



Manual

Structure and Reaction Editor

JavaScript Version 3.0.4

Spring 2016

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1 Introduction

Due to increasing difficulties with Java and Java applets in general with the newest generation of most of the common browsers, InfoChem has in addition to the applet version of the editor developed an HTML5 based, JavaScript editor. Of course the IEDIT JavaScript version supports all features known by the applet and needed by a chemical query editor for structures and reactions.

ICEDIT is also available as Windows application and as the above mentioned applet for all platforms supporting Java.

The IEDIT Windows application offers full editing functionalities (chemical as well as display functionalities). The Windows version 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.

Depending on the individual configuration of IEdit for a specific web page, some features may not be available (please refer to the technical documentation for details on the configuration options).

2 General Information

2.1 Button bars

The JavaScript application of ICEDIT has two button bars. The upper one represents the main button bar whereas the lower one represents the sub-button bar.

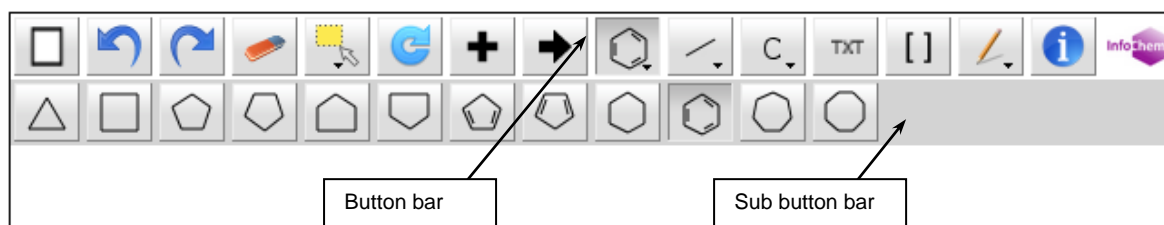


Fig. 1: The ICEDIT button bars.

The buttons displayed in the sub button bar depend on the selected button of the main button bar. The buttons from the sub button bar show further functionality belonging to the selected main button.

For example the template button  opens the following sub button bar:



For a detailed description of the buttons please see chapter 3.

2.2 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:** Opens the “Edit Bond” or “Edit Atom” dialog window. The currently selected atom(s) or bond(s) can now be edited.
- **Copy:** Copies the selected object(s) (into an internal buffer).
- **Paste:** Pastes the selected object(s) (from an internal buffer).
- **Duplicate Object(s):** Duplicates the selected object(s).
- **Delete:** Deletes the currently selected atom(s) or bond(s). (Keyboard shortcut: DEL).
- **Expand Superatom:** Expands a selected superatom.
- **Contract Superatom:** Contracts a selected superatom.
- **Create Chiral Flag:** Creates a chiral flag on the selected molecule(s). Please refer to chapter 7 for further details.
- **Group:** Merges multiple selected chemical objects.
- **Ungroup:** Ungroups a selected group of chemical objects.
- **Create No-Structure:** Opens the “Create No-Structure” dialog window to create a No-Structure label. Please refer to chapter 9 for further details on No-Structures.

Please note: The three methods “Copy”, “Paste” and “Duplicate Object(s)” work only internally within IEDIT. Therefore, you cannot copy/paste from/into other Windows applications via the clipboard.

2.3 Keyboard Shortcuts

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

- **Ctrl+A:** Selects all objects within the drawing area.
- **Ctrl+Z:** Undoes the last operation.
- **Ctrl+Y:** Redoes the last undone operation.

3 Buttons

Various edit and template buttons are provided in the button bars. 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.

3.1 Buttons from main bar



Clear screen.

Deletes all objects from the drawing area.



Undo last operation.

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



Redo last operation.

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



Delete object.

The object(s) (atom, bond, molecule, text) you are selecting with the selection rectangle will be deleted. (Keyboard shortcut: DEL).



Show Select button bar.

The Select button bar contains two select buttons:



For a detailed description see chapter 3.2.1.



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.

Adds a reaction arrow to the drawing area.

Please note: Only one arrow per reaction is supported.



Show Template button bar.

The Template button bar consists of the following template buttons:



For a detailed description see chapter 3.2.2.



Show Bond button bar

The Bond button bar contains various standard bond buttons and the bond dialog button:

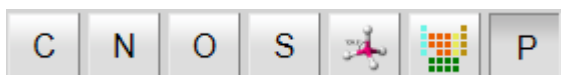


For a detailed description see chapter 3.2.3.



Show Atom button bar

The Atom menu bar contains four atom buttons (configurable), the atom dialog button, the periodic table button and one atom button which shows the last selected atom from the periodic table (here: P-atom).



For a detailed description see chapter 3.2.4.



Draw text.

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



Draw Brackets.

Draws a pair of brackets. Please refer to chapter 8 for further details.



Show enhanced chemical functionality button bar

The enhanced chemical functionality menu bar consists of two Rgroup and two mapping buttons:



For a detailed description see chapter 3.2.5.



Show info dialog.

Shows information about IEDIT, the used components and their version numbers and provides a link to open the IEDIT manual.

3.2 Buttons from Sub button bars

3.2.1 Select Buttons

The Select button bar contains two select buttons:



Select.

Use this tool either to select a single object or a group of objects in a rectangle. The selected objects can then be moved, deleted or copied using either the context menu or the appropriate buttons



Select object.

Use this tool to select whole objects at once. Click on a specific object as soon as it is marked by a red frame to select the complete object. The selected objects can then be moved, deleted or copied using either the context menu, the menu bar or the appropriate keyboard shortcuts.

3.2.2 Molecule Template Buttons

The IEDIT JavaScript application provides various structure templates via the molecule template button:



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.

3.2.3 Standard Bond Buttons

The Bond button bar contains various standard bond buttons and the bond dialog button:



Draw single bonds or change existent bonds.

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 single 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.

Please note: It is only possible to convert a double bond to a triple bond if the valence on the C 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.



Draw double bonds or change existent bonds to double bonds.

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



Draw triple bonds or change existent bonds to triple bonds.

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



Draw up wedges or change existent 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 existent 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).

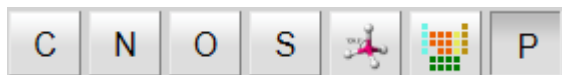


Draw a chain.

Draws a chain of C-C single bonds.

3.2.4 Standard Atom Buttons

The Atom menu bar contains four atom buttons (configurable), the atom dialog button, the periodic table button and one atom button which shows the last selected atom from the periodic table (here: P-atom).



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.



Open "Edit Atom" dialog.

Use the dialog window to define atom properties and atom query features.

