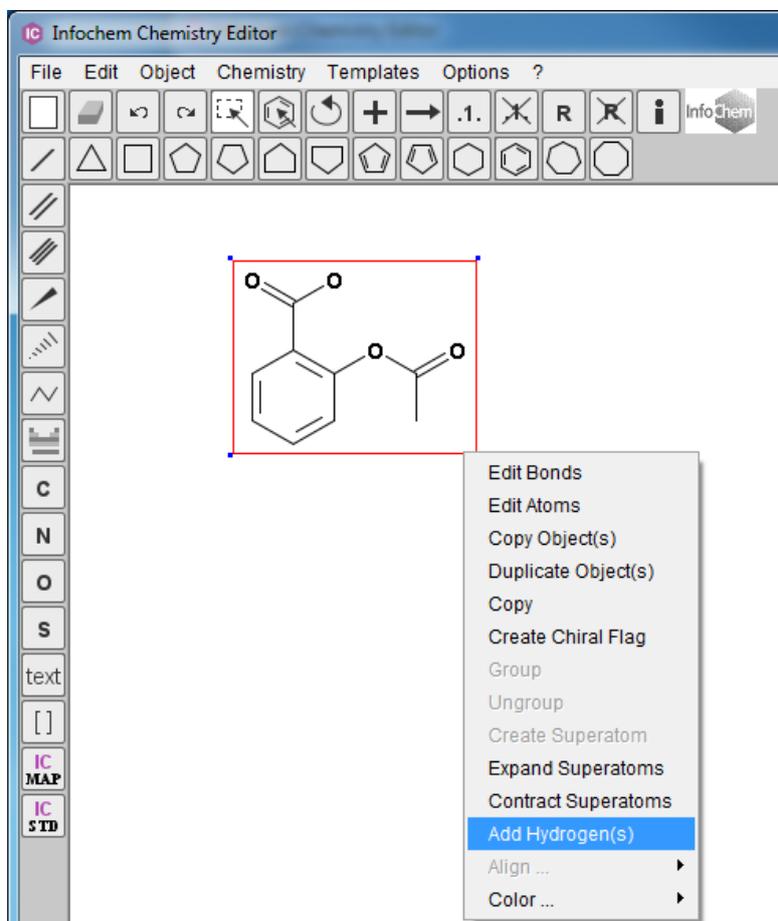
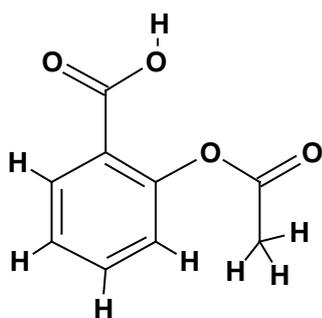


Fig. 33: “Add Hydrogen(s)” functionality.

Result:



**Please note:** The “Add Hydrogen(s)” functionality does only support single molecules without query features. Multiple (non-grouped) molecules must be selected separately, fragments or query features are not supported yet.

## 11 Automap a Reaction

Please select the desired reaction and click the “Automap the reaction” button  to add mapping numbers and reaction center information automatically to the reaction. To remove the mapping and reaction center information please use the “Remove mappings” button from the button bar . The “Automap the reaction” button automatically maps atoms and automatically adds reaction centers whereas the “Map atoms” button  allows the manual input of mapping numbers (see above).

**Please note:** The “Automap the reaction” button is only available if the automap functionality is included in your license. Please contact us for further licensing information ([iceditsupport@infochem.de](mailto:iceditsupport@infochem.de)).

## 12 Standardize a Structure/Reaction

Please select the desired structure or reaction and click the “Standardize the structure” button  to standardize the selected molecule or reaction in accordance with InfoChem’s standardization rules.

For further details on applied standardization rules please refer to the document “Standardization Rules” in the “Documentation” folder in the IEDIT installation path. Please use the undo button to restore your previously drawn structure/reaction if the standardization does not meet your requirements.

