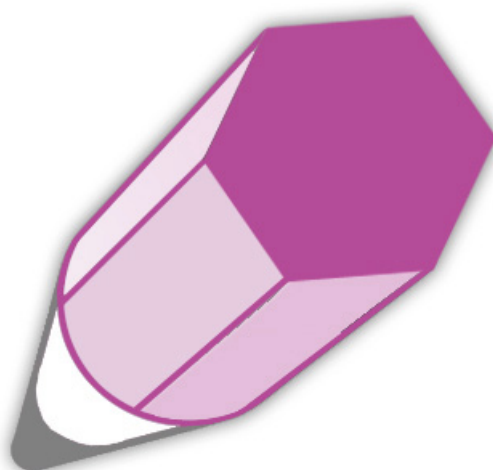


**IC***EDIT*



**Manual**

Structure and Reaction Editor

Version 1.7.3.3

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# Table of Contents

<b>1</b>	<b>Preface</b>	<b>1</b>
<b>2</b>	<b>Getting Started</b>	<b>1</b>
..	Overview of the Java applet.....	1
<b>3</b>	<b>Description of the Menu Bar</b>	<b>2</b>
3.1	File.....	2
3.2	Edit.....	3
3.3	Templates.....	4
3.4	? - Menu.....	4
<b>4</b>	<b>Description of Standard Edit Buttons</b>	<b>5</b>
<b>5</b>	<b>General Information</b>	<b>10</b>
5.1	Drawing.....	10
5.2	Context Menus.....	10
5.3	Keyboard Shortcuts.....	10
<b>6</b>	<b>User defined Templates</b>	<b>11</b>
<b>7</b>	<b>Embedded as OLE-Server</b>	<b>11</b>
7.1	Integration in MSOffice.....	11
7.2	OLE Interfaces.....	11
<b>8</b>	<b>Additional clipboard formats</b>	<b>11</b>
<b>9</b>	<b>Programming Interface - API</b>	<b>13</b>
9.1	Functions.....	13
9.2	Events.....	14
9.3	Using ICEDIT in Visual Basic 6.0.....	14
<b>10</b>	<b>Additional Tools</b>	<b>15</b>
10.1	Add-in for MSExcel.....	15
10.2	ICEDIT as ActiveX Control (ICEditOcx).....	15
10.3	ICRENDIT.....	15

# 1 Preface

The chemical structure editor ICEDIT is available as applet for all Java supporting platforms 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, Access, PowerPoint)
- Application Programming Interface (API) for Java, VB 6, VBA and .NET

# 2 Getting Started

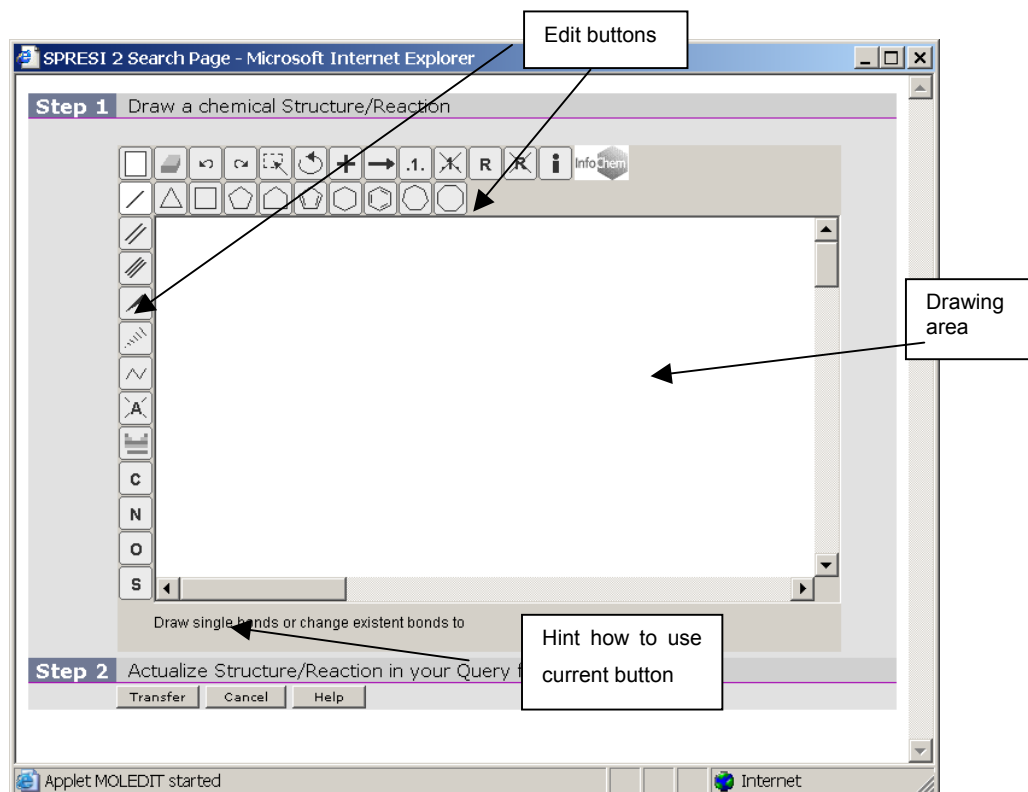
## *Windows application only*

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!

## 2.1 Overview of the Java applet



**Fig. 1:** The ICEDITJava applet

## 3 Description of the Menu Bar

*Windows application only*

### 3.1 File

#### 3.1.1 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)

#### 3.1.2 New

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

#### 3.1.3 Open

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

#### 3.1.4 Save

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

#### 3.1.5 Save As

Saves a structure file with a different file name.

#### 3.1.6 Export - Mol/Rxnfile

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

#### 3.1.7 Export - Skcfile

Exports a structure or reaction to MDLSketch file format.

#### 3.1.8 Import - Molfile

Imports a structure from MDL MOL file format.

#### 3.1.9 Import - Rxnfile

Imports a reaction from MDL RXN file format.

#### 3.1.10 Import - Skcfile

Imports a structure or reaction from MDL Sketch file format.

#### 3.1.11 Import - Smiles

Imports a structure from the Smiles format and generates coordinates.

### **3.1.12 Import - Cdxfile**

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

### **3.1.13 Exit**

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

## **3.2 Edit**

### **3.2.1 Undo**

Undo last operation. (Keyboard shortcut CTRL + Z)

### **3.2.2 Redo**

Redo last operation. (Keyboard shortcut CTRL + Y)

### **3.2.3 Copy**

Copies the current structure into the windows clipboard.

Transfer to ISIS/Draw, MDLDraw and Microsoft Office products is supported. (Keyboard shortcut CTRL + C)

### **3.2.4 Paste**

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

### **3.2.5 Delete**

Deletes the selected objects. (Keyboard shortcut DEL)

### **3.2.6 Select all**

Selects all objects. (Keyboard shortcut CTRL + A)

### **3.2.7 Duplicate**

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

## 3.3 Templates

### 3.3.1 Open

Opens the Templates Dialog.

#### 3.3.1.1 Insert Templates

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

It is possible to select the docking point (atom or bond) from the template. This atom or bond is highlighted in the template dialog. By clicking at an attachment point in the structure within the drawing area, the template will be connected.

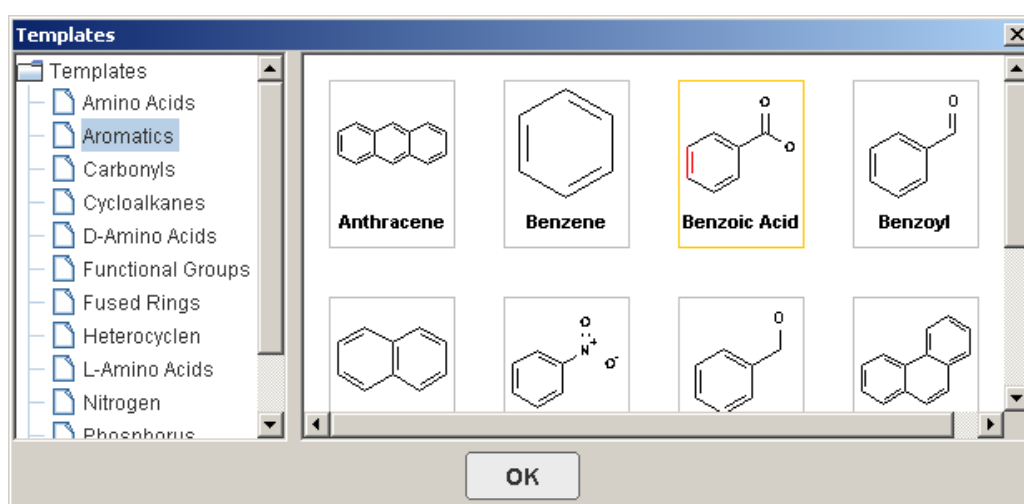


Fig. 2: Use the dialog to insert a template at a specific bond.

## 3.4 ? - Menu

### 3.4.1 Help

Open the PDF-documentation file.

### 3.4.2 About

Shows information about IEDIT and its version number.

## 4 Description of Standard Edit Buttons

Standard buttons provided by the applet and the Windows application:



Clear screen

Deletes all objects from the drawing area.



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.



Undo last operation



Redo last operation



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 by using either the context menu or the appropriate keyboard shortcuts.



Rotate selected objects



Add reaction plus



Add reaction arrow

Please note: At the moment there is only one arrow per reaction supported.



### 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 map reactant atoms with product atoms.



### 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.



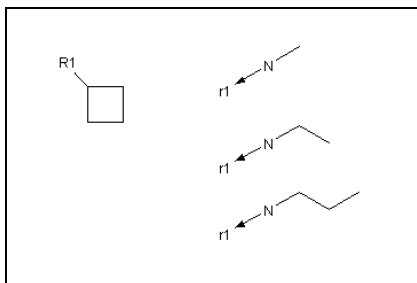
### Define R-groups

Draw a core structure and several R-groups.

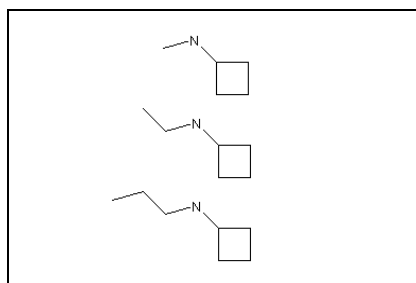
First click on the position of the core structure, where you want to have the R-Group attached. Then click on the connection position of the R-Groups.

Examples:

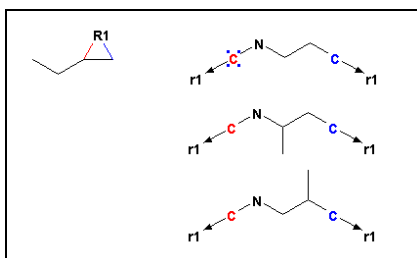
#### R-Query



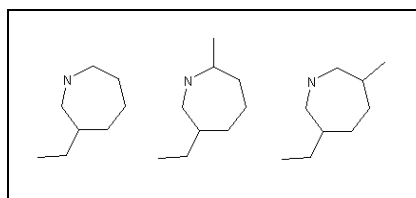
#### resolved single Queries:



#### R-Query



#### resolved single Queries:



**Please note:** to specify two different attachments in one R-group, 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 R-Group numbering, please click at the object you want to edit and enter the new number with your keyboard. To do this the "Define R-groups" button must be selected!



Remove R-group Info from atom



Show info dialog

Shows information about ICDIT and its version number.

### Standard templates

Select a standard template in the button bar. The selected template button is selected. Click in the drawing area to place the selected template. By clicking at an attachment point in the structure within the drawing area, the template will be connected.

Templates provided:



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



Show/hide atom numbers



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 a double or triple bond.



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. Additional clicks on it change its direction.



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. Additional clicks on it change its direction.

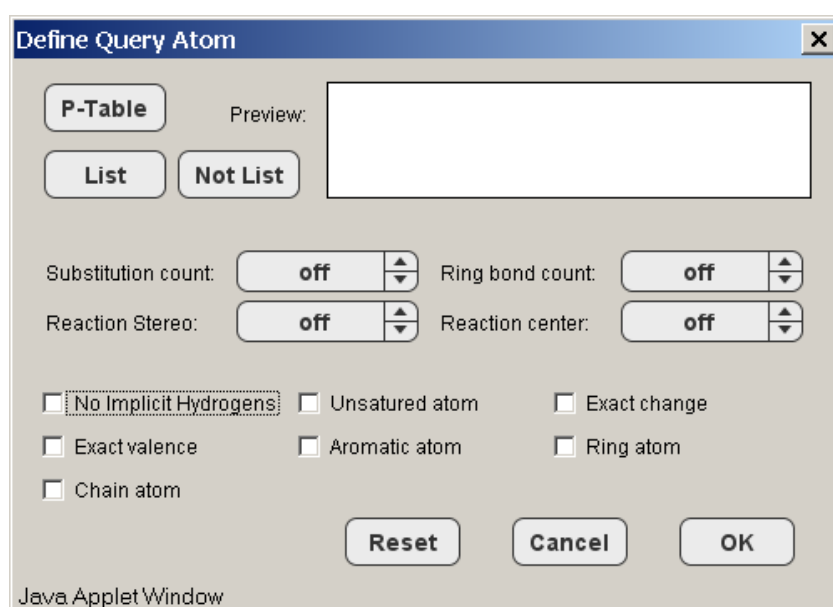


Draw chain

Draws a chain of C-C single bonds.



Edit query atom



**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.

**P-Table** has additional buttons for not standard 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)



Open Periodic Table of the Elements to select an atom

Opens a dialog with the Periodic Table of the Elements to select additional elements besides C,O,N,S. Use this dialog to define charge, isotope, radical, and valence. After selection click in the drawing area to place the atom.



Draw atom C

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



Draw atom N

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



Draw atom O

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



Draw atom S

Draws a S atom or converts an existing atom into a S 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.



Transfer structure back to calling application

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

## 5 General Information

### 5.1 Drawing

To draw atoms or bonds, click the corresponding button to activate the drawing mode.

To draw rings click the corresponding template button and click once for one ring. To fuse rings, click on an existing ring bond. To connect rings as spiro molecules click on a ring atom.

You can change the alignment of atoms, bonds or templates by dragging the object into the desired direction before releasing the mouse button. Please note, that rings will be fused automatically, if the distance between two rings falls below a certain threshold.

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).

### 5.2 Context Menus

Context menus are available by right clicking on the drawing surface. Use the context menu to:

- **Copy** selected objects into an internal buffer.
- **Paste** objects from the internal buffer into your drawing.
- **Duplicate** the selected objects.
- **Edit** the currently selected atom, bond or selection.
- **Delete** the currently selected atom or bond.

### 5.3 Keyboard Shortcuts

The following keyboard shortcuts are available in IEDIT:

- **Ctrl+C**: Copy the current structure into the windows clipboard.
- **Ctrl+V**: Paste a structure from the clipboard.
- **Ctrl+B**: Transfer structure to calling application.
- **Ctrl+N**: New window (clear screen)
- **Ctrl+O**: Open file
- **Ctrl+S**: Save structure/reaction as \*.icf file (default file name and default directory)
- **Ctrl+A**: Select all objects within the drawing area
- **Ctrl+E**: Exit IEDIT

## 6 User defined Templates

Draw the structure you want to use as template in *ICEDIT* and save it to the subdirectory **Templates** of your *ICEDIT* installation directory (e.g. 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).

## 7 Embedded as OLE-Server

*Windows application only*

### 7.1 Integration in MSOffice

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

- To start *ICEDIT* in MSWord, MSEXcel, etc. choose the item 'ICEdit Document' from menu Insert – Object.
- Click the button 'Back' to transfer the structure from *ICEDIT* back to MSOffice.
- Double-clicking the structure starts *ICEDIT*.
- Choose 'Copy' from *ICEDIT* menu Edit to copy your structure via clipboard to MSWord, MSEXcel, etc.
- Choose 'Paste' to insert a structure from MSOffice into *ICEDIT* via clipboard.

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

### 7.2 OLE Interfaces

The following OLE Interfaces are supported:

- IDataObject.GetData for format "MDLCT"
- IDataObject.SetData for format "MDLCT"

## 8 Additional clipboard formats

*Windows application only*

*ICEDIT* application offers the following additional clipboard formats:

- MDLCT



## 9 Programming Interface - API

### *Windows application only*

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

### 9.1 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.
- **ICEDIT.SetMDLCT(mdct )**  
Displays the transferred structure in MDLCT format in the current ICEDIT window.
- **ICEDIT.SetMDLCTClip(mdct, len )**  
Displays the transferred structure in MDLCTClip<sup>1)</sup> 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. <sup>9.1.1)</sup>
- **ICEDIT.PasteFromClipboard( )**  
Pastes a structure from the clipboard to the ICEDIT object.
- **ICEDIT.CopyMdCt (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

<sup>1)</sup> 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.

#### 9.1.1 Format of parameter 'rosdal'

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

Allowed main tags:

Tag name	Description
ICEdit	To use only, if the structure is made by Icedit. The structure won't 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

Tag name	Description	Required
RECTANGLE	Dimension of the bounding box.	yes

## 9.2 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'.

## 9.3 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.

## 10 Additional Tools

### 10.1 Add-in for MSEXcel

*Windows application only*

Under development – not yet supported

### 10.2 IC<sub>EDIT</sub> 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.

#### 10.2.1 Integration of ICEditOcx in HTML

<AppDir>/ICedit/Examples/ActiveXCtrl 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>
```

### 10.3 IC<sub>RENDIT</sub>

IC<sub>RENDIT</sub> is a small Signed Applet which can be implemented in a web page to show chemical structures.

#### 10.3.1 Context menu

The context menu offers the following functionalities:

- **Copy:** Copy the structure as OLE-Object to 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

### 10.3.2 Integration of IC<sub>RENDIT</sub> 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>
```

### 10.3.3 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	

### 10.3.4 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()
```

### 10.3.5 Copyright

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