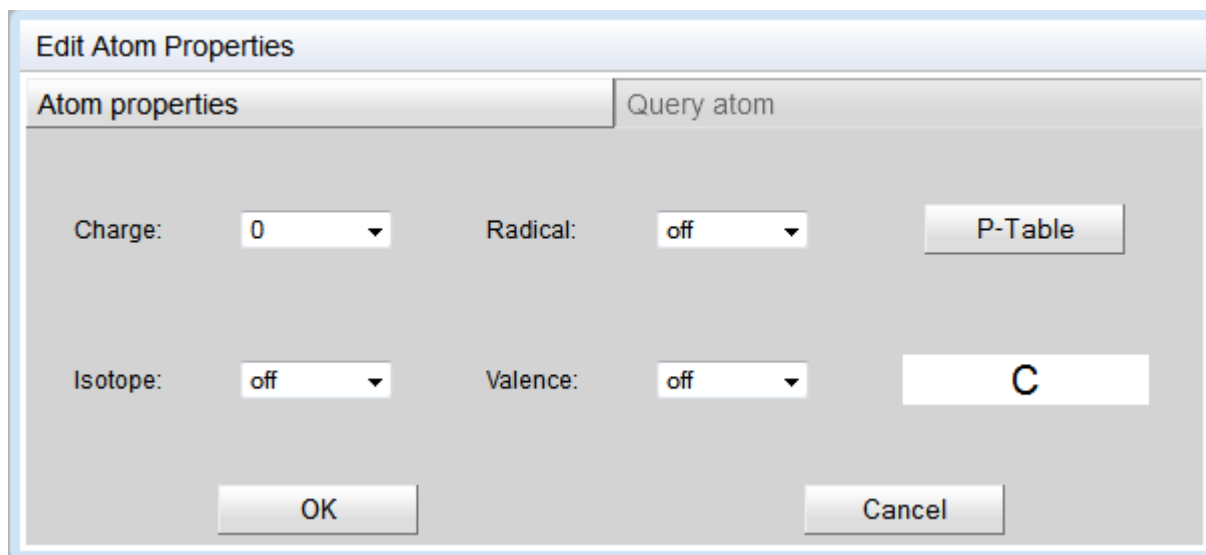
Atom properties:

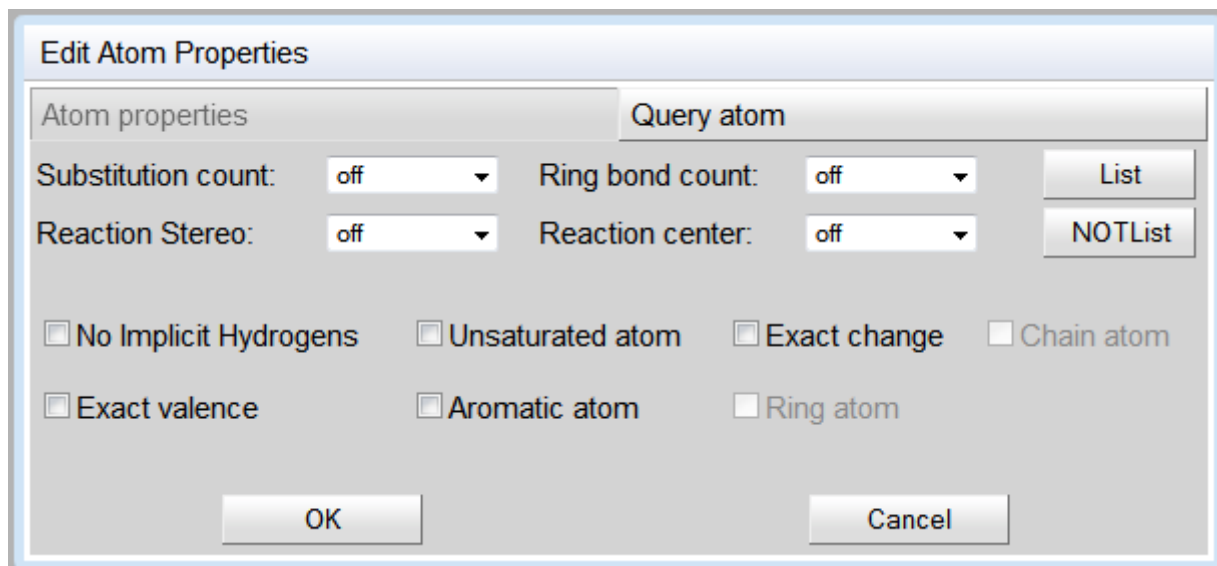
Fig. 2: Atom properties dialog window, main tab.

Use this dialog window 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.

Query atom:**Fig. 3:** Atom properties dialog window, Query atom tab.

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.

Please read the ICFSE_Tutorial.pdf from the download area of the InfoChem homepage (<http://www.infochem.de/>) for further information on the input and use of query features.



Open "Periodic Table" dialog.

Use the dialog window to select another atom type. The result will be displayed as button label to the right of the Periodic Table button.

Example:

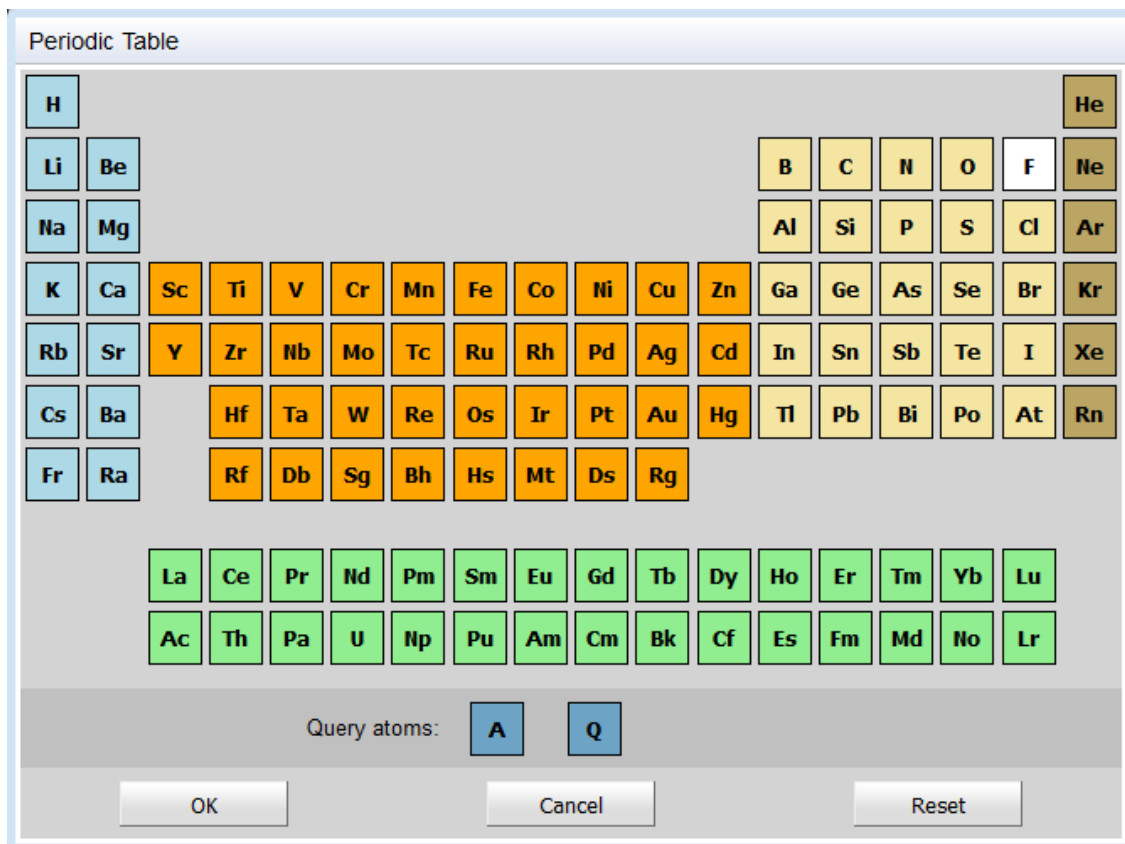


Fig. 4: Periodic Table dialog window.

Select the Si atom type and click ok.



The button on the right hand side of the Periodic Table will be updated to "Si" and can be used to draw further Si atoms.

3.2.5 Enhanced chemical functionality buttons

The enhanced chemical functionality bar contains two Rgroup and two mapping buttons:

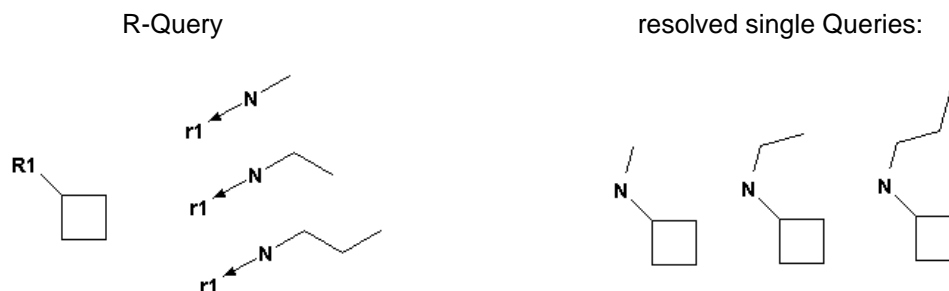


Define Rgroups.

Draw a core structure and several Rgroups.

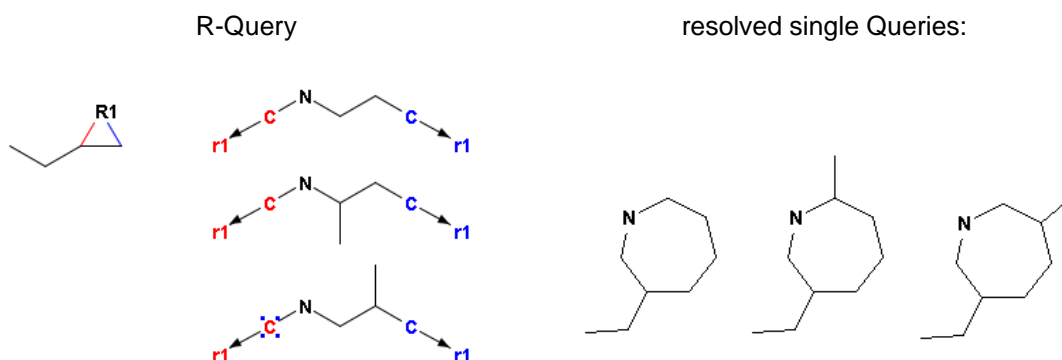
First click on the position of the core structure, where you want to have the Rgroup attached. Then click on the connection position of the Rgroups.

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.

Example:



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!



Remove Rgroup Info from atom.

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

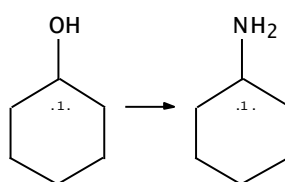


Map atoms.

Adds mapping numbers to the atoms you select. In order to do so, please mark 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.

4 Using the Editor

4.1 Draw Objects

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.

4.2 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.

Or choose the "Select Object" button to select whole objects at once.

4.3 Scale Objects

To scale one or more objects please select first the objects and then use the double headed arrow in one of the four corners of the selection frame to change the size of the objects.

4.4 Edit Objects

4.4.1 Edit Atoms

You can change the atom symbol of a selected atom by using the keyboard. Please insert an atom label and press enter. The input of atom symbols 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 different atom types by simple drawing a bond, typing the atom label and pressing enter. The keyboard input of charge and isotopes is supported as well:

- 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).

In addition you can change an atom symbol using the “Edit Atom” dialog window. To open the dialog window please use either the “Edit Atom” button, the context menu “Edit Atom” or double-click a specific atom. For details of the “Edit Atom” dialog window please see chapter **Error! Reference source not found.**

4.4.2 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.

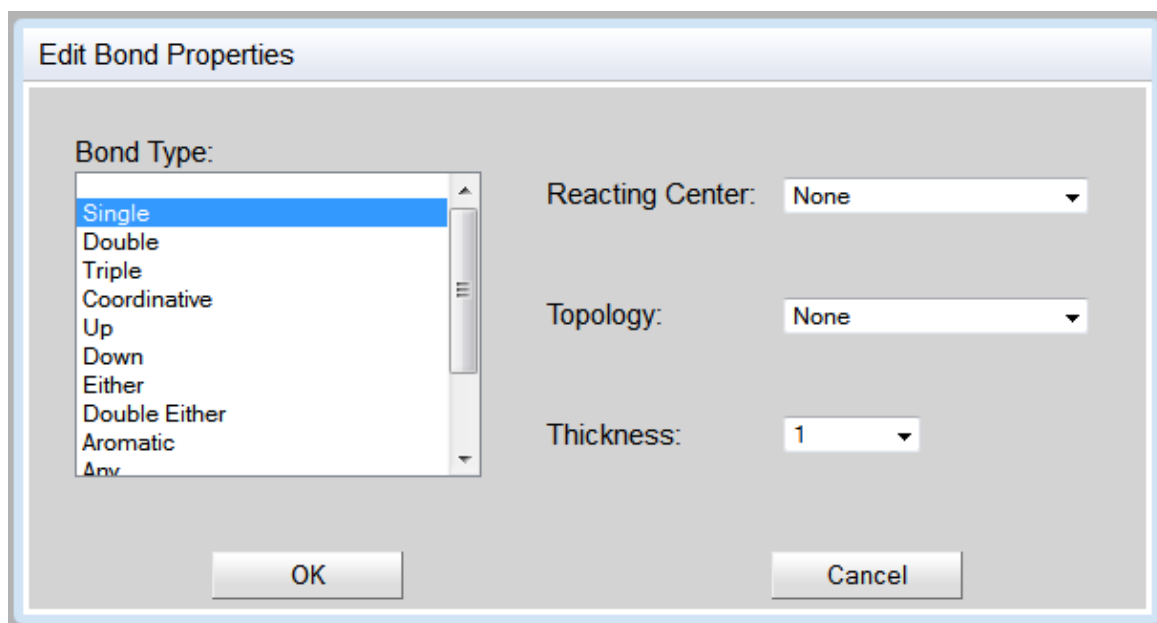







Fig. 5: “Edit Bond” dialog window.

The following bond types are supported:

	Single		Double Either
	Double		Aromatic
	Triple		Any
	Up		Single/Double
	Down		Single/Aromatic
	Either		Double/Aromatic

The following reaction query features are supported:

Reacting Center

	Not Center
	Make & Change
	Change
	Make/Break
	Center

Topology

	Chain		Ring
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4.4.3 Group or Ungroup Chemical Objects

Group

To group multiple chemical objects please select the desired objects and use the context menu item "Group".

The selected multiple items are now grouped and will be treated as a solely object, visible at the 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 the context menu option "Ungroup".

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

Example:

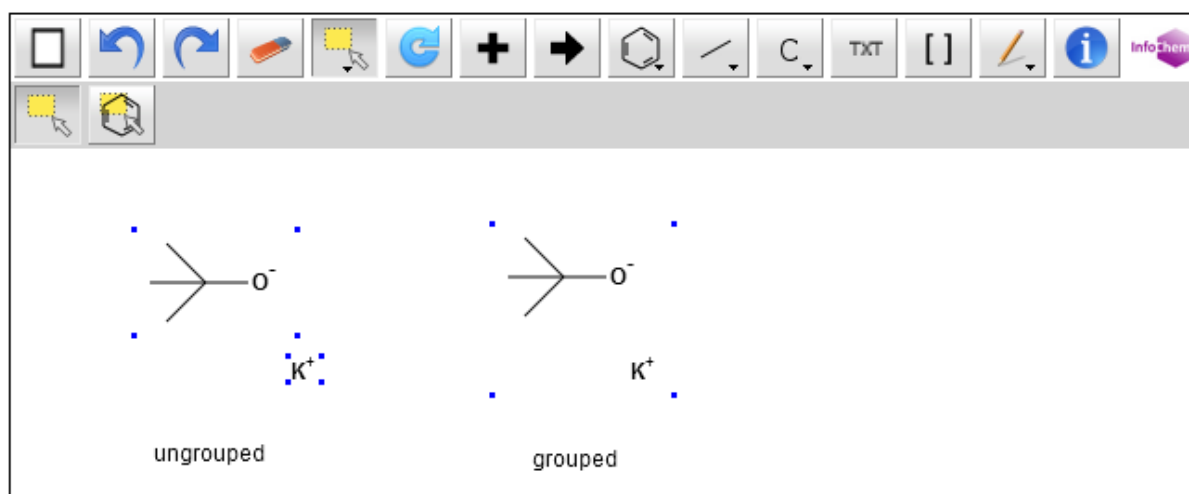



Fig. 6: Ungrouped and grouped objects.

4.5 Insert Text



Please use the text button  from the upper menu bar to enter a text string.

To edit any text please select the select button and double-click the text label or right-click the text label to open the context menu and choose “Edit Text” to open the “Edit Text” dialog window.

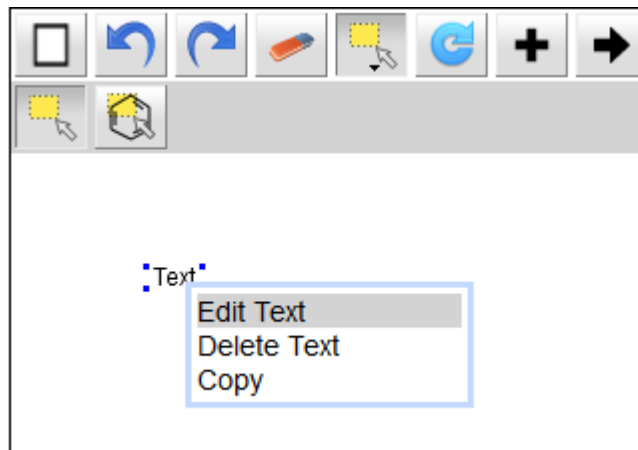


Fig. 7: Text context menu.

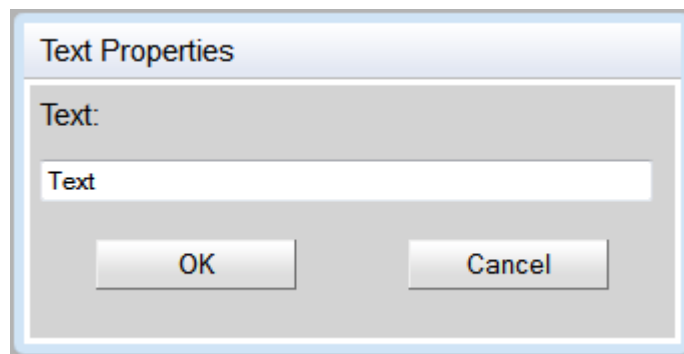


Fig. 8: The “Edit Text” dialog window.

4.6 Create Superatoms

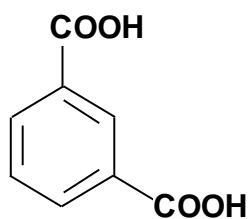
4.6.1 General

In the default Javascript Version only self-defined superatoms can be created. For the support of common superatoms like COOH, CN, NO₂ an enhanced version of the Javascript editor is required (see chapter 4.6.3 and technical documentation).

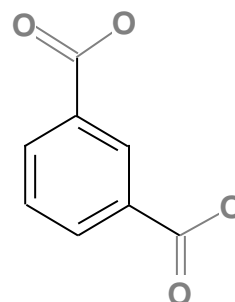
The expanded structure of the superatom is highlighted in gray. The expanded structure parts can be contracted again.