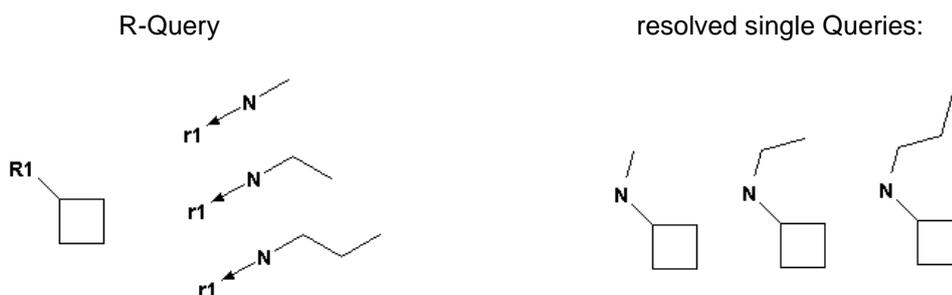
**Please note:** The “Standardize the structure” button is only available if the standardization functionality is included in your license. Please contact us for further licensing information ([iceditsupport@infochem.de](mailto:iceditsupport@infochem.de)).

## 13 RGroup Queries

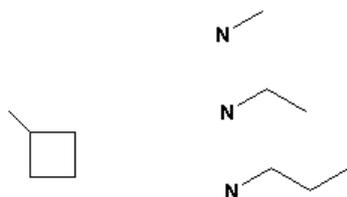
An RGroup search finds molecule records in a database that contain a desired core structure with defined variable functional groups or structure parts. Instead of performing multiple queries you can combine a parent structure with variable RGroups to use one single query to retrieve the desired records.

The following examples demonstrate how to input Rgroup queries.

### Example 1: Rgroups with one attachment

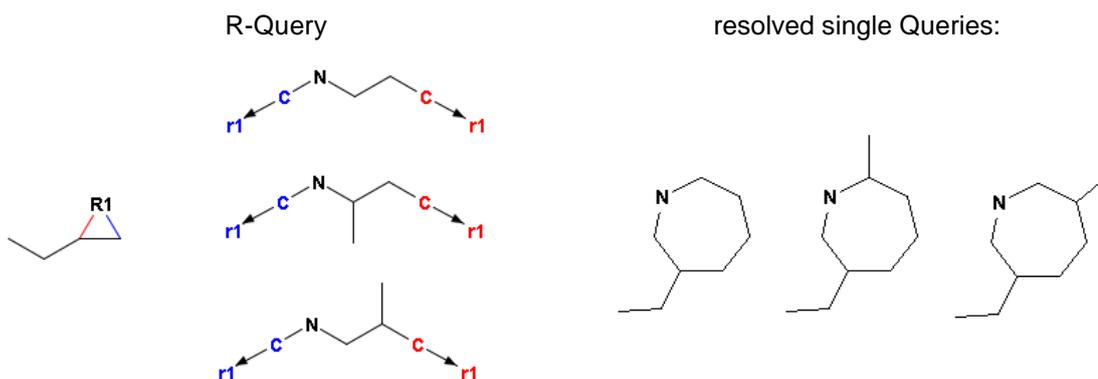


1. First draw the core structure and the Rgroup fragments as follows:

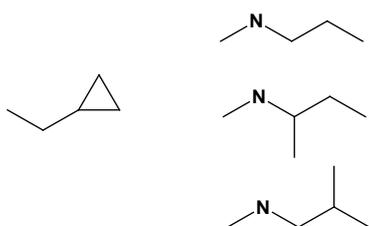


2. Select the button  in the toolbar.
3. Click on the position of the core structure, where you want to have the Rgroup fragments attached. Then click on the connection positions of the Rgroup fragments.  
The program will generate R1 and r1 labels with arrows.

