

A stylized graphic of a purple and white pencil or marker, oriented diagonally from the bottom-left towards the top-right. The tip of the pencil is a dark grey cone.

ICEDIT

Manual

Structure and Reaction Editor

Version 1.8.0

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1 Preface

The chemical structure editor ICEDIT is available as applet for all platforms supporting Java and as Windows application.

The applet version can be integrated into a web site. It has not the full functionality of the Windows application.

The Windows application of ICEDIT provides the following additional features:

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

2 Getting Started

2.1 Setup

Windows application only

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

IMPORTANT: If you want to uninstall ICEDIT please use 'Add/Remove Programs'. Do not use Setup.exe to uninstall ICEDIT!

2.2 Overview of the Windows Application

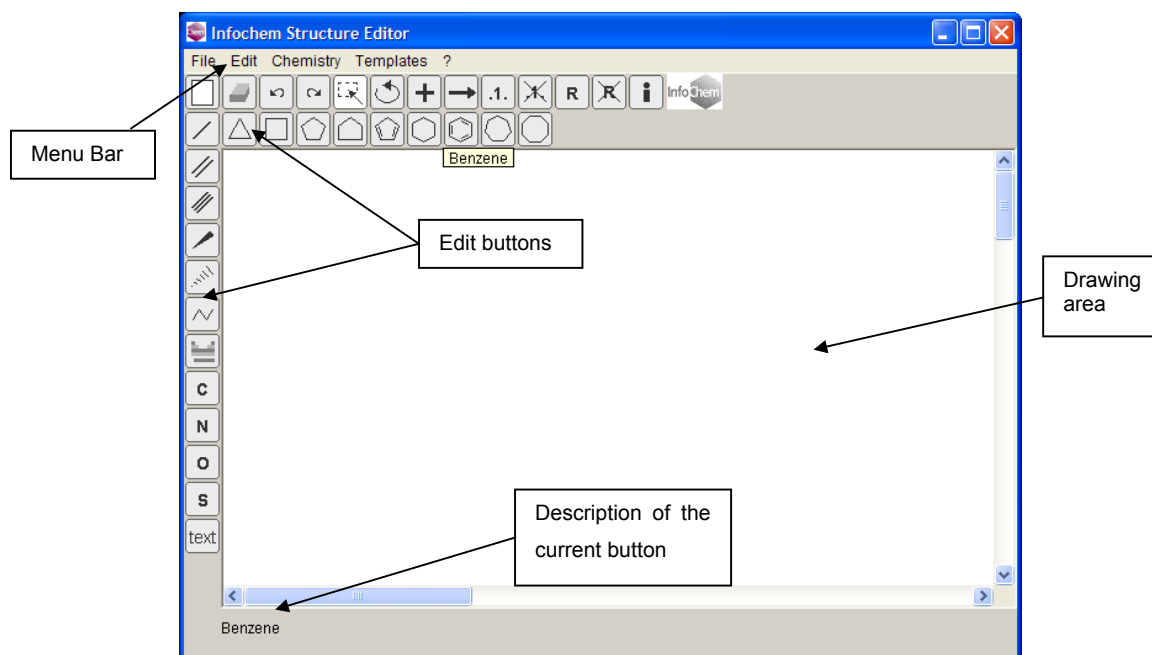


Fig. 1: The ICEDIT Windows application.