- **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".

Example:



Contracted form



Expanded form

4.6.2 Creation of 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.

Example:

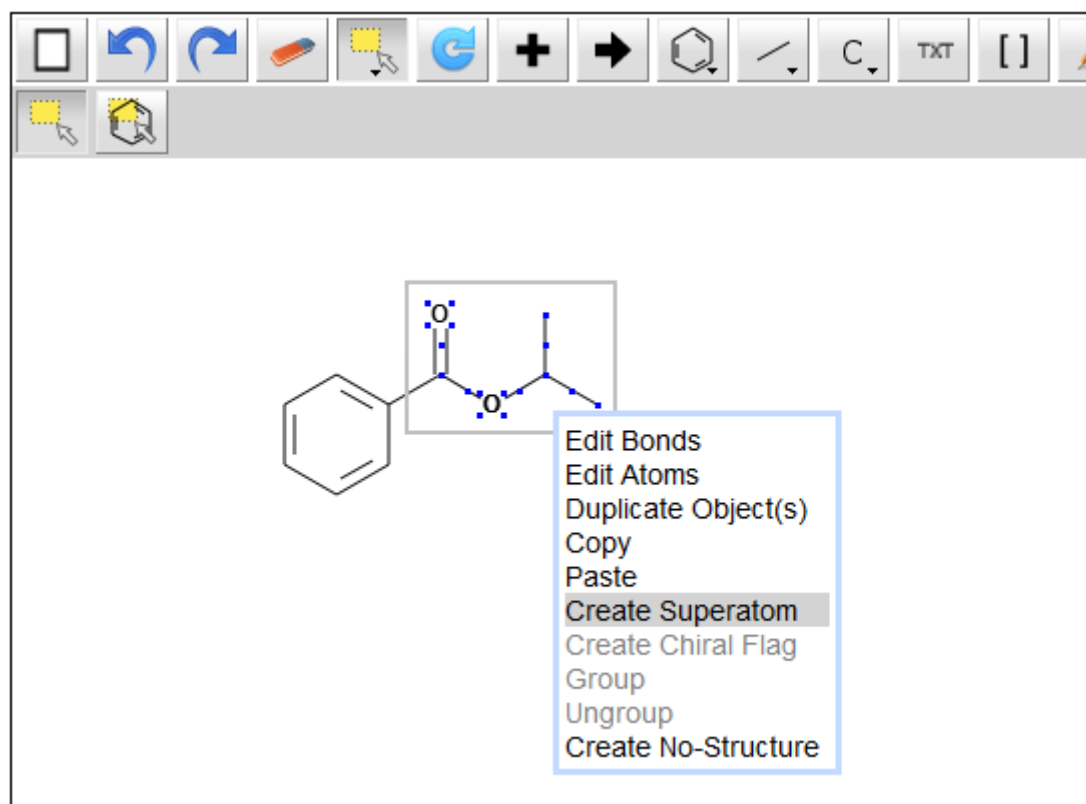


Fig. 9: Create Superatom context menu.

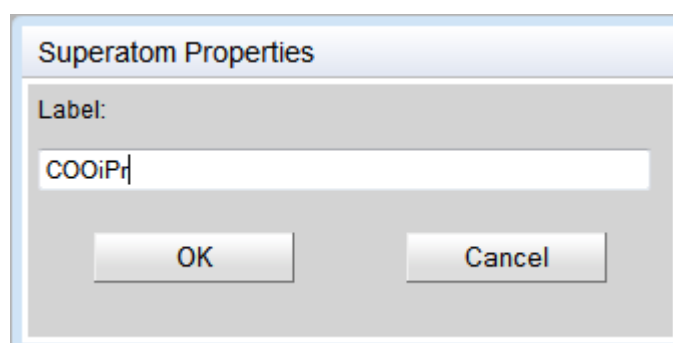


Fig. 10: Superatom Properties Dialog window.

Result:

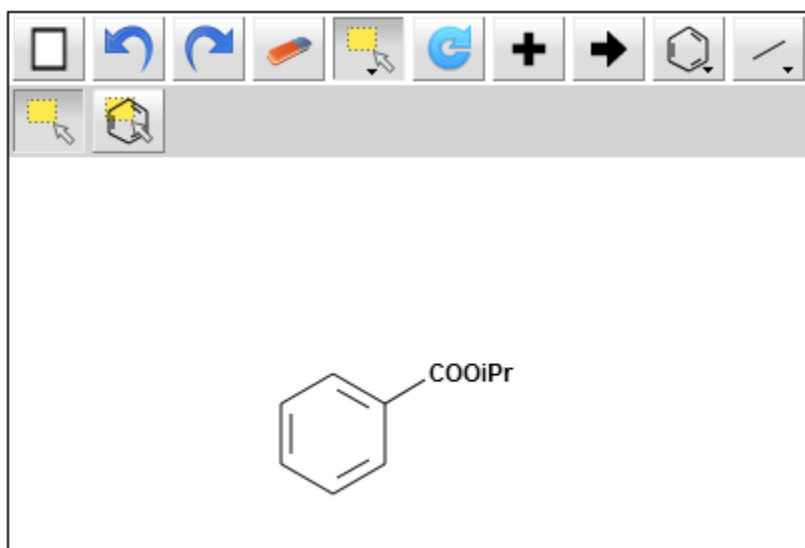


Fig. 11: Create Superatom action result.

Please note: A molecule containing a self-defined superatom can be copied, saved or exported like any other usual molecule.

Please note for user of the enhanced version: 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.

4.6.3 Support of common superatoms

The input and automatic recognition of superatom labels is supported by the enhanced JavaScript Editor. For the setup please see the technical documentation.

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.

4.6.3.1 Input of superatoms

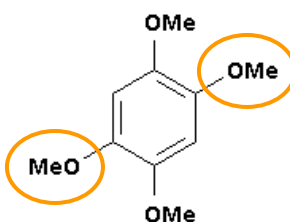
The input of superatoms is case sensitive.

- 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

4.6.3.2 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 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 “Supported Superatom labels.pdf” on the InfoChem home page to find a full list of supported superatoms and superatom labels.

4.7 Create 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:

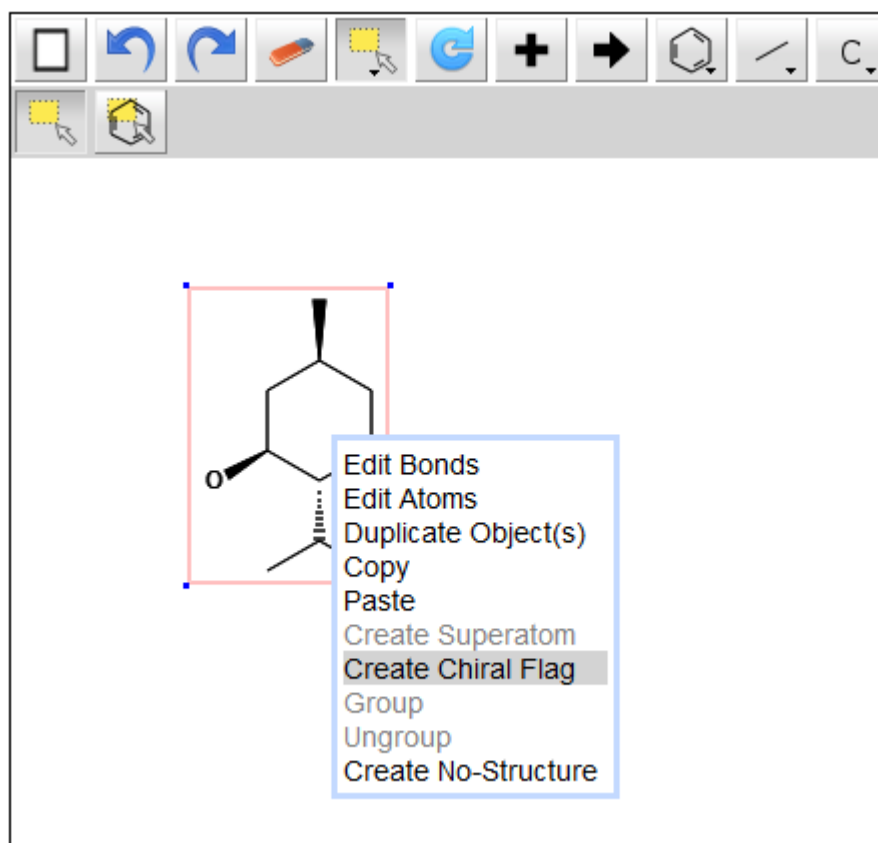


Fig. 12: Context menu item "Create Chiral Flag".

Result:

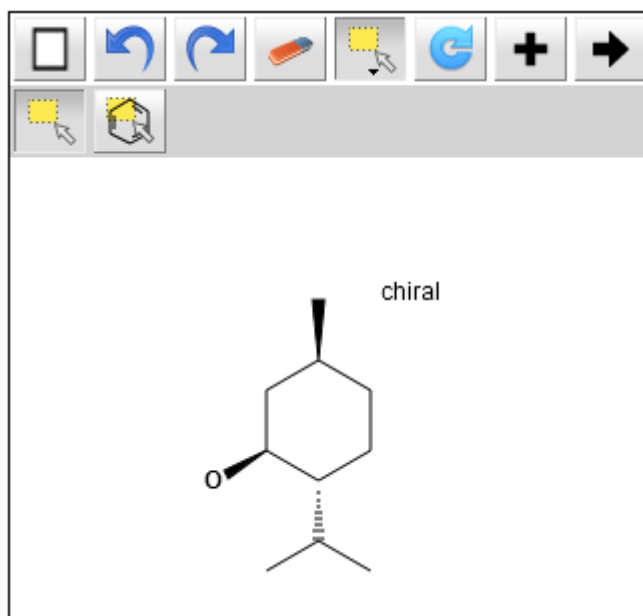



Fig. 13: Molecule labeled as chiral.

4.8 Create Brackets

To draw a bracket, please select the bracket  button from the upper menu bar 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. Therefore please make sure that the height is fitting before releasing the mouse button.

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.

Example:

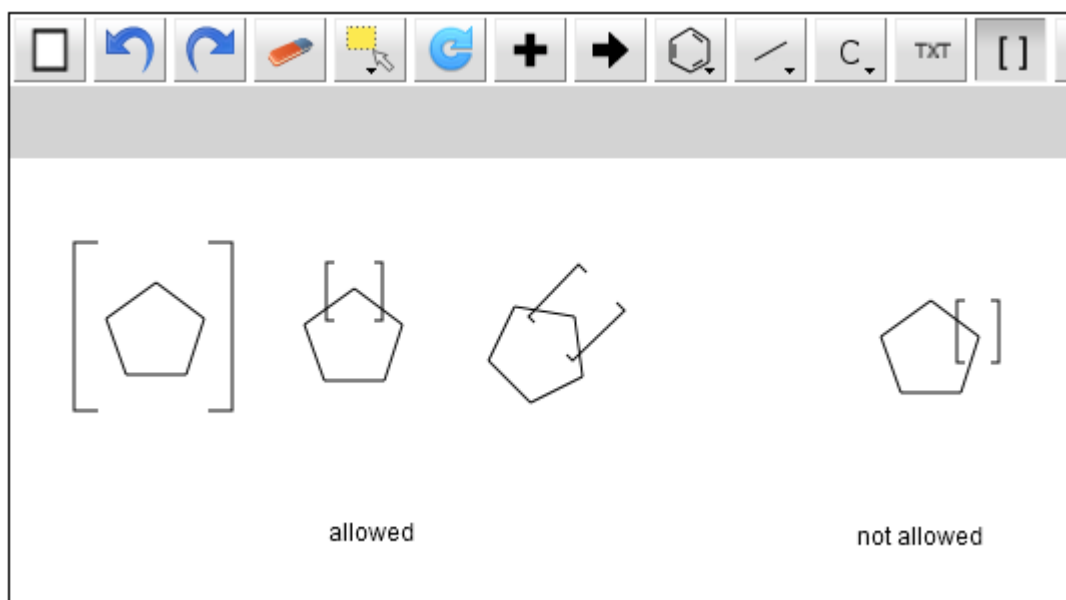


Fig. 14: Allowed/not allowed bracket positions.

You can edit or delete 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.

Example:

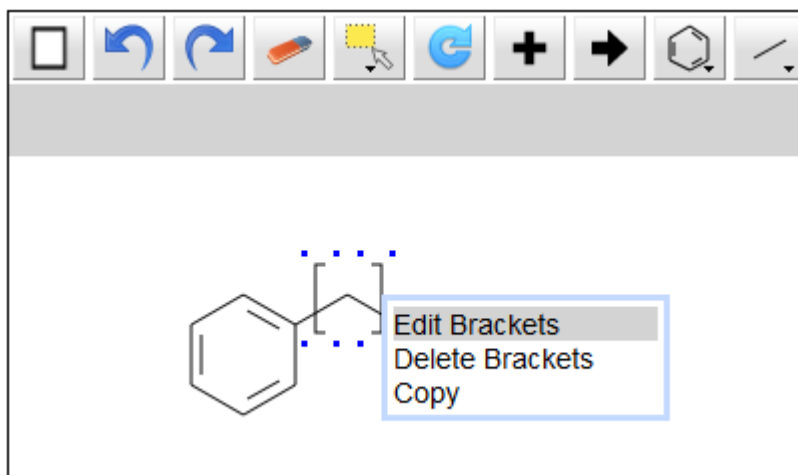


Fig. 15: Bracket context menu.

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:

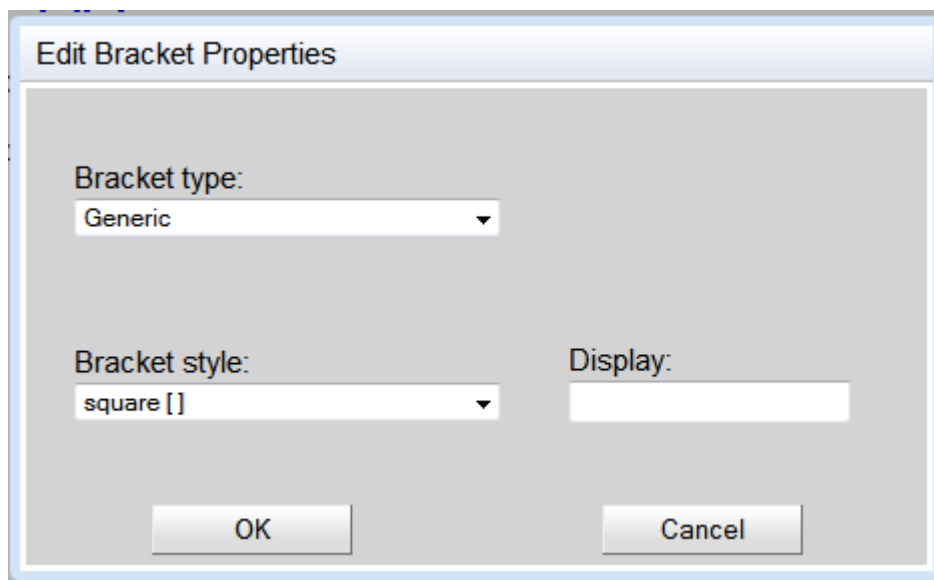


Fig. 16: The “Edit brackets” dialog window with bracket type “Generic”.

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 be not 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 enclosed part is multiplied.

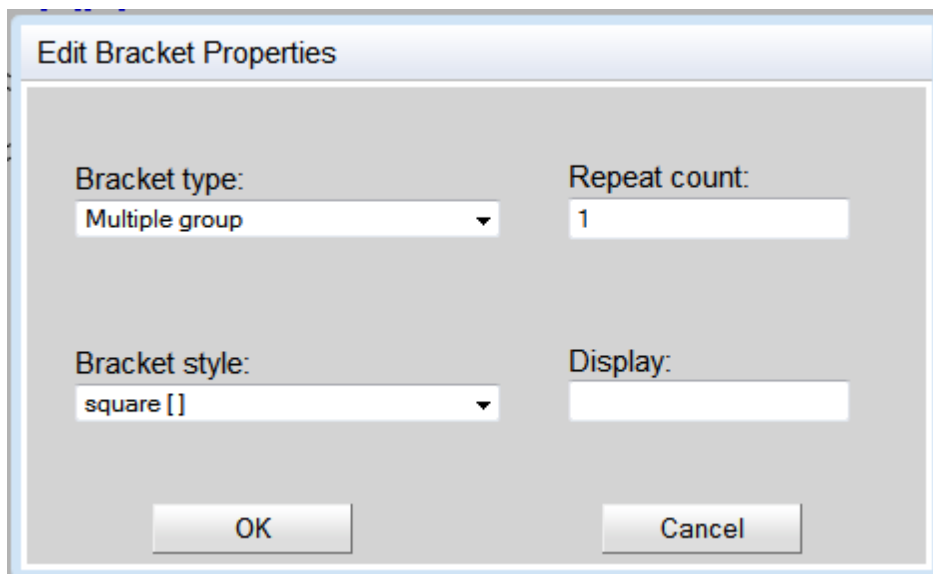


Fig. 17: The “Edit brackets” dialog window with bracket type “Multiple group”.

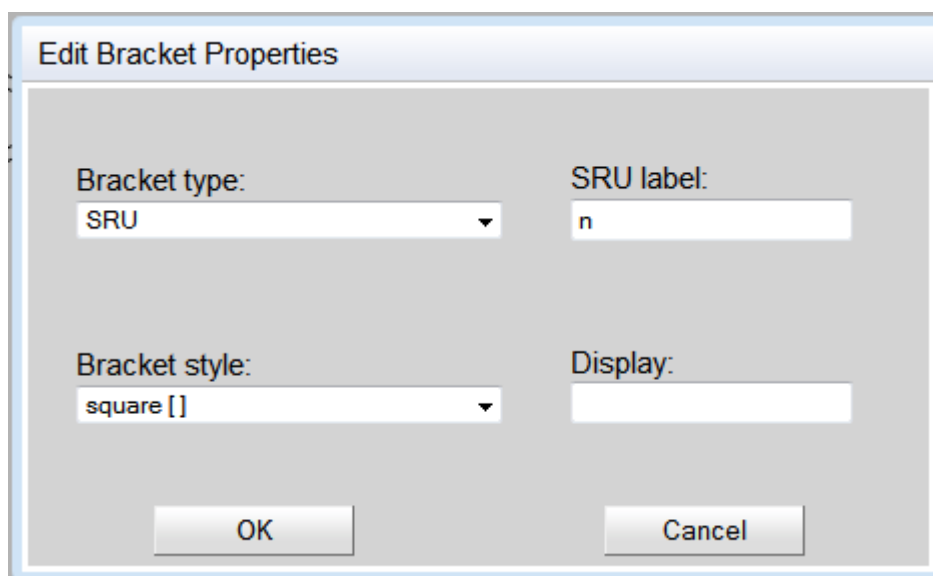


Fig. 18: The “Edit brackets” dialog window with bracket type “SRU”.

Edit the Bracket Style:

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

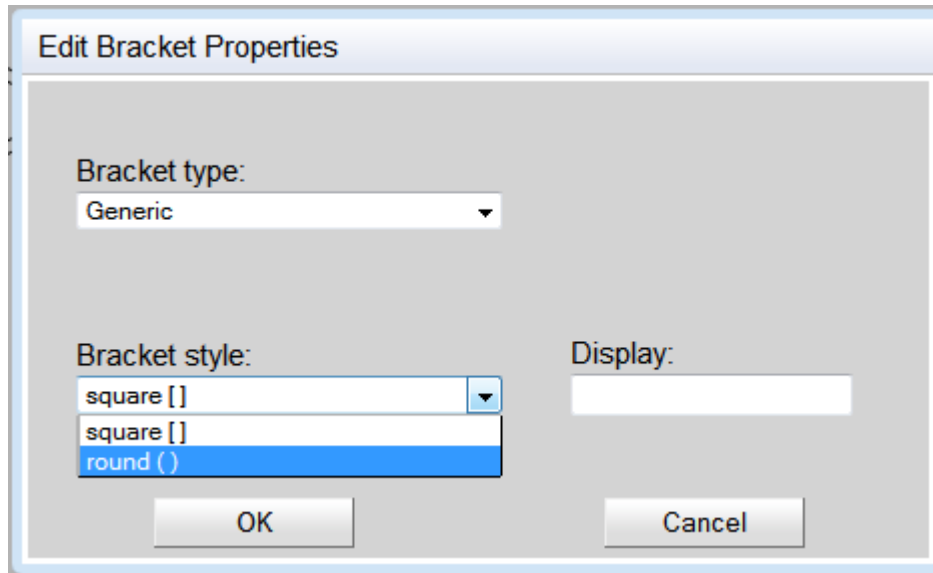


Fig. 19: The “Edit brackets” dialog window with two different bracket styles.

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.

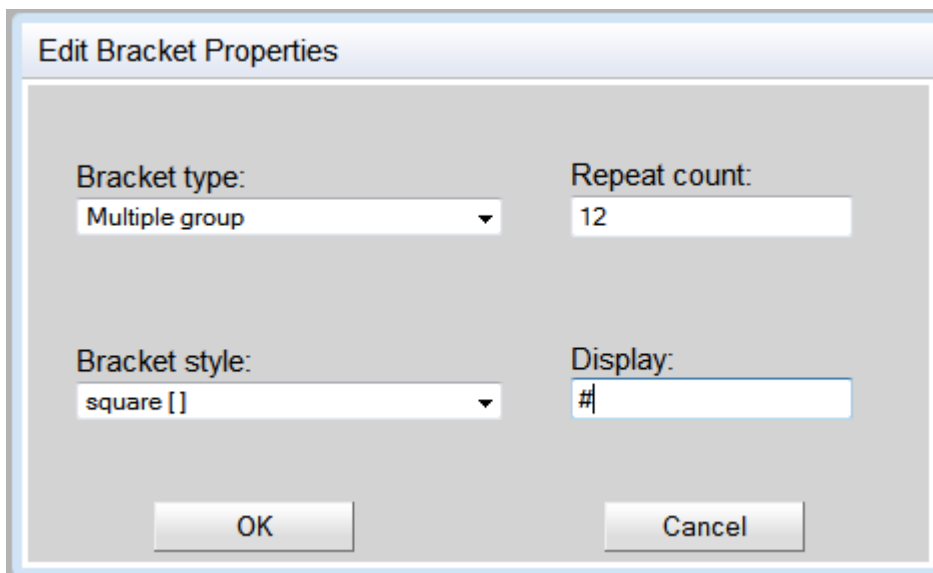


Fig. 20: The “Edit brackets” dialog window with additional display information.

Result:

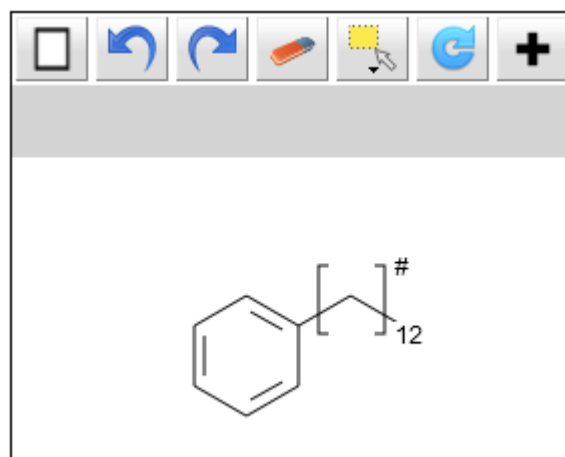


Fig. 21: Molecule with Multiple group bracket.

Delete Brackets:

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

4.9 Create 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 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 the context menu item "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".

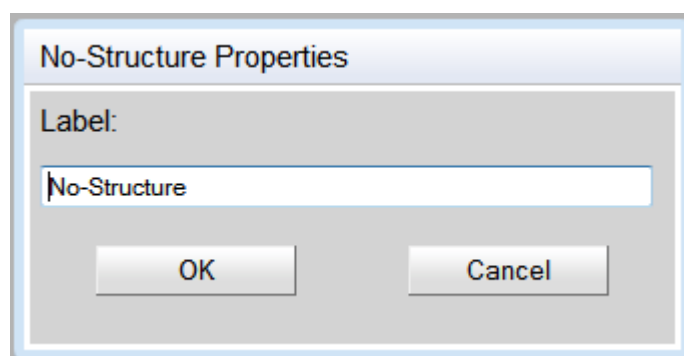


Fig. 22: The "Create No-Structure" dialog window.

Edit a No-Structure:

You can edit or delete 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.

Example:

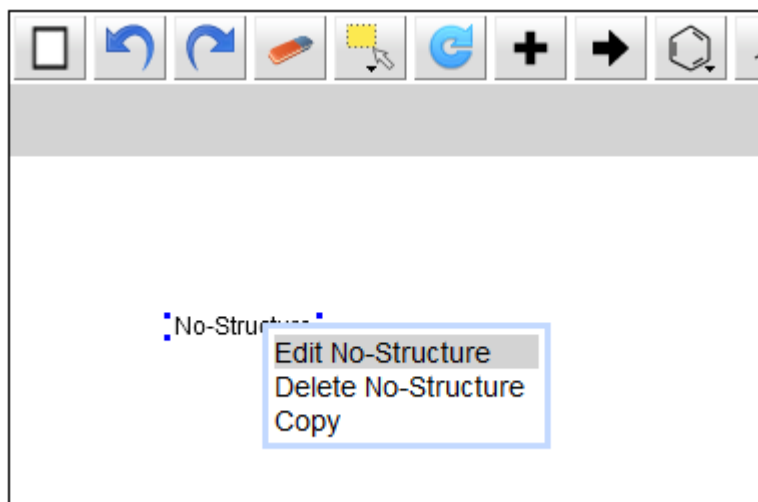


Fig. 23: The “No-Structure” context menu.

Please note: A reaction or molecule containing a self-defined No-Structure can be copied like any other usual molecule.

5 Customer Support

Please contact us to receive technical support or license information:

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