### Example 2: Rgroups with two attachments at different positions

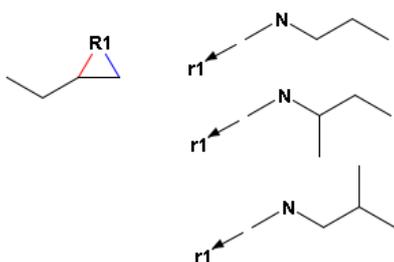


1. Draw the core structure and the Rgroup fragments as follows:



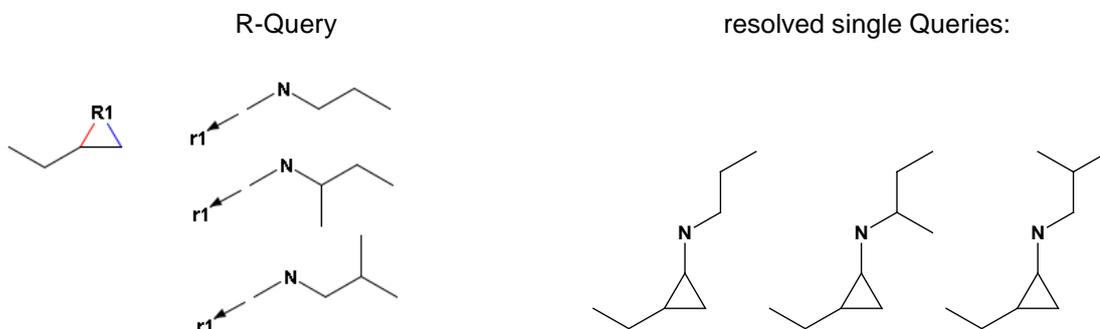
2. Select the button  in the toolbar.
3. Click on the connection position in the core structure. Then click on the first attachment point of the Rgroup fragments.

The program will generate R1 and r1 labels with arrows. In the core structure both attachment bonds are marked in blue and red colors, but the coloring of the Rgroups is not visible yet (see picture below).



4. Click on the second attachment point in the Rgroups.
- All the attachment positions of the Rgroups are now colored correspondingly as shown in the R-Query above.

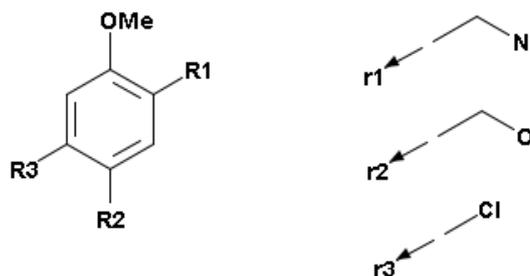
### Example 3: Rgroups with two attachments at the same position



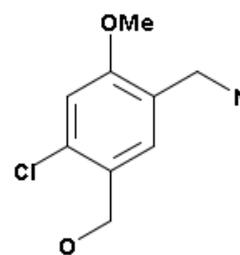
Repeat the first three steps in Example 2 to create the R-Query where both attachment points are at the same position.

**Example 4: Molecules with several Rgroups**

R-Query



resolved single Query:



1. First draw the core structure and the Rgroup fragments.
2. Select the button  in the toolbar.
3. Click on the connection position in the core structure. Then click on the first attachment point of the first Rgroup fragment.
4. Repeat step 3 successively for all other Rgroup fragments (R2 and R3).

**Please note:** If you accidentally mixed up the Rgroups, e.g. R1 and R2 positions should be exchanged, you can change the Rgroup numbering by clicking on the position in the core or in the Rgroup, where you want to edit, and then enter the new Rgroup number with the keyboard. The  button must be selected.

**Please note:** To remove Rgroup information from atoms please select the  "Remove Rgroup Info from atom" button and click on the corresponding atoms.

## 14 User-defined Templates

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

## 15 OLE-Server Functionalities

### 15.1 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" or use the keyboard shortcut CTRL + B 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 item "Edit", the context menu or use the keyboard shortcut CTRL+C 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.

## 16 Technical Documentation

In addition to this ICEDIT user manual a detailed technical documentation is available. Please refer to the document ICEDIT\_Technical\_Documentation.pdf in the "Documentation" folder in the ICEDIT 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.
- ICEDIT as ActiveX Control (ICEDITOCX).

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