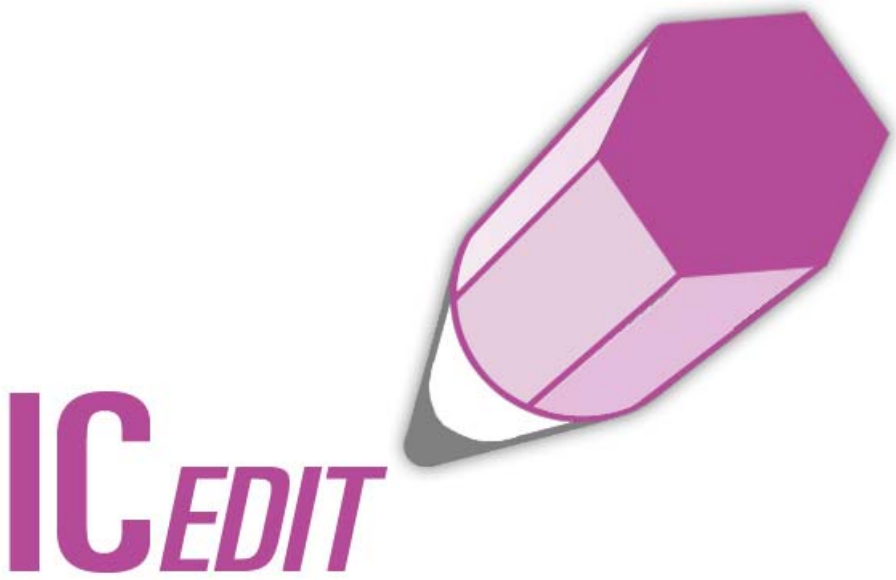
InfoChem



Technical Documentation

Structure and Reaction Editor

Version 2.2

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Table of Contents

1 Preface 1

2 Configuration of Standard Edit and Drawing Buttons 2

2.1 Default XML String 4

2.2 Button Definition 7
2.2.1 Standard Edit Buttons 7
2.2.2 Standard Molecule Templates 10
2.2.3 Standard Bond Buttons 12
2.2.4 Standard Atom Buttons 13
2.2.5 Others 15

2.3 Description of the XML String 16
2.3.1 Toolbars 20
2.3.2 Configuration of Buttons 22

3 Embedded as OLE-Server 26

3.1 Integration in MS Office 26

3.2 OLE Interfaces 26
3.2.1 Standard OLE-Interface 26
3.2.2 Additional COM Interfaces 27

4 Programming Interface - API 30

4.1 Using IC*EDIT* in Visual Basic 6.0 30

5 Additional Clipboard Formats 31

6 Additional Tools 32

6.1 Add-in for MSExcel 32

6.2 IC*EDIT* as ActiveX Control (IC*EDITOCX*) 32
6.2.1 Integration of IC*EDITOCX* in HTML 32
6.2.2 Programming Interface – API 32

6.3 IC*EDIT* Java Applet 34
6.3.1 Enhanced IC*EDIT* Java Applet 34
6.3.2 Installation 35

6.4 IC*RENDIT* 36
6.4.1 Context Menu 36
6.4.2 Integration of IC*RENDIT* in HTML 36
6.4.3 Applet Parameter 37
6.4.4 Public Applet Methods 37
6.4.5 Usage without an IC*EDIT* Installation 38
6.4.6 Copyright 38

7 Customer Support 39

1 Preface

This documentation gives a detailed technical description of IC*EDIT* and its components.

Here you can find information about:

- IC*RENDIT*
- IC*EDITOCX*
- Configuration of IC*EDIT* button bars
- OLE-Server functionalities
- Add-in for MSExcel
- Clipboard formats
- Programming interfaces

Please note: For the use of IC*EDIT* please refer to the IC*EDIT* user manual. It can be found either by opening the IC*EDIT* application and selecting “Help” from the “?” menu or opening the “ICEditManual.pdf” from the “Documentation” folder of the installation path of IC*EDIT*.

2 Configuration of Standard Edit and Drawing Buttons

In this chapter you will find a brief description on how to arrange the buttons and toolbars from either the IC*EDIT* applet in your internet or intranet environment or the IC*EDIT* application.

- **IC*EDIT* application:** To adjust the configuration of the IC*EDIT* toolbars please edit the file iceditcfg.xml from the IC*EDIT* installation path according to the description given below.
  Please note: The file iceditcfg_orig.xml from the installation path can be used to restore the default value if the format of the configured icedit.xml file is corrupt.
- **IC*EDIT* applet:** To adjust the configuration of the IC*EDIT* toolbars please edit the applet parameter "config" according to the description given below.

Various standard edit and template buttons are provided in the following three button bars (toolbars):

- Standard edit buttons (1st horizontal toolbar)

- Standard molecule templates and single bond (2nd horizontal toolbar)

- Standard bond buttons, standard atom buttons and others (vertical toolbar)

The edit and template buttons can be configured in the following way:

(i) The position of the complete toolbar - vertical or horizontal - can be defined (chapter 2.3.1).
Please note: Several horizontal toolbars, but only one vertical toolbar is supported currently.

(ii) The order of buttons in-between one toolbar can be changed (chapter 2.3.2).

(iii) Buttons can be allocated from one to another toolbar (chapter 2.3.2).

(iv) The generation of new atom buttons is possible (e.g. creation of “P” button, chapter 2.3.2).

(v) The generation of new toolbars is possible (e.g. separation of bond and atom buttons in two individual toolbars, chapter 2.3.1).

The incorporation of **new** template buttons (e.g. the incorporation of a benzoic acid button) is under investigation and will be supported in future.

2.1 Default XML String

To restore or recover the default button configuration, please use the following original XML string (please remove new-line characters (carriage return line feed CRLF) between lines for use).

```
<toolbars>
  <toolbar>
    <vertical>false</vertical>
    <polygonbutton>
      <drawmode>19</drawmode>
      <toggle>false</toggle>
      <description>Clear screen</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>17</drawmode>
      <toggle>true</toggle>
      <description>Delete object</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>20</drawmode>
      <toggle>false</toggle>
      <description>Undo last operations</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>31</drawmode>
      <toggle>false</toggle>
      <description>Redo last operations</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>21</drawmode>
      <toggle>true</toggle>
      <description>Select</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>48</drawmode>
      <toggle>true</toggle>
      <description>Select object</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>22</drawmode>
      <toggle>true</toggle>
      <description>Rotate selected object</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>33</drawmode>
      <toggle>true</toggle>
      <description>Add reaction plus</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>34</drawmode>
      <toggle>true</toggle>
      <description>Add reaction arrow</description>
    </polygonbutton>
    <button>
      <drawmode>35</drawmode>
      <toggle>true</toggle>
      <description>Maps atoms</description>
      <label>.1.</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
    <polygonbutton>
      <drawmode>36</drawmode>
      <toggle>true</toggle>
      <description>Remove mapping from atoms</description>
    </polygonbutton>
    <button>
      <drawmode>37</drawmode>
      <toggle>true</toggle>
      <description>Define Rgroups</description>
      <label>R</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
    <polygonbutton>
```

```
            <drawmode>38</drawmode>
            <toggle>true</toggle>
            <description>Remove Rgroup Info from atom</description>
        </polygonbutton>
        <polygonbutton>
            <drawmode>23</drawmode>
            <toggle>false</toggle>
            <description>Show Info dialog</description>
        </polygonbutton>
    </toolbar>
    <toolbar>
        <vertical>false</vertical>
        <polygonbutton>
            <drawmode>1</drawmode>
            <toggle>true</toggle>
            <description>Draw single bonds</description>
        </polygonbutton>
        <templatebutton>
            <name>Cyclopropane</name>
            <description>Cyclopropane</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclobutane</name>
            <description>Cyclobutane</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclopentane</name>
            <description>Cyclopentane</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclopentane2</name>
            <description>Cyclopentane</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclopentane1</name>
            <description>Cyclopentane</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclopentane3</name>
            <description>Cyclopentane</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclopentadiene</name>
            <description>Cyclopentadiene</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclopentadiene1</name>
            <description>Cyclopentadiene</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclohexane</name>
            <description>Cyclohexane</description>
        </templatebutton>
        <templatebutton>
            <name>Benzene</name>
            <description>Benzene</description>
        </templatebutton>
        <templatebutton>
            <name>Cycloheptane</name>
            <description>Cycloheptane</description>
        </templatebutton>
        <templatebutton>
            <name>Cyclooctane</name>
            <description>Cyclooctane</description>
        </templatebutton>
    </toolbar>
    <toolbar>
        <vertical>true</vertical>
        <polygonbutton>
            <drawmode>2</drawmode>
            <toggle>true</toggle>
            <description>Draw double bonds</description>
        </polygonbutton>
        <polygonbutton>
            <drawmode>3</drawmode>
            <toggle>true</toggle>
            <description>Draw triple bonds</description>
        </polygonbutton>
        <polygonbutton>
            <drawmode>5</drawmode>
            <toggle>true</toggle>
            <description>Draw up wedges</description>
        </polygonbutton>
        <polygonbutton>
            <drawmode>6</drawmode>
            <toggle>true</toggle>
```

```
            <description>Draw down wedges</description>
        </polygonbutton>
        <polygonbutton>
            <drawmode>15</drawmode>
            <toggle>true</toggle>
            <description>Draw chain</description>
        </polygonbutton>
        <polygonbutton>
            <drawmode>24</drawmode>
            <toggle>true</toggle>
            <description>Draw an atom</description>
        </polygonbutton>
        <button>
            <drawmode>18</drawmode>
            <toggle>true</toggle>
            <description>Draw carbon atoms</description>
            <label>C</label>
            <font>
                <size>14</size>
                <style>1</style>
            </font>
        </button>
        <button>
            <drawmode>18</drawmode>
            <toggle>true</toggle>
            <description>Draw nitrogen atoms</description>
            <label>N</label>
            <font>
                <size>14</size>
                <style>1</style>
            </font>
        </button>
        <button>
            <drawmode>18</drawmode>
            <toggle>true</toggle>
            <description>Draw oxygen atoms</description>
            <label>O</label>
            <font>
                <size>14</size>
                <style>1</style>
            </font>
        </button>
        <button>
            <drawmode>18</drawmode>
            <toggle>true</toggle>
            <description>Draw sulfur atoms</description>
            <label>S</label>
            <font>
                <size>14</size>
                <style>1</style>
            </font>
        </button>
        <button>
            <drawmode>16</drawmode>
            <toggle>true</toggle>
            <description>Draw text</description>
            <label>text</label>
            <font>
                <size>14</size>
                <style>0</style>
            </font>
        </button>
        <button>
            <drawmode>42</drawmode>
            <toggle>true</toggle>
            <description>Bracket</description>
            <label>[ ]</label>
            <font>
                <size>16</size>
                <style>0</style>
            </font>
        </button>
    </toolbar>
</toolbars>
```

2.2 Button Definition

Please find below the description of all buttons and templates together with their XML string. To change the position of a button it is necessary to (i) localize (ii) select (iii) and drag and drop the complete XML string. For an easier identification we have listed all XML strings below (please remove new-line characters (carriage return line feed CRLF) between lines for use).

2.2.1 Standard Edit Buttons

 Clear screen.

```
<polygonbutton>
   <drawmode>19</drawmode>
   <toggle>false</toggle>
   <description>Clear screen</description>
</polygonbutton>
```

 Delete object.

```
<polygonbutton>
   <drawmode>17</drawmode>
   <toggle>true</toggle>
   <description>Delete object</description>
</polygonbutton>
```

 Undo last operation.

```
<polygonbutton>
   <drawmode>20</drawmode>
   <toggle>false</toggle>
   <description>Undo last operations</description>
</polygonbutton>
```

 Redo last operation.

```
<polygonbutton>
   <drawmode>31</drawmode>
   <toggle>false</toggle>
   <description>Redo last operations</description>
</polygonbutton>
```

 Select object.

```
<polygonbutton>
   <drawmode>21</drawmode>
   <toggle>true</toggle>
   <description>Select</description>
</polygonbutton>
```

 Select object.

```
<polygonbutton>
   <drawmode>48</drawmode>
   <toggle>true</toggle>
   <description>Select object</description>
</polygonbutton>
```

 Rotate selected objects.

```
<polygonbutton>
   <drawmode>22</drawmode>
   <toggle>true</toggle>
   <description>Rotate selected object</description>
</polygonbutton>
```

 Add reaction plus.

```
<polygonbutton>
   <drawmode>33</drawmode>
   <toggle>true</toggle>
   <description>Add reaction plus</description>
</polygonbutton>
```

 Add reaction arrow.

```
<polygonbutton>
   <drawmode>34</drawmode>
   <toggle>true</toggle>
   <description>Add reaction arrow</description>
</polygonbutton>
```

 Map atoms.

```
<button>
   <drawmode>35</drawmode>
   <toggle>true</toggle>
   <description>Maps atoms</description>
   <label>.1.</label>
  <font>
     <size>14</size>
     <style>1</style>
   </font>
</button>
```

 Remove mappings from atoms and reaction center information from bonds.

```
<polygonbutton>
   <drawmode>36</drawmode>
   <toggle>true</toggle>
   <description>Remove mapping from atoms</description>
</polygonbutton>
```

 Define Rgroups.

```
<button>
   <drawmode>37</drawmode>
   <toggle>true</toggle>
   <description>Define Rgroups</description>
   <label>R</label>
  <font>
     <size>14</size>
     <style>1</style>
   </font>
</button>
```

 Remove Rgroup Info from atom.

```
<polygonbutton>
   <drawmode>38</drawmode>
   <toggle>true</toggle>
   <description>Remove Rgroup Info from atom</description>
</polygonbutton>
```

 Show info dialog.

```
<polygonbutton>
   <drawmode>23</drawmode>
   <toggle>false</toggle>
   <description>Show Info dialog</description>
</polygonbutton>
```

2.2.2 Standard Molecule Templates

 Cyclopropane.

```
<templatebutton>
   <name>Cyclopropane</name>
   <description>Cyclopropane</description>
</templatebutton>
```

 Cyclobutane.

```
<templatebutton>
   <name>Cyclobutane</name>
   <description>Cyclobutane</description>
</templatebutton>
```

 Cyclopentane.

```
<templatebutton>
   <name>Cyclopentane</name>
   <description>Cyclopentane</description>
</templatebutton>
```

 Cyclopentane.

```
<templatebutton>
   <name>Cyclopentane2</name>
   <description>Cyclopentane</description>
</templatebutton>
```

 Cyclopentane.

```
<templatebutton>
   <name>Cyclopentane1</name>
   <description>Cyclopentane</description>
</templatebutton>
```

 Cyclopentane.

```
<templatebutton>
   <name>Cyclopentane3</name>
   <description>Cyclopentane</description>
</templatebutton>
```

 Cyclopentadiene.

```
<templatebutton>
   <name>Cyclopentadiene</name>
   <description>Cyclopentadiene</description>
</templatebutton>
```

 Cyclopentadiene.

```
<templatebutton>
   <name>Cyclopentadiene1</name>
   <description>Cyclopentadiene</description>
</templatebutton>
```

 Cyclohexane.

```
<templatebutton>
   <name>Cyclohexane</name>
   <description>Cyclohexane</description>
</templatebutton>
```

 Benzene.

```
<templatebutton>
   <name>Benzene</name>
   <description>Benzene</description>
</templatebutton>
```

 Cycloheptane.

```
<templatebutton>
   <name>Cycloheptane</name>
   <description>Cycloheptane</description>
</templatebutton>
```

 Cyclooctane.

```
<templatebutton>
   <name>Cyclooctane</name>
   <description>Cyclooctane</description>
</templatebutton>
```

2.2.3 Standard Bond Buttons

 Draw single bonds or change an existing bond.

```
<polygonbutton>
   <drawmode>1</drawmode>
   <toggle>true</toggle>
   <description>Draw single bonds</description>
</polygonbutton>
```

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

```
<polygonbutton>
   <drawmode>2</drawmode>
   <toggle>true</toggle>
   <description>Draw double bonds</description>
</polygonbutton>
```

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

```
<polygonbutton>
   <drawmode>3</drawmode>
   <toggle>true</toggle>
   <description>Draw triple bonds</description>
</polygonbutton>
```

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

```
<polygonbutton>
   <drawmode>5</drawmode>
   <toggle>true</toggle>
   <description>Draw up wedges</description>
</polygonbutton>
```

 Draw down wedges or change an existing bond to down wedge.

```
<polygonbutton>
   <drawmode>6</drawmode>
   <toggle>true</toggle>
   <description>Draw down wedges</description>
</polygonbutton>
```

 Draw chain.

```
<polygonbutton>
   <drawmode>15</drawmode>
   <toggle>true</toggle>
   <description>Draw chain</description>
</polygonbutton>
```

2.2.4 Standard Atom Buttons

 Draw atom.

```
<polygonbutton>
   <drawmode>24</drawmode>
   <toggle>true</toggle>
   <description>Draw an atom</description>
</polygonbutton>
```

 Draw atom C.

```
<button>
   <drawmode>18</drawmode>
   <toggle>true</toggle>
   <description>Draw carbon atoms</description>
   <label>C</label>
  <font>
     <size>14</size>
     <style>1</style>
   </font>
</button>
```

 Draw atom N.

```
<button>
   <drawmode>18</drawmode>
   <toggle>true</toggle>
   <description>Draw nitrogen atoms</description>
   <label>N</label>
  <font>
     <size>14</size>
     <style>1</style>
   </font>
</button>
```

 Draw atom O.

```
<button>
   <drawmode>18</drawmode>
   <toggle>true</toggle>
   <description>Draw oxygen atoms</description>
   <label>O</label>
  <font>
     <size>14</size>
     <style>1</style>
   </font>
</button>
```

Draw atom S.

```
<button>
   <drawmode>18</drawmode>
   <toggle>true</toggle>
   <description>Draw sulfur atoms</description>
   <label>S</label>
  <font>
     <size>14</size>
     <style>1</style>
   </font>
</button>
```

2.2.5 Others

Draw text.

```
<button>
   <drawmode>16</drawmode>
   <toggle>true</toggle>
   <description>Draw text</description>
   <label>text</label>
  <font>
     <size>14</size>
     <style>0</style>
   </font>
</button>
```

Draw Bracket.

```
<button>
   <drawmode>42</drawmode>
   <toggle>true</toggle>
   <description>Bracket</description>
   <label>[ ]</label>
  <font>
     <size>16</size>
     <style>0</style>
   </font>
</button>
```

2.3 Description of the XML String

The XML string is defined by a start tag, the toolbar information, including button, polygonbutton and template button elements and an end tag (please remove new-line characters (carriage return line feed CRLF) between lines for use).

start tag: <toolbars>

Content of the three toolbars: Here visualized in red, blue and green.

end tag: </toolbars>

```
<toolbars>
  <toolbar>
    <vertical>false</vertical>
    <polygonbutton>
      <drawmode>19</drawmode>
      <toggle>false</toggle>
      <description>Clear screen</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>17</drawmode>
      <toggle>true</toggle>
      <description>Delete object</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>20</drawmode>
      <toggle>false</toggle>
      <description>Undo last operations</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>31</drawmode>
      <toggle>false</toggle>
      <description>Redo last operations</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>21</drawmode>
      <toggle>true</toggle>
      <description>Select</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>48</drawmode>
      <toggle>true</toggle>
      <description>Select object</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>22</drawmode>
      <toggle>true</toggle>
      <description>Rotate selected object</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>33</drawmode>
      <toggle>true</toggle>
      <description>Add reaction plus</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>34</drawmode>
      <toggle>true</toggle>
      <description>Add reaction arrow</description>
    </polygonbutton>
    <button>
      <drawmode>35</drawmode>
      <toggle>true</toggle>
      <description>Maps atoms</description>
      <label>.1.</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
```

```
    <polygonbutton>
      <drawmode>36</drawmode>
      <toggle>true</toggle>
      <description>Remove mapping from atoms</description>
    </polygonbutton>
    <button>
      <drawmode>37</drawmode>
      <toggle>true</toggle>
      <description>Define Rgroups</description>
      <label>R</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
    <polygonbutton>
      <drawmode>38</drawmode>
      <toggle>true</toggle>
      <description>Remove Rgroup Info from atom</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>23</drawmode>
      <toggle>false</toggle>
      <description>Show Info dialog</description>
    </polygonbutton>
  </toolbar>
  <toolbar>
    <vertical>false</vertical>
    <polygonbutton>
      <drawmode>1</drawmode>
      <toggle>true</toggle>
      <description>Draw single bonds</description>
    </polygonbutton>
    <templatebutton>
      <name>Cyclopropane</name>
      <description>Cyclopropane</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclobutane</name>
      <description>Cyclobutane</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclopentane</name>
      <description>Cyclopentane</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclopentane2</name>
      <description>Cyclopentane</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclopentane1</name>
      <description>Cyclopentane</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclopentane3</name>
      <description>Cyclopentane</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclopentadiene</name>
      <description>Cyclopentadiene</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclopentadiene1</name>
      <description>Cyclopentadiene</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclohexane</name>
      <description>Cyclohexane</description>
    </templatebutton>
    <templatebutton>
      <name>Benzene</name>
      <description>Benzene</description>
    </templatebutton>
    <templatebutton>
      <name>Cycloheptane</name>
```

```
      <description>Cycloheptane</description>
    </templatebutton>
    <templatebutton>
      <name>Cyclooctane</name>
      <description>Cyclooctane</description>
    </templatebutton>
  </toolbar>
  <toolbar>
    <vertical>true</vertical>
    <polygonbutton>
      <drawmode>2</drawmode>
      <toggle>true</toggle>
      <description>Draw double bonds</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>3</drawmode>
      <toggle>true</toggle>
      <description>Draw triple bonds</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>5</drawmode>
      <toggle>true</toggle>
      <description>Draw up wedges</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>6</drawmode>
      <toggle>true</toggle>
      <description>Draw down wedges</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>15</drawmode>
      <toggle>true</toggle>
      <description>Draw chain</description>
    </polygonbutton>
    <polygonbutton>
      <drawmode>24</drawmode>
      <toggle>true</toggle>
      <description>Draw an atom</description>
    </polygonbutton>
    <button>
      <drawmode>18</drawmode>
      <toggle>true</toggle>
      <description>Draw carbon atoms</description>
      <label>C</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
    <button>
      <drawmode>18</drawmode>
      <toggle>true</toggle>
      <description>Draw nitrogen atoms</description>
      <label>N</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
    <button>
      <drawmode>18</drawmode>
      <toggle>true</toggle>
      <description>Draw oxygen atoms</description>
      <label>O</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
    <button>
      <drawmode>18</drawmode>
      <toggle>true</toggle>
      <description>Draw sulfur atoms</description>
      <label>S</label>
      <font>
```

```
            <size>14</size>
            <style>1</style>
          </font>
        </button>
        <button>
          <drawmode>16</drawmode>
          <toggle>true</toggle>
          <description>Draw text</description>
          <label>text</label>
          <font>
            <size>14</size>
            <style>0</style>
          </font>
        </button>
        <button>
          <drawmode>42</drawmode>
          <toggle>true</toggle>
          <description>Bracket</description>
          <label>[ ]</label>
          <font>
            <size>16</size>
            <style>0</style>
          </font>
        </button>
      </toolbar>
</toolbars>
```

2.3.1 Toolbars

Toolbars are defined by the following XML tag:

```
<toolbar>
   <vertical>true</vertical>
   button information
</toolbar>
```

2.3.1.1 Generate New Toolbars

To generate a new toolbar add this XML string on the desired position and insert the preferred button elements.

Shown example: Addition of a third horizontal toolbar (brown):

Default XML string of the toolbars

```
<toolbars>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>true</vertical>
      button information
   </toolbar>
</toolbars>
```

Addition of a new horizontal toolbar

```
<toolbars>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>true</vertical>
      button information
   </toolbar>
</toolbars>
```

2.3.1.2 Set Position of the Toolbars

To set the position (horizontal, vertical) of the toolbar, please set the vertical information as desired:

For horizontal toolbars:	*<vertical>false</vertical>*
For vertical toolbar:	*<vertical>true</vertical>*

Please note: Several horizontal toolbars, but only one vertical toolbar is supported currently.

The order of the horizontal toolbars is as ordered in the XML string (1st horizontal toolbar, 2nd horizontal toolbar, 3rd horizontal toolbar, ..). To change the order please (i) select and (ii) drag and drop the whole toolbar tag and place it on the desired position.

Shown example: The order of the 1st and the 2nd horizontal toolbar is changed.

Default order of the horizontal toolbars

```
<toolbars>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>true</vertical>
      button information
   </toolbar>
</toolbars>
```

Changed order of the horizontal toolbars

```
<toolbars>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>false</vertical>
      button information
   </toolbar>
   <toolbar>
      <vertical>true</vertical>
      button information
   </toolbar>
</toolbars>
```

2.3.2 Configuration of Buttons

2.3.2.1 Change the Position of Buttons

To change the position of a button please select the complete button element string of the desired button and drag and drop it to the preferred position.

Please note: Please take care that the complete XML string of a button element is selected. The XML button element begins with the start tag and ends with the end tag, as shown below.

for buttons:	<*button*>button information</*button*>
for templatebuttons:	<*templatebutton*>button information</*templatebutton*>
for polygonbuttons:	<*polygonbutton*>button information</*polygonbutton*>

Whenever a XML string is cut the XML string is not valid any more. In this case a warning is shown when the applet is started and the default values are loaded.

Short example:

Default XML string

```
<toolbar>
   <vertical>true</vertical>
   <polygonbutton>button_information</polygonbutton>
   <polygonbutton>button_information></polygonbutton>
   <polygonbutton>button_information</polygonbutton>
   <button> button_information</button>
</toolbar>
```

Changed button position – the first button is now the last one

```
<toolbar>
   <vertical>true</vertical>
   <polygonbutton>button_information></polygonbutton>
   <polygonbutton>button_information</polygonbutton>
   <button> button_information</button>
   <polygonbutton>button_information</polygonbutton>
</toolbar>
```

Real example (please remove new-line characters (carriage return line feed CRLF) between lines for use):
The text button will be moved to the standard edit button toolbar between the “remove R-Group” button and the “information” button:

1) Please select the complete XML string of the text button:

```
<toolbars>
  <toolbar>
    <vertical>false</vertical>
    <polygonbutton>
      <drawmode>19</drawmode>
      <toggle>false</toggle>
      <description>Clear screen</description>
    </polygonbutton>
...
    <polygonbutton>
```

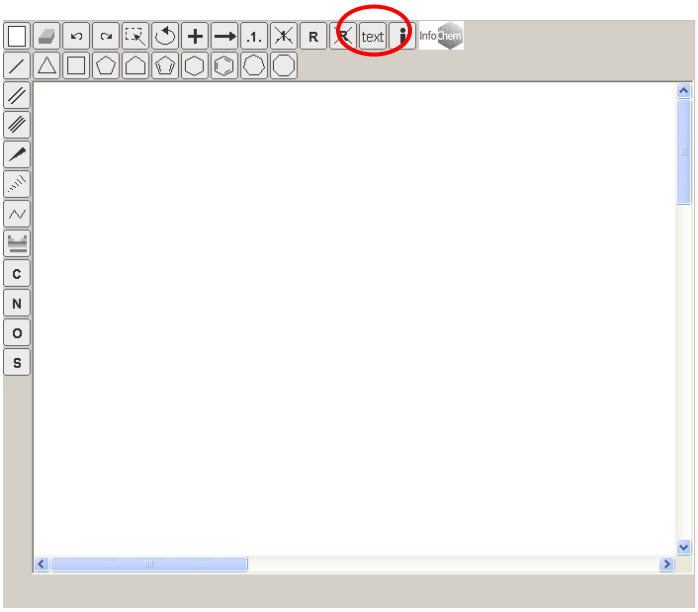
```
            <drawmode>23</drawmode>
            <toggle>false</toggle>
            <description>Show Info dialog</description>
          </polygonbutton>
        </toolbar>
        <toolbar>
...
        </toolbar>
        <toolbar>
          <vertical>true</vertical>
          <polygonbutton>
            <drawmode>2</drawmode>
            <toggle>true</toggle>
            <description>Draw double bonds</description>
          </polygonbutton>
...
          <button>
            <drawmode>18</drawmode>
            <toggle>true</toggle>
            <description>Draw sulfur atoms</description>
            <label>S</label>
            <font>
              <size>14</size>
              <style>1</style>
            </font>
          </button>
          <button>
            <drawmode>16</drawmode>
            <toggle>true</toggle>
            <description>Draw text</description>
            <label>text</label>
            <font>
              <size>14</size>
              <style>0</style>
            </font>
          </button>
        </toolbar>
      </toolbars>
```

2) Drag and drop the selected part to the desired position

```
<toolbars>
  <toolbar>
    <vertical>false</vertical>
    <polygonbutton>
      <drawmode>19</drawmode>
      <toggle>false</toggle>
      <description>Clear screen</description>
    </polygonbutton>
...
    <button>
      <drawmode>37</drawmode>
      <toggle>true</toggle>
      <description>Define Rgroups</description>
      <label>R</label>
      <font>
        <size>14</size>
        <style>1</style>
      </font>
    </button>
    <button>
      <drawmode>16</drawmode>
      <toggle>true</toggle>
      <description>Draw text</description>
      <label>text</label>
      <font>
        <size>14</size>
        <style>0</style>
      </font>
    </button>
```

```
        <polygonbutton>
          <drawmode>38</drawmode>
          <toggle>true</toggle>
          <description>Remove Rgroup Info from atom</description>
        </polygonbutton>
        <polygonbutton>
          <drawmode>23</drawmode>
          <toggle>false</toggle>
          <description>Show Info dialog</description>
        </polygonbutton>
      </toolbar>
      <toolbar>
...
      </toolbar>
      <toolbar>
        <vertical>true</vertical>
        <polygonbutton>
          <drawmode>2</drawmode>
          <toggle>true</toggle>
          <description>Draw double bonds</description>
        </polygonbutton>
...
        <button>
          <drawmode>18</drawmode>
          <toggle>true</toggle>
          <description>Draw sulfur atoms</description>
          <label>S</label>
          <font>
            <size>14</size>
            <style>1</style>
          </font>
        </button>
      </toolbar>
    </toolbars>
```

3) New window:



2.3.2.2 Delete Buttons

Please delete the complete XML string of the desired button to remove it from the ICEDIT window.

Example:

Default XML string

```
<toolbar>
  <vertical>true</vertical>
  <polygonbutton>button_information</polygonbutton>
  <polygonbutton>button_information></polygonbutton>
  <polygonbutton>button_information</polygonbutton>
  <button> button_information</button>
</toolbar>
```

The green button is now deleted

```
<toolbar>
  <vertical>true</vertical>
  <polygonbutton>button_information</polygonbutton>
  <polygonbutton>button_information></polygonbutton>
  <button> button_information</button>
</toolbar>
```

2.3.2.3 Add New Atom Buttons

Please insert the following input string to insert for example a P atom (please remove new-line characters (carriage return line feed CRLF) between lines for use):

```
<button>
  <drawmode>18</drawmode>
  <toggle>true</toggle>
  <description>Draw phosphorous atoms</description>
  <label>P</label>
  <font>
    <size>14</size>
    <style>1</style>
  </font>
</button>
```

For atoms others than P please change the red parts correspondingly.

Please note: Only the generation of new atom buttons is supported currently. The generation of new bond or template buttons will be supported in a later version!

3 Embedded as OLE-Server

Windows application only

3.1 Integration in MS Office

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

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

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

3.2 OLE Interfaces

The IC*EDIT* application is a registered OLE-Server, which supports the standard OLE interface as well as a additional COM interface described in a type library named ICEditOleSvr.tlb.

3.2.1 Standard OLE-Interface

Standard OLE interface methods like:

- IDataObject.GetData for the formats "mdlct", "metafile" and "enhanced metafile"
- IDataObject.SetData for format "mdlct" and "infochem rosdal"
- IOleObject.DoVerb
- IOleObject.Close

are supported.

3.2.2 Additional COM Interfaces

3.2.2.1 Interface IApplication

- ***BringToFront ( )***
  Moves the active editor window to the front.
- ***CopyMdlCt (mdlct, width, height, showMapps, showRkz, showSter, showNumb, showInvRet, queryDisplay, showResidue)***
  Copies the specified structure in MDLCT format to the Windows clipboard.
  width, height Picture width and height in pixel
  showMapps, … Display flags
- ***CopyToClipboard (rosdal)***
  Copies the specified structure in ROSDAL format to the Windows clipboard.
- ***Exit ( )***
  Closes the active window and terminates the session.
- ***ExitForce ( )***
  Closes the active window and terminates the session forced.
- ***GetMDLCT ( )***
  Returns the current structure in MDLCT format.[1]
- ***GetMdlCtClipFromClipboard ( )***
  Returns a structure in MDLCT clipboard format from the clipboard.[2]
- ***GetMdlCtFromClipboard ( )***
  Returns a structure in MDLCT format from the clipboard.[1]
- ***PasteFromClipboard ( )***
  Pastes a structure from the clipboard to the ICEDIT object.
- ***SetMDLCT(mdlct)***
  Displays the transferred structure in MDLCT file format in the current ICEDIT window.[1]
- ***SetMDLCTClip (mdlct, len)***
  Displays the transferred structure in MDLCTClip[2] format in the current ICEDIT window.
  len Length of mdlct (mdlct may contain 0-values)
- ***Show ( )***
  Displays an empty ICEDIT window.
- ***ShowICF (icf)***
  Displays a new ICEDIT window, which contains the specified structure in ICF format.

---

[1] For details see: CTFile formats, http://accelrys.com/products/informatics/cheminformatics/ctfile-formats/no-fee.php.

[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.

- ***ShowMDLCT(mdlct)***
  Displays a new IC*EDIT* window, which contains the specified structure in MDLCT format.[1]
- ***ShowRosdal (rosdal)***
  Displays a new IC*EDIT* window, which contains the specified structure in InfoChem ROSDAL format.
- ***ShowWaitMDLCT(mdlct)***
  Displays a new IC*EDIT* window, which contains the specified structure in MDLCT format.[1]
  This method returns not until the application has been closed.

3.2.2.2 Interface IDocument

- ***GetRosdal ( )***
  Returns the current structure in InfoChem ROSDAL format.
- ***Release ( )***
  Releases this object from memory.
- ***SetICF (icf)***
  Sets the specified structure in ICF format for this object.
- ***SetMDLCT (mdlct)***
  Sets the specified structure in MDLCT[1] format for this object.
- ***SetRosdal (rosdal)***
  Sets the specified structure in InfoChem ROSDAL format for this object.

  Description of parameter ROSDAL:

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

Main tags	Description
IC*EDIT*	To use only, if the structure is made by IC*EDIT*. The structure will not be scaled!
XML	To use in all other cases. The structure will be scaled!

Sub tags	Description	Required
ROSDAL	Structure in ROSDAL format.	yes
RECTANGLE	Dimension of the bounding box.	yes

3.2.2.3 Interface IEvent

- ***RosdalEvent (rosdal [out])***
  This event is thrown if the user has closed the window. The specified buffer contains information about the current structure in InfoChem ROSDAL format and the action, which has occurred this event.
- ***MdlCtEvent (mdlct [out])***
  This event is thrown if the user has closed the window. The specified buffer contains information about the current structure in MDLCT format[2] and the action, which has occurred this event.

4 Programming Interface - API

Windows application only

You can integrate IC*EDIT* as object in your source code in VisualBasic or .NET projects.
An IC*EDIT* object supports the same methods as the COM interface IApplication (chapter 3.2.2.1) and can throw the same events described in chapter 3.2.2.3 (IEvent).

4.1 Using IC*EDIT* in Visual Basic 6.0

The following steps are necessary to work with an IC*EDIT* 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.

5 Additional Clipboard Formats

Windows application only

The IC*EDIT* application offers the following additional clipboard formats:

- MDLCT

6 Additional Tools

6.1 Add-in for MSExcel

Windows application only

Under development – not yet supported.

6.2 IC*EDIT* as ActiveX Control (IC*EDITOCX*)

Windows application only, Internet Explorer only

IC*EDITOCX* can be used as ActiveX Control in Internet Explorer.

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

6.2.1 Integration of IC*EDITOCX* in HTML

<ApplDir>/ICEdit/Examples/ActiveXCtl contains the example html file ICEditocxTest.htm.

To create a reference to IC*EDITOCX*, 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>
```

6.2.2 Programming Interface – API

6.2.2.1 Methods

IC*EDITOCX* supports the following methods:

- ***ICEditOcx.startEditor (rosdal);***
  Displays the transferred structure in ROSDAL format in a new IC*EDIT* 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 IC*EDIT* 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 IC*EDITOCX*.
- ***ICEditOcx.getInfo ( );***
  Returns an information string.
- ***ICEditOcx.getReady ( );***
  Returns true if a structure has been drawn.

6.2.2.2 Events

IC*EDITOCX* supports the following events:

- ***ICEditOcx.Editready()***
  Occurs after a structure has been drawn.

6.3 IC*EDIT* Java Applet

The IC*EDIT* Java applet is an Internet browser based query editor for the input of chemical structures and reactions.
Features such as

- easy integration in any desktop or web application
- advanced options for the definition of query features
- support of complex R-group query specification

make IC*EDIT* an ideal tool to create queries for searching structure and reaction databases.

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

The IC*EDIT* Java applet supports the following methods:

- ***ICEditApplet.setRosdal (rosdal);***
  Transfers a chemical structure in InfoChem ROSDAL format to the applet.
- ***ICEditApplet.getRosdal ();***
  Returns from the applet the current chemical structure in InfoChem ROSDAL format.

6.3.1 Enhanced IC*EDIT* Java Applet

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

6.3.2 Installation

Create an applet tag at your html page:

```
<applet
      code="de.infochem.icedit.applet.ICEditApplet.class"
      archive="icedit.jar"
      name="ICEdit"
      width="550"
      height="500"
      codebase="."
      MAYSCRIPT
      class="border">
      Trouble instantiating applet!!<br/>
      Enable Java and JavaScript please.
</applet>
```

Parameter description:

code	the main class of the applet
archive	the name of the applets jar file
width	the width of the applet
height	the height of the applet
codebase	the directories where the applets jar file is located
config (optional)	contains a data stream with the configuration of the ICEDIT (see chapter 2.3.2 for more information)

6.4 IC*RENDIT*

IC*RENDIT* is a small trusted Java applet primarily used to render chemical structures and reactions in HTML documents. An editing functionality is implemented by connecting to an IC*EDIT* installation at the client side. IC*RENDIT* is based on the full application and therefore, all IC*EDIT* application functionalities like the full support of superatoms, templates and general setting display features are supported.
Optionally, IC*RENDIT* can be used without an installation of the IC*EDIT* application (see also chapter 6.4.5).
Please note: If IC*RENDIT* is used without an IC*EDIT* installation it is only possible to render chemical structures and reactions. For any editing functionalities an installation of the IC*EDIT* application is required.

6.4.1 Context Menu

The context menu offers the following functionalities:

- **Copy**: Copies the structure as OLE-Object to the Windows clipboard[3].
- **Save**: Saves the structure as MOL/RXNFILE.
- **Edit**: Launches IC*EDIT* to edit the structure[3].
- **Load**: Loads a MOL/RXNFILE.
- **Paste**: Pastes a structure from the Windows clipboard[3].
- **Display**: For the adjustment of display properties.
- **Version**: Returns the actual version of IC*RENDIT.*

6.4.2 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>
```

[3] Requires an IC*EDIT* installation

6.4.3 Applet Parameter

Parameter	Type	Optional	Default value
width	numeric	no	
height	numeric	no	
mdlct	string	yes	
editor	boolean	yes	false
no_editor_installed	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

6.4.4 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()

6.4.5 Usage without an IC*EDIT* Installation

IC*RENDIT* can be used without an installation of the IC*EDIT* application. In this case, the context menu entries “Copy”, “Paste” and “Edit” cannot be used and should be disabled by changing the applet parameter “no_editor_installed” to true (default: false).

Instead of an IC*EDIT* installation on the client side, the following four files have to be copied to the “Windows\system32” directory manually (or any other directory listed in the environment variable “PATH”): icchemaddin.dll, icauxiliary.dll, ICImage.dll and StructConvertCPPDLL.dll.

Please note: If IC*RENDIT* is used without an IC*EDIT* installation, it is only possible to render chemical structures and reactions. For any editing functionalities an installation of the IC*EDIT* application is required.

6.4.6 Copyright

IC*RENDIT* is using **com4j:**

7 Customer Support

Please contact us to receive technical support or license information:

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