2.3 Overview of the Java Applet

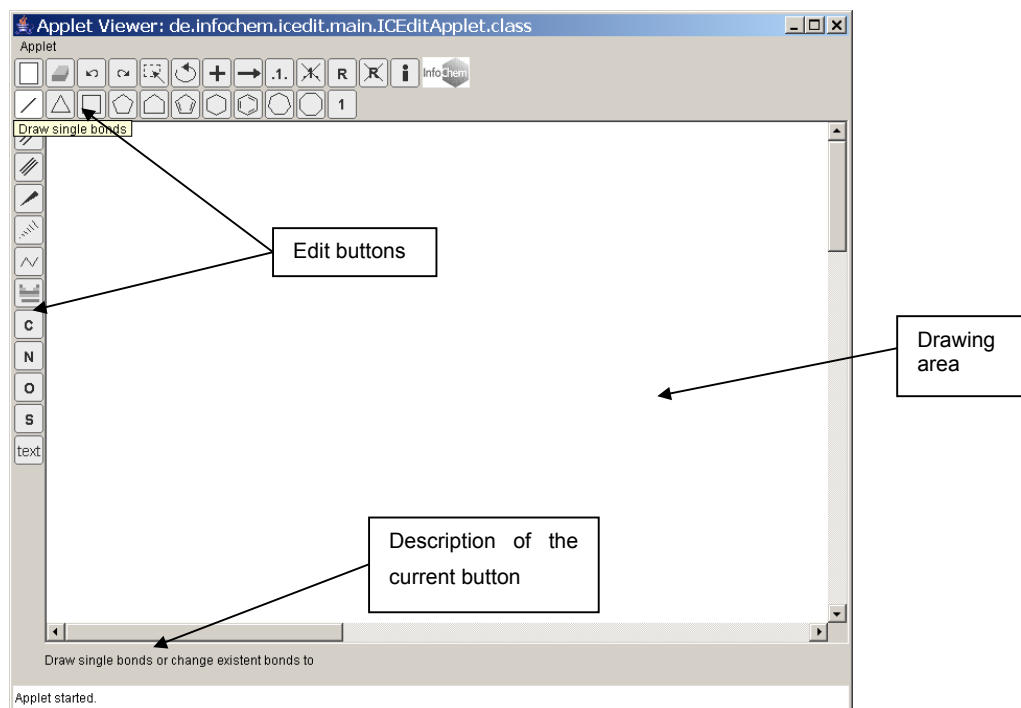


Fig. 2: The ICEDIT Java applet.

3 General Information

3.1 Description of the Menu Bar

Windows application only

3.1.1 'File'-Menu

Transfer to client

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

New

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

Open

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

Save

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

Save As

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

Export - Mol/Rxnfile

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

Export - Skcfile

Exports a structure or reaction to MDL Sketch file format.

Please note: Complex schemes are not yet supported.

Import - Molfile

Imports a structure from MDL MOL file format.

Import - Rxnfile

Imports a reaction from MDL RXN file format.

Import - Skcfile

Imports a structure or reaction from MDL Sketch file format.

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

Import - SMILES

Imports a structure from the SMILES format and generates coordinates.

Import - Cdxfile

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

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

Exit

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

3.1.2 'Edit'-Menu**Undo**

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

Redo

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

Copy

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

Paste

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

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

Delete

Deletes the selected objects. (Keyboard shortcut DEL).

Select all

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

Duplicate

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

3.1.3 'Chemistry'-Menu**Superatoms - Expand all**

Expands all superatoms.

Superatoms - Contract all

Contracts all superatoms.

Superatoms - Show Info

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

Molecule Values - Calculate

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

The following molecule values are supported:

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

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

The calculated values can be pasted in the drawing area using the 'Paste' button. Information not required can be unselected and will not be transferred into the drawing area.

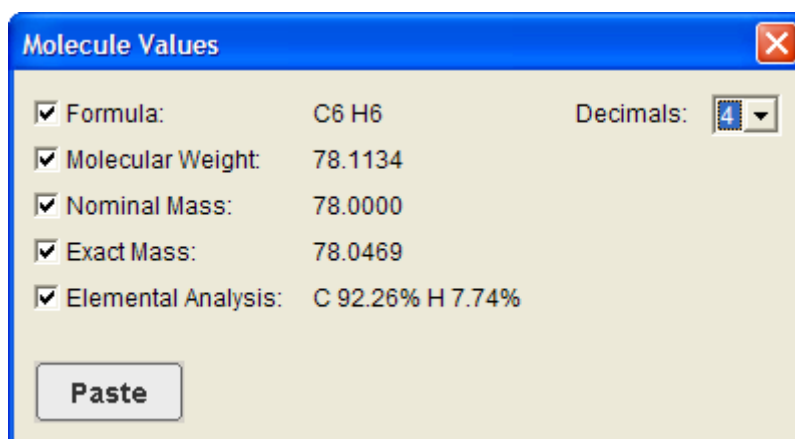


Fig. 3: 'Molecule Values' dialog window.

Atom Numbers - Show

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

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

3.1.4 'Templates'-Menu

Open

Opens the 'Templates' dialog.

Insert templates:

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

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

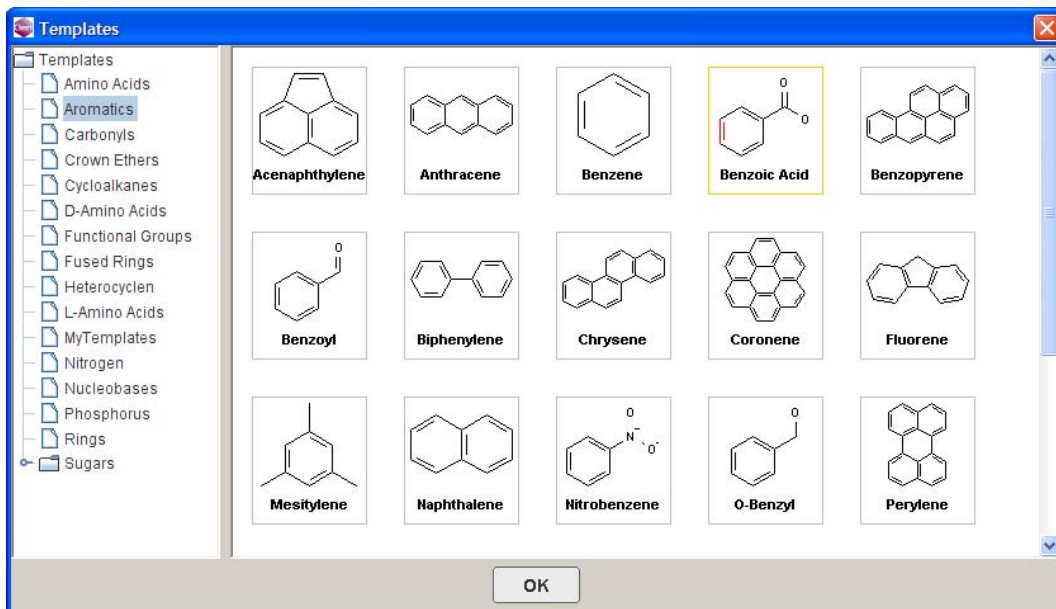


Fig. 4: The 'Templates' dialog window.

3.1.5 '?' - Menu

Help

Opens the PDF-documentation file.

About

Shows information about Icedit and its version number.

3.2 Context Menus

Context menus are available by right clicking (i) on the drawing surface, (ii) on specific bonds, (iii) on specific atoms, (iv) on selected objects. Use the context menu to:

- **Copy** selected objects (into the Windows clipboard). (Keyboard shortcut CTRL + C).
- **Paste** objects (from the Windows clipboard) into your drawing area. (Keyboard shortcut CTRL + V).
- **Copy Molecule:** copies the selected object (into an internal buffer).
- **Paste Molecule:** pastes the selected object (from an internal buffer).
- **Duplicate Molecule:** duplicates the selected object.

- **Edit** the currently selected atoms or bonds.
- **Delete** the currently selected atom or bond. (Keyboard shortcut DEL).
- **Expand Superatom**: expands a selected superatom.
- **Contract Superatom**: contract a selected superatom.
- **Create Superatom**: creates a self-defined superatom.

3.3 Keyboard Shortcuts

The following keyboard shortcuts are available in *ICEDIT*:

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

4 Description of Standard Edit Buttons

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

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

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

4.1 Standard Edit Buttons



Clear screen

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



Delete object

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



Undo last operation.

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



Redo last operation.

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



Select object

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



Rotate selected objects

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



Add reaction plus



Add reaction arrow


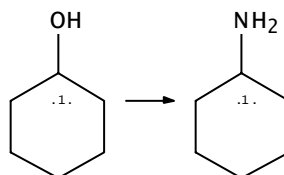
Please note: Only one arrow per reaction is supported. Complex schemes will be supported in future.

.1. Map atoms

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

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

Example:

 Remove mappings from atoms and reaction center information from bonds.

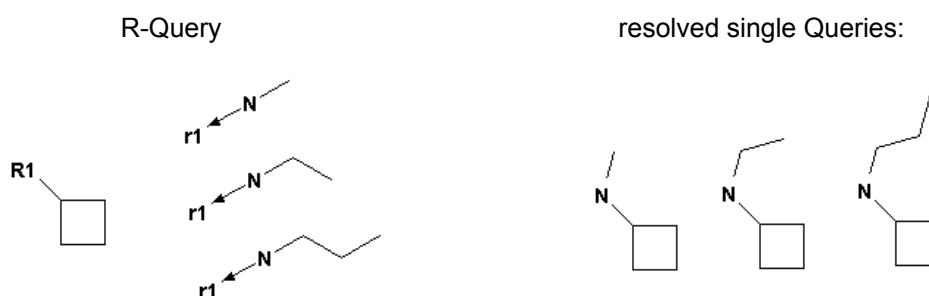
Click single atoms/bonds or draw a rectangle to remove mappings or reaction center information from multiple atoms/bonds.

R Define Rgroups

Draw a core structure and several Rgroups.

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

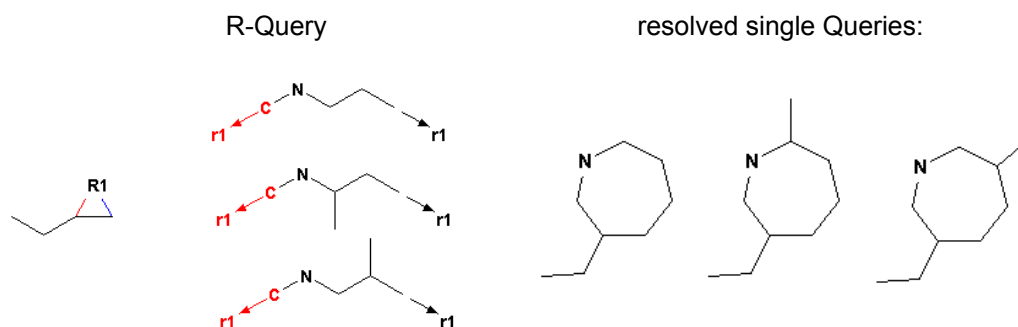
Example:



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

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

Example:



Remove Rgroup Info from atom.

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



Show info dialog

Shows information about ICEDIT and its version number.



Transfer structure back to calling application

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

4.2 Standard Templates

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

4.2.1 Standard Molecule Templates



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

4.2.2 Standard Bond Buttons



Draw single bonds or change existing 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 bond, you can convert it into:

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



Draw double bonds or change 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 its direction.

Please note: The orientation of up wedges is important (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 its direction.

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



Draw chain

Draws a chain of C-C single bonds.

4.2.3 Standard Atom Buttons



Draw atom

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

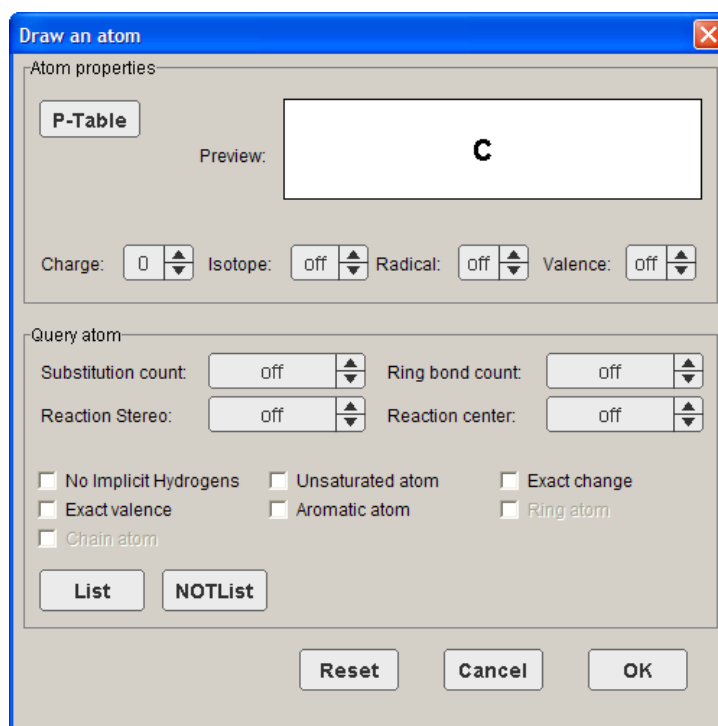


Fig. 5: 'Draw an Atom' dialog window.

Atom properties:

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

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

- A:** Draws an A query atom: any atom excluding H.
- Q:** Draws a Q query atom: any atom excluding H and C.
- X:** Draws a X atom; atom type used for halogens (no valid query feature).
- R:** Draws a R atom (no valid query feature).


Query atom:

The following query features are implemented and can be adjusted


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

In addition the following query settings can be adjusted

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

 Draw atom C


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

 Draw atom N

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

 Draw atom O

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

 Draw atom S

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

 Draw text

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

5 Drawings

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

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

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

5.1 Select objects

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

5.2 Edit atoms

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

- For a charged atom please insert (i) an atom symbol, (ii) the amount of charge, (iii) the charge type (e.g. S2-).
- For isotopic information please insert (i) the nuclear number, (ii) the atom symbol (e.g. 2H).

In addition you can change an atom symbol by the use of the 'Edit Atom' dialog window. To open the dialog window please click on either the template button 'Draw an atom' or the context menu 'Edit Atom'. For details of the 'Edit Atom' dialog please see chapter 4.

5.3 Edit bonds

Select a bond and click on the right mouse button. Select 'Edit Bonds' from the context menu. The 'Edit bond' interface opens.

The following bond types are supported:

	Single		Triple
	Double		Up



	Down		Any
	Either		Single/Double
	Double Either		Single/Aromatic
	Aromatic		Double/Aromatic

In addition reaction query features can be adjusted:

Reacting Center

	Not Center		Make/Break
	Make & Change		Center
	Change		

Topology

	Chain
	Ring

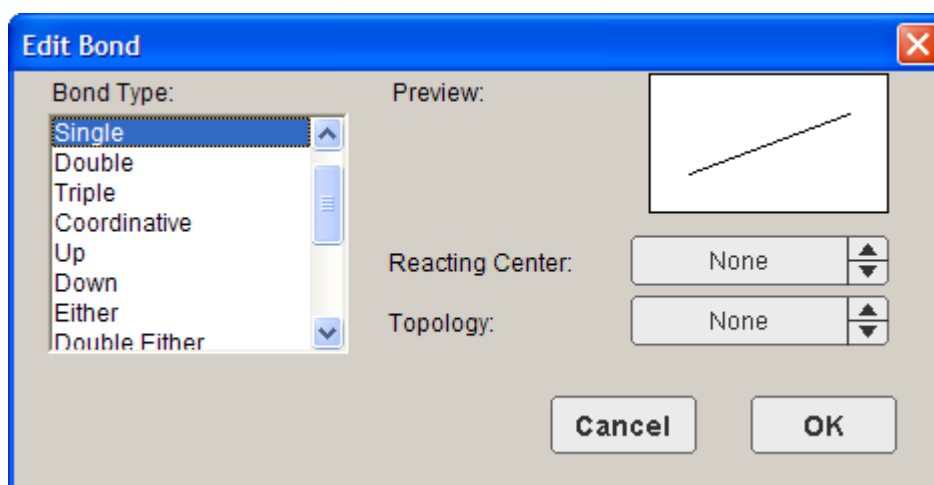


Fig. 6: 'Edit Bond' dialog window.

6 Superatoms

The input and recognition of superatoms is supported.

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

If a superatom is recognized the label is shown in default font format.

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

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

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

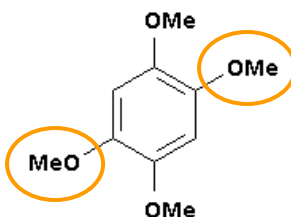
Input of superatoms:

The input of superatoms is case sensitive.

- All atom symbols from superatoms have to be drawn as represented in the Periodic Table of the Elements (e.g. **COOH**, **OMe**, **SiMe₃**).
- Abbreviations are case sensitive as well. They are supported in the most common notation (e.g. Me is supported, me or ME is not supported). The standard typing of abbreviations is as follows:
 - Bn, Boc, Bt, Bu, Bz
 - Cbz, Cy
 - EE, Et
 - Fmoc
 - Me, MEM, Mes, MOM, MPM, Ms
 - Naph, NPhth
 - Ph, Piv, PMB, PNB, Pr
 - SEM, Su
 - TBDMS, TBDPS, TBS, TES, Tf, THP, TIPS, TMS, Tol, Tr, Ts

Display of superatom labels:

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



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

Please note: Abbreviations do not change their order.

Examples:

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

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

6.1 Self-defined Superatoms

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

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

At the moment the storage of self-defined superatoms as user defined template is not yet supported but will be supported in a future version.

7 User defined Templates

Draw the structure you want to use as template in IEDIT and save it to the subdirectory 'Templates' of your IEDIT installation directory (e.g. My Templates at C:/Program files/Infochem/ICedit/Templates). To group the templates choose an existing subdirectory or create a new subdirectory (multiple levels of subdirectories are supported).

8 Embedded as OLE-Server

Windows application only

8.1 Integration in MSOffice

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

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

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

8.2 OLE Interfaces

The following OLE Interfaces are supported:

- IDataObject.GetData for format 'MDLCT'
- IDataObject.SetData for format 'MDLCT'
- IOleObject.DoVerb
- IOleObject.Close

9 Additional clipboard formats

Windows application only

ICEDIT application offers the following additional clipboard formats:

- MDLCT

10 Programming Interface - API

Windows application only

You can integrate ICEDIT as object in your source code in VisualBasic or .NET projects.

10.1 Functions

An ICEDIT object supports the following functions:

- **ICEdit.Show()**
Displays the ICEDIT window.
- **ICEdit.ShowRosdal(rosdal)**
Displays the transferred structure in ROSDAL format in a new ICEDIT window.
- **ICEdit.ShowMDLCT(mdct)**
Displays the transferred structure in MDLCT format in a new ICEDIT window.¹
- **ICEdit.SetMDLCT(mdct)**
Displays the transferred structure in MDLCT file format in the current ICEDIT window.
- **ICEdit.SetMDLCTClip(mdct, len)**
Displays the transferred structure in MDLCTClip¹ format in the current ICEDIT window.
len Length of mdct (mdct may contain 0-values)
- **mdct = ICEdit.GetMDLCT()**
Returns the current structure in MDLCT format.
- **ICEdit.CopyToClipboard(rosdal)**
Copies the transferred structure in ROSDAL format to the Windows clipboard.²
- **ICEdit.PasteFromClipboard()**
Pastes a structure from the clipboard to the ICEDIT object.
- **ICEdit.CopyMdIct (mdct, width, height, showMapps, showRkz, showSter, showNumb, showInvRet, queryDisplay, showResidue);)**
Copies the a structure in MSDLCT format to the Windows clipboard.
width, height Picture width and height in pixel
showMapps, ... Display flags

¹ For details see: CTFfile Formats, <http://www.mdl.com/downloads/public/ctfile/ctfile.pdf>.

² In Format MDLCTClip all line breaks of the corresponding MOL/RXNFILE are replaced by a numeric value which holds the number of characters per line.

10.1.1 Format of parameter 'rosdal'

```
<XML>
  <ROSDAL type='MOL'>1 (X238,Y-137), ...</ROSDAL>
  <RECTANGLE>
    <WIDTH>200</WIDTH>
    <HEIGHT>100</HEIGHT>
  </RECTANGLE>
</XML>
```

Allowed main tags:

Tag name	Description
ICedit	To use only, if the structure is made by ICEDIT. The structure will not be scaled!
XML	To use in all other cases. The structure will be scaled!

Sub tags:

Tag name	Description	Required
ROSDAL	Structure in rosdal format.	yes
RECTANGLE	Dimension of the bounding box.	yes

10.2 Events

An ICEDIT object can throw the following events:

- **RosdalEvent (rosdal)**
An ICEDIT object generates this event by closing the window and by pushing the button 'Back'.

10.3 Using ICEDIT in Visual Basic 6.0

The following steps are necessary to work with an ICEDIT object in VisualBasic 6:

- Check the item 'ICeditOleSvr' in the menu Projects – References of your VB-Application.
- Declare your object:
`Public WithEvents icedit As ICeditOleSvr.Application`
- Create an instance of your object:
`Set icedit = CreateObject("ICeditOleSvr.Application")`

Please see the project ICeditOleTestClient in the examples directory.

11 Additional Tools

11.1 Add-in for MSEXCEL

Windows application only

Under development – not yet supported

11.2 ICEDIT as ActiveX Control (ICEDITOCX)

Windows application only

Internet Explorer only

ICEDITOCX can be used as ActiveX Control in Internet Explorer.

As well as a Signed Applet it offers the full functionality of a Windows application.

11.2.1 Integration of ICEDITOCX in HTML

<AppDir>/ICedit/Examples/ActiveXctl contains the example html file ICeditocxTest.htm.

To create a reference to ICEDITOCX, the following tag is necessary:

```
<OBJECT id=ICeditCtrl type=application/x-oleobject
classid=CLSID:DB9FCC1E-10A4-4B39-898E-48B4264B9DF9 name=ICeditCtrl
CLSID="{DB9FCC1E-10A4-4B39-898E-48B4264B9DF9}"></OBJECT>
```

11.2.2 Programming Interface – API

11.2.2.1 Methods

ICEDITOCX supports the following methods:

- **ICeditOcx.startEditor (rosdal);**

Displays the transferred structure in ROSDAL format in a new ICEDIT window.

Example:

```
ICeditOcx.startEditor("1 (X839, Y-617) , 2 (X1037, Y-617) , 3S, 3 (X938, Y-445) , 1!2, 1!3, 2!3.");
```

- **ICeditOcx.startEditor ("");**

Displays the ICEDIT window.

Example:

```
ICeditOcx.startEditor("");
```

- **ICeditOcx.Data("");**

Returns the current structure in MDLCT format.

Return:

```
<ICEDIT version='version' action='FINISHED'>
  <MDLCT>mdlct</MDLCT>
</ICEDIT>
```

- **ICEDITOcx.Data("ROSDAL");**

Returns the current structure in Infochem Rosdal format.

Return:

```
<ICEDIT version='version' action='FINISHED'>
<ROSDAL type='type'>rosdal</ROSDAL>
<RECTANGLE><WIDTH>width</WIDTH><HEIGHT>height</HEIGHT></RECTANGLE>
</ICEDIT>
```

- **ICEDITOcx.getVersion ();**

Returns the current version of ICEDITOcx.

- **ICEDITOcx.getInfo ();**

Returns an information string.

- **ICEDITOcx.getReady ();**

Returns true if a structure has been drawn.

11.2.2.2 Events

ICEDITOcx supports the following events:

- **ICEDITOcx.Editready()**

Occurs after a structure has been drawn.

11.3 IC_{RENDIT}

IC_{RENDIT} is a small Signed Applet which can be implemented in a web page to show chemical structures.

11.3.1 Context menu

The context menu offers the following functionalities:

- **Copy:** Copy the structure as OLE-Object to the windows clipboard
- **Paste:** Pastes a structure from the windows clipboard
- **Save:** Save the structure as MOL/RXNFILE
- **Edit:** Launch ICEDIT to edit the structure
- **Load:** Load a MOL/RXNFILE
- **Display:** Change set display properties

11.3.2 Integration of IC*RENDIT* in HTML

Applet tag:

```
<applet
  code="de.infochem.icedit.main.ICRenditApplet.class"
  archive="icrendit.jar"
  name="ICRendit"
  width="200"
  height="200"
  codebase="icrendit"
  queryDisp=true
  editor=true
  MAYSCRIPT
  mdlct="|      MDL-Draw  0208081626|| 10 10 ..."
  class="border">
  <param
    name="javascriptCallback"
  value="document.getElementById('mdlct').value=document.ICRendit.getMdlCt();">
</applet>
```

11.3.3 Applet parameter

Parameter	Type	Optional	Default value
width	numeric	no	
height	numeric	no	
mdlct	string	yes	
editor	boolean	yes	false
showMappings	boolean	yes	false
showRxnCenter	boolean	yes	false
showStereo	boolean	yes	false
showNumbers	boolean	yes	false
showInvRet	boolean	yes	false
showResidue	boolean	yes	false
queryDisp	boolean	yes	false
javascriptCallback	string	yes	false
debug	boolean	yes	false

11.3.4 Public applet methods

```
void setMdlCt(java.lang.String)
void setMdlCt(java.lang.String,char)
java.lang.String getMdlCt()
void setDispInvRet(boolean)
void setDispMappings(boolean)
```

```
void setDispNumbers(boolean)
void setDispQueryFeatures(boolean)
void setDispResidue(boolean)
void setDispRxnCenter(boolean)
void setDispStereo(boolean)
void showEditor()
void save()
void load()
void copy()
```

11.3.5 Copyright

ICRENDIT is using **com4j**:

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