Table of Contents

Before You Begin ............................................................................................ viii
    About This Reference Manual ........................................................................ viii
    Mouse Conventions ......................................................................................... viii
    For More Information ...................................................................................... ix
        How to Contact Us ....................................................................................... ix
        Online Updates ............................................................................................. ix

1. Introduction ........................................................................................................ 1
    1.1 About ACD/ChemSketch ................................................................................. 1
    1.2 Additional Modules ....................................................................................... 1
    1.3 What’s New? .................................................................................................. 2
    1.4 Freeware Version .......................................................................................... 3

2. Interface Overview ................................................................................................ 4
    2.1 Objectives ...................................................................................................... 4
    2.2 Common Window Elements .......................................................................... 4
        2.2.1 Toolbar Customization .......................................................................... 5
    2.3 Title Bar ......................................................................................................... 5
    2.4 Color Palette .................................................................................................. 6
    2.5 RSS News bar ................................................................................................ 6
        2.5.1 RSS Channels Dialog Box ..................................................................... 6
        2.5.2 HTTP Proxy Parameters Dialog Box .................................................... 7
    2.6 Status Bar ..................................................................................................... 8
    2.7 Structure and Draw Modes .......................................................................... 9

3. Structure Mode .................................................................................................... 10
    3.1 Objectives ..................................................................................................... 10
    3.2 General Information ....................................................................................... 10
    3.3 Screen ........................................................................................................... 11
    3.4 Menu Bar ...................................................................................................... 12
    3.5 General Toolbar ........................................................................................... 12
        3.5.1 Delete Button ......................................................................................... 14
        3.5.1.1 Structure Mode .................................................................................. 15
        3.5.1.2 Draw Mode ......................................................................................... 15
        3.5.2 Zoom In and Zoom Selection Buttons .................................................. 16
        3.5.3 Zoom Out Button ................................................................................... 16
        3.5.4 Zoom Box ............................................................................................... 16
        3.5.5 3D Viewer Button .................................................................................. 17
    3.6 Structure Toolbar .......................................................................................... 17
        3.6.1 Select/Move Button ............................................................................... 19
        3.6.2 Select/Rotate/Resize Button .................................................................. 21
        3.6.3 3D Rotation Button ............................................................................... 22
        3.6.4 Lasso On/Off Button ............................................................................. 23
        3.6.5 Draw Normal Button ............................................................................. 23
        3.6.6 Draw Continuous Button ...................................................................... 24
        3.6.7 Draw Chains Button .............................................................................. 25
        3.6.8 Up Stereo Bonds Button ...................................................................... 26
        3.6.9 Down Stereo Bonds Button .................................................................. 27
        3.6.10 Coordinating Bonds Buttons ............................................................... 27
## Table of Contents

3.6.11 Special Bonds Buttons ................................................................. 28  
3.6.12 Solid / Dotted Delocalization Curve Buttons ............................... 28  
3.6.13 Markush Bond Buttons ............................................................... 29  
3.6.14 Reaction Plus Button ................................................................. 31  
3.6.15 Reaction Arrow Buttons ............................................................... 32  
3.6.16 Reaction Arrow Labeling Button .................................................. 32  
3.6.17 Reaction Calculator Button ......................................................... 34  
3.6.18 Atom-Atom Map Button .............................................................. 35  
3.6.19 Polymers Button .......................................................... 36  
3.6.20 Change Position Button ............................................................. 37  
3.6.21 Set Bond Horizontally Button ...................................................... 38  
3.6.22 Set Bond Vertically Button .......................................................... 38  
3.6.23 Flip on Bond Button ................................................................... 38  
3.6.24 Flip Top to Bottom Button ............................................................ 39  
3.6.25 Flip Left to Right Button .............................................................. 39  
3.6.26 Instant Template Button ............................................................... 39  
3.6.27 Calculate Parameters of Substituent Button ................................... 40  

### 3.7 Atoms Toolbar................................................................................. 40

3.7.1 Query Atom Buttons ................................................................. 41  
3.7.2 Query Bond Buttons ................................................................. 41  
3.7.3 Atom Buttons ........................................................................... 42  
3.7.4 Edit Atom Label Button ............................................................. 44  
3.7.5 Pseudo Atom and Radical Label Buttons ...................................... 45  
3.7.6 Charges/Radicals Buttons ............................................................ 46  
3.7.6.1 Increment (+) Charge and Decrement (–) Charge Buttons .......... 46  
3.7.6.2 Radicals Buttons .................................................................... 46  
3.7.7 Atom Chemical Properties Button ................................................ 47  
3.7.8 Manual Numbering Button ........................................................... 48  

### 3.8 References Toolbar......................................................................... 49

### 3.9 File Menu ......................................................................................... 49

3.9.1 New ............................................................................... 49  
3.9.2 Open ............................................................................. 50  
3.9.3 Close ............................................................................. 50  
3.9.4 Save ............................................................................. 51  
3.9.5 Save As ........................................................................... 51  
3.9.5.1 Windows Bitmaps Export Options, TIFF Export Options, and Portable Network Graphics Export Options Dialog Boxes ................................................. 52  
3.9.6 Save All ........................................................................... 52  
3.9.7 Export ........................................................................... 52  
3.9.8 Import ............................................................................ 53  
3.9.9 Run ChemBasic ..................................................................... 53  
3.9.10 Forms Manager ................................................................. 53  
3.9.11 Page Setup ........................................................................ 54  
3.9.11.1 Page Setup Dialog Box: Size & Orientation Tab ................... 55  
3.9.11.2 Page Setup Dialog Box: Margins Tab .................................. 56  
3.9.11.3 Page Setup Dialog Box: Poster Tab .................................... 56  
3.9.12 Print ............................................................................... 57  
3.9.13 Print Preview ....................................................................... 57  
3.9.14 Properties ......................................................................... 59  
3.9.15 Send > As Is / As PDF ......................................................... 60  
3.9.16 File Associations ................................................................. 60  
3.9.17 Exit ............................................................................... 61  
3.9.18 Recent Files ....................................................................... 61  

### 3.10 Edit Menu .............................................................................. 62

3.10.1 Undo ............................................................................. 62  
3.10.2 Redo ............................................................................. 62
Table of Contents

3.10.3 Cut ................................................................. 62
3.10.4 Copy ............................................................ 63
3.10.5 Paste > Default ............................................... 63
3.10.6 Paste > In Place ............................................... 63
3.10.7 Paste > Special ............................................... 64
3.10.8 Paste > Structure ........................................... 64
3.10.9 Paste > Table .................................................. 64
3.10.10 Delete .......................................................... 65
3.10.11 Select All ..................................................... 65
3.10.12 Insert Object ............................................... 65
3.10.13 Edit Object ................................................... 65
3.11 Pages Menu ...................................................... 66
3.11.1 New ............................................................. 66
3.11.2 Insert ........................................................... 66
3.11.3 Change Order ............................................... 66
3.11.4 Delete .......................................................... 67
3.11.5 Rename ........................................................ 67
3.11.6 Color ............................................................ 67
3.11.7 Header and Footer > Edit ............................... 68
3.11.8 Header and Footer > Load ............................... 69
3.11.9 Header and Footer > Save ............................. 69
3.11.10 Header and Footer > Set As Default .......... 69
3.11.11 Header and Footer > Clear ......................... 70
3.11.12 Header and Footer > Show ......................... 70
3.11.13 Header and Footer > Show ......................... 70
3.11.14 Previous ..................................................... 71
3.11.15 Next ............................................................ 71
3.11.16 First ............................................................ 71
3.11.17 Last ............................................................. 71
3.12 Tools Menu ....................................................... 71
3.12.1 Structure Properties ....................................... 71
3.12.1.1 Properties Panel: Common Tab ............... 72
3.12.1.2 Properties Panel: Atom Tab .................... 73
3.12.1.3 Properties Panel: Bond Tab .................... 75
3.12.1.4 Properties Panel: Special Tab ................ 76
3.12.2 Clean Structure ............................................ 77
3.12.3 Check Tautomeric Forms .............................. 77
3.12.3.1 ACD/Tautomers Algorithm .................... 78
3.12.4 3D Structure Optimization ........................... 79
3.12.5 Calculate Boiling Point ................................. 80
3.12.6 MassSpec Scissors ....................................... 81
3.12.7 Show Aromaticity ........................................ 81
3.12.8 Hide Aromaticity ......................................... 81
3.12.9 Expand Shorthand Formulae ....................... 82
3.12.10 Add Explicit Hydrogens ............................. 82
3.12.11 Remove Explicit Hydrogens ....................... 83
3.12.12 Bring Bond(s) to Front .............................. 83
3.12.13 Send Bond(s) to Back ................................ 83
3.12.14 Auto Renumbering .................................... 84
3.12.15 Clear Numbering ....................................... 84
3.12.16 Generate > Name for Structure ................ 84
3.12.17 Generate > Structure from Name ............. 86
3.12.17.1 ACD/Name to Structure Options Dialog Box 88
3.12.18 Generate > Stereo Descriptors ................. 89
3.12.19 Generate > Stereo Descriptors Options .... 90
3.12.20 Generate > SMILES Notation ................. 90
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.12.21</td>
<td>Generate &gt; Structure from SMILES</td>
<td>91</td>
</tr>
<tr>
<td>3.12.22</td>
<td>Generate &gt; InChI for Structure</td>
<td>91</td>
</tr>
<tr>
<td>3.12.23</td>
<td>Generate &gt; InChI Options</td>
<td>91</td>
</tr>
<tr>
<td>3.12.24</td>
<td>Generate &gt; Structure from InChI</td>
<td>94</td>
</tr>
<tr>
<td>3.12.25</td>
<td>Search for Structure</td>
<td>94</td>
</tr>
<tr>
<td>3.12.25.1</td>
<td>Look Through Files Dialog Box</td>
<td>97</td>
</tr>
<tr>
<td>3.12.25.2</td>
<td>Search Options Dialog Box</td>
<td>98</td>
</tr>
<tr>
<td>3.12.25.3</td>
<td>Similarity Search Options Dialog Box</td>
<td>101</td>
</tr>
<tr>
<td>3.12.26</td>
<td>Calculate &gt; &lt;Property Name&gt;</td>
<td>101</td>
</tr>
<tr>
<td>3.12.27</td>
<td>Calculate &gt; All Properties</td>
<td>102</td>
</tr>
<tr>
<td>3.12.28</td>
<td>Calculate &gt; Select Properties to Calculate</td>
<td>102</td>
</tr>
<tr>
<td>3.12.29</td>
<td>Calculate &gt; Selected Properties</td>
<td>103</td>
</tr>
<tr>
<td>3.13</td>
<td>Templates Menu</td>
<td>104</td>
</tr>
<tr>
<td>3.13.1</td>
<td>Template Window</td>
<td>104</td>
</tr>
<tr>
<td>3.13.2</td>
<td>Template Organizer</td>
<td>106</td>
</tr>
<tr>
<td>3.13.3</td>
<td>Save User Template</td>
<td>107</td>
</tr>
<tr>
<td>3.13.4</td>
<td>Table of Radicals</td>
<td>108</td>
</tr>
<tr>
<td>3.13.5</td>
<td>Periodic Table</td>
<td>109</td>
</tr>
<tr>
<td>3.13.6</td>
<td>Dictionary</td>
<td>111</td>
</tr>
<tr>
<td>3.14</td>
<td>Options Menu</td>
<td>112</td>
</tr>
<tr>
<td>3.14.1</td>
<td>Preferences</td>
<td>112</td>
</tr>
<tr>
<td>3.14.1.1</td>
<td>Preferences Dialog Box: General Tab</td>
<td>113</td>
</tr>
<tr>
<td>3.14.1.2</td>
<td>Preferences Dialog Box: Structure Tab</td>
<td>115</td>
</tr>
<tr>
<td>3.14.1.3</td>
<td>Preferences Dialog Box: Reaction Tab</td>
<td>118</td>
</tr>
<tr>
<td>3.14.1.4</td>
<td>Preferences Dialog Box: Clean Tab</td>
<td>119</td>
</tr>
<tr>
<td>3.14.2</td>
<td>Show Grid</td>
<td>120</td>
</tr>
<tr>
<td>3.14.3</td>
<td>Snap on Grid</td>
<td>120</td>
</tr>
<tr>
<td>3.14.4</td>
<td>Show Palette</td>
<td>120</td>
</tr>
<tr>
<td>3.14.5</td>
<td>Show RSS</td>
<td>120</td>
</tr>
<tr>
<td>3.14.6</td>
<td>Set Structure Drawing Style Submenu</td>
<td>120</td>
</tr>
<tr>
<td>3.14.7</td>
<td>Add-On Organizer</td>
<td>121</td>
</tr>
<tr>
<td>3.14.8</td>
<td>ChemBasic Organizer</td>
<td>122</td>
</tr>
<tr>
<td>3.14.8.1</td>
<td>ChemBasic Program Dialog Box</td>
<td>123</td>
</tr>
<tr>
<td>3.15</td>
<td>Documents Menu</td>
<td>124</td>
</tr>
<tr>
<td>3.15.1</td>
<td>Next</td>
<td>124</td>
</tr>
<tr>
<td>3.15.2</td>
<td>Previous</td>
<td>124</td>
</tr>
<tr>
<td>3.15.3</td>
<td>Close All</td>
<td>124</td>
</tr>
<tr>
<td>3.16</td>
<td>Add-Ons Menu</td>
<td>124</td>
</tr>
<tr>
<td>3.17</td>
<td>I-Lab Menu</td>
<td>125</td>
</tr>
<tr>
<td>3.18</td>
<td>ACD/Labs Menu</td>
<td>126</td>
</tr>
<tr>
<td>3.18.1</td>
<td>Next Loaded</td>
<td>126</td>
</tr>
<tr>
<td>3.18.2</td>
<td>Anchor—New to 12.0!</td>
<td>126</td>
</tr>
<tr>
<td>3.18.3</td>
<td>Exit All</td>
<td>126</td>
</tr>
<tr>
<td>3.18.4</td>
<td>Setup Style—New to 12.0!</td>
<td>126</td>
</tr>
<tr>
<td>3.19</td>
<td>Help Menu</td>
<td>127</td>
</tr>
<tr>
<td>3.19.1</td>
<td>Help Topics</td>
<td>127</td>
</tr>
<tr>
<td>3.19.2</td>
<td>Using Help</td>
<td>127</td>
</tr>
<tr>
<td>3.19.3</td>
<td>Tip of the Day</td>
<td>127</td>
</tr>
<tr>
<td>3.19.4</td>
<td>Instructions for Authors</td>
<td>127</td>
</tr>
<tr>
<td>3.19.5</td>
<td>ChemBasic Help</td>
<td>127</td>
</tr>
<tr>
<td>3.19.6</td>
<td>Message Box Preferences</td>
<td>128</td>
</tr>
<tr>
<td>3.19.7</td>
<td>Documents</td>
<td>129</td>
</tr>
<tr>
<td>3.19.8</td>
<td>Visit ACD/Labs Web Site</td>
<td>129</td>
</tr>
<tr>
<td>3.19.9</td>
<td>Bug Report / Feature Request</td>
<td>129</td>
</tr>
<tr>
<td>3.19.10</td>
<td>Bug Report Settings</td>
<td>130</td>
</tr>
</tbody>
</table>
Table of Contents

3.19.11 About ACD/ChemSketch ................................................................................................. 130

4. Draw Mode ................................................................................................................................... 131

4.1 Objectives .................................................................................................................................. 131
4.2 General Information .................................................................................................................. 131
4.3 Screen ...................................................................................................................................... 132
4.4 Menu Bar .................................................................................................................................. 133
4.5 General Toolbar ........................................................................................................................ 133
4.6 Editing Toolbar .......................................................................................................................... 134
  4.6.1 Select/Move/Resize Button .................................................................................................. 135
  4.6.2 Select/Move/Rotate Button ................................................................................................. 136
  4.6.3 Edit Nodes Button .............................................................................................................. 136
    4.6.3.1 Node Toolbar ............................................................................................................... 137
  4.6.4 Edit Text Button .................................................................................................................. 138
    4.6.4.1 Text Toolbar ............................................................................................................... 139
4.7 Drawing Toolbar ....................................................................................................................... 139
  4.7.1 Line Button .......................................................................................................................... 140
  4.7.2 Arc Buttons .......................................................................................................................... 141
  4.7.3 Curve Button ....................................................................................................................... 141
  4.7.4 Polyline Button .................................................................................................................... 141
  4.7.5 Arrow Button ....................................................................................................................... 142
  4.7.6 Rectangle Button ................................................................................................................ 143
  4.7.7 Rounded Rectangle Button ............................................................................................... 143
  4.7.8 Ellipse Button ..................................................................................................................... 143
  4.7.9 Polygon Button .................................................................................................................... 144
  4.7.10 Insert Image Button .......................................................................................................... 144
  4.7.11 Text Button ....................................................................................................................... 145
  4.7.12 Table Button ..................................................................................................................... 145
    4.7.12.1 Table Toolbar ............................................................................................................. 145
  4.7.13 Brackets Buttons ............................................................................................................... 146
  4.7.14 Callout Buttons ................................................................................................................ 147
  4.7.15 Report Template Button ................................................................................................. 147
4.8 File Menu .................................................................................................................................. 148
4.9 Edit Menu .................................................................................................................................. 148
4.10 Pages Menu ............................................................................................................................. 148
4.11 Tools Menu ............................................................................................................................... 148
  4.11.1 Pen Style Panel ................................................................................................................. 149
  4.11.2 Fill Style Panel .................................................................................................................. 150
  4.11.3 Arrow Style Panel ............................................................................................................ 151
  4.11.4 Font Panel ........................................................................................................................ 152
  4.11.5 Paragraph Panel .............................................................................................................. 153
  4.11.6 Table Panel ........................................................................................................................ 154
  4.11.7 Update Object Style Panel ............................................................................................... 155
    4.11.7.1 Objects Panel: Common ............................................................................................ 156
    4.11.7.2 Objects Panel: Structure .......................................................................................... 157
    4.11.7.3 Objects Panel: Lines & Arrows ................................................................................. 158
    4.11.7.4 Objects Panel: Shapes ............................................................................................... 159
    4.11.7.5 Objects Panel: Text .................................................................................................... 160
    4.11.7.6 Objects Panel: NMR Spectrum ............................................................................... 162
    4.11.7.7 Objects Panel: Spectrum .......................................................................................... 163
    4.11.7.8 Objects Panel: 2D Spectrum ..................................................................................... 165
    4.11.7.9 Objects Panel: Table .................................................................................................. 167
  4.11.8 Style Organizer Panel ....................................................................................................... 169
    4.11.8.1 Save User Style Dialog Box ..................................................................................... 170
  4.11.9 Generate Submenu ............................................................................................................. 171
Appendix C. Goodies ..................................................................................... 184
Appendix B. Calculated Properties............................................................... 177
Appendix A. Running ACD/ChemSketch from Command Line .................. 176

4.11.10 Search for Structure........................................................................... 171
4.12 Object Menu.............................................................................................. 171
  4.12.1 Group/Ungroup.................................................................................... 171
  4.12.2 Bring to Front...................................................................................... 172
  4.12.3 Send to Back....................................................................................... 172
  4.12.4 Flip Left to Right................................................................................ 172
  4.12.5 Flip Top to Bottom............................................................................. 172
  4.12.6 Rotate 90° ......................................................................................... 173
  4.12.7 Align Horizontally > Left/Center/Right ............................................ 173
  4.12.8 Align Vertically > Top/Center/Bottom ............................................. 173
  4.12.9 Fit Horizontally.................................................................................. 173
  4.12.10 Fit Vertically .................................................................................... 174
  4.12.11 Convert to Polyline........................................................................... 174
  4.12.12 Connect Lines................................................................................... 174
4.13 Templates Menu....................................................................................... 174
4.14 Options Menu......................................................................................... 174
4.15 Documents Menu.................................................................................... 174
4.16 I-Lab Menu............................................................................................. 175
4.17 ACD/Labs Menu....................................................................................... 175
4.18 Help Menu............................................................................................... 175

Appendix A. Running ACD/ChemSketch from Command Line ................. 176

Appendix B. Calculated Properties............................................................... 177

Overview ........................................................................................................ 177
Algorithms for Calculating Properties.............................................................. 177
  Molar Volume, MV .................................................................................... 178
  Molar Refractivity, MR ............................................................................ 178
  Parachor, P ............................................................................................... 178
  Density, d ................................................................................................. 179
  Refractive Index, n .................................................................................. 179
  Surface Tension, γ .................................................................................. 179
  Dielectric Constant, ε (Permittivity) .......................................................... 179
  Polarizability ............................................................................................ 179
  Monoisotopic, Nominal, Average Masses and other Mass Values .................. 180

Correlation Statistics with Experimental Data ................................................ 180
  Distribution of Molar Refractivity Prediction Error .................................... 180
  Distribution of Molar Volume Prediction Error .......................................... 181
  Distribution of the Parachor Prediction Error ............................................ 181
  Distribution of the Refractive Index Prediction Error .................................. 182
  Distribution of the Density Prediction Error ............................................. 182
  Distribution of the Surface Tension Prediction Error ............................... 183
  Distribution of the Dielectric Constant (Permittivity) Estimation Error ....... 183

Appendix C. Goodies ..................................................................................... 184

What are “Goodies”?..................................................................................... 184
Where Can I Get Them?............................................................................... 184
Goodies ........................................................................................................ 184
  Insert Page............................................................................................... 184
  Clone Page .............................................................................................. 185
  Move/Copy Page ................................................................................... 185
  Reorder Pages ....................................................................................... 185
  Delete Pages ......................................................................................... 185
  Rename Pages ....................................................................................... 185
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Insert Page Numbers/ Annotations</td>
<td>186</td>
</tr>
<tr>
<td>Annotate Document</td>
<td>186</td>
</tr>
<tr>
<td>Document Browse</td>
<td>186</td>
</tr>
<tr>
<td>Create HTML</td>
<td>186</td>
</tr>
<tr>
<td>Sketch-to-VRML Converter</td>
<td>187</td>
</tr>
<tr>
<td>SDF-to-Sketch Converter</td>
<td>187</td>
</tr>
<tr>
<td>Sketch-To-SDF Converter</td>
<td>187</td>
</tr>
<tr>
<td>Table Wizard</td>
<td>187</td>
</tr>
<tr>
<td>Replace Element</td>
<td>188</td>
</tr>
<tr>
<td>Solution Calculator</td>
<td>188</td>
</tr>
<tr>
<td>Label Printer</td>
<td>188</td>
</tr>
<tr>
<td>Peptide Builder</td>
<td>188</td>
</tr>
<tr>
<td>Carbohydrate Builder</td>
<td>189</td>
</tr>
<tr>
<td>Remove Spectator Ions (Desalt)</td>
<td>189</td>
</tr>
<tr>
<td>Nucleic Acid Builder</td>
<td>189</td>
</tr>
<tr>
<td>Column Selector</td>
<td>189</td>
</tr>
</tbody>
</table>
Before You Begin

Thank you for purchasing ACD/ChemSketch—an integrated software package from Advanced Chemistry Development, Inc. (ACD/Labs) for drawing chemical structures, reactions, and schematic diagrams, and designing other chemistry-related reports and presentations.

About This Reference Manual

This manual provides a comprehensive description of all of the options available in ACD/ChemSketch, it is designed for either online use or to be printed and used as a “hard copy” version.

The screen shots shown throughout this reference manual have been taken with a relatively small window size.

The colors and other properties of the window elements described throughout this manual correspond to the Windows Classic Theme (with dismissed gradients) of the operating system’s Display Properties.

This reference manual is provided in electronic form, readable with Adobe software. If you cannot locate an index topic you need please do a text string search for the relevant word or phrase, or related words.

Mouse Conventions

You may perform several actions during your work with this software; the following specific words are used to describe them:

- **Point to** means move the mouse pointer to an item.
- **Click** means point to an item, and quickly press and release the left mouse button.
- **Right-click** means point to an item, and quickly press and release the right mouse button.
- **Double-click** means point to an item, and quickly press and release the left mouse button twice.
- **Drag** means point to an item, and press and hold down the left mouse button while you move the item.
- **Select** means highlight or make an interface element active either by clicking it or dragging over it (other actions are possible if specified in documentation). If used in “select the check box”, it means that the check box should be marked with a tick (as opposed to “clear the check box” when the check box should be cleared, without a mark).
For More Information...

To see the latest in ACD/Labs software and services, please visit our Web site at  
http://www.acdlabs.com/

Our Web site is being accessed at the rate of tens of thousands of “hits” per day. There’s a reason for this: much is offered through our Web site. We offer free ACD/ChemSketch, an ACD/LogP Freeware Add-on for ChemSketch, a free ISIS 3D Add-in, free ChemDraw extensions, and a free 2-week demo key for “Interactive Laboratory” sessions where you can run test calculations using Java applets without purchasing software. There are TechSmith Camtasia-based movies which show the operation of many of our software packages (especially ACD/ChemSketch). The movies can be run from the ACD/Labs software folder, \MOVIES.

We are constantly updating the information on our Web site. The Web site will tell you at which scientific conferences you can visit the ACD/Labs booth. You can browse the Frequently Asked Questions page or drop in and “chat” on our newsgroup, which can also be reached via our Web site.

If you would like to stay informed of the latest developments in chemical software at ACD/Labs, please be sure to sign up for e-mail broadcasts at our Web site page:  
http://www.acdlabs.com/newsletters/

How to Contact Us

We are accessible through our Web site, phone, fax, and regular mail, but by far the most popular way to contact us is via electronic mail. Questions on pricing, sales, availability, and general issues should be directed to:

info@acdlabs.ru

Technical and scientific support issues should be addressed by visiting:

http://www.acdlabs.com/support/

Please tell us the name of the software purchaser; the product name, version number, build number, and license ID of the product you are contacting us about (from the Help menu, choose About to find this information); as well as a description of the problem you are having. If applicable, please tell us the name of the distributor from whom you purchased the software.

Online Updates

Updates of our Desktop and Enterprise products are made throughout the year. These intermediate releases (bringing the actual version number of a program, for example, from N.00 to N.01) often contain new functionality along with additional bug fixes and support for new file formats. To check if there is a new update available and to have this sent to you, please contact your local agent or our Technical Support Department. Before calling, we recommend that you have ready the name of the software purchaser, the product name, version number, build number, and license ID of the product you are contacting us about. All Desktop ACD/Labs software contains the capability to have software updates delivered online. You will need the registration numbers of the software and an Internet connection from the same computer on which the software is installed. For more information, refer to the ACD/Updater User’s Guide located in the ACD/Labs documentation folder, \DOCS\UP_CLNT.PDF.
1. Introduction

1.1 About ACD/ChemSketch

ACD/ChemSketch is an integrated software package from Advanced Chemistry Development, Inc., developed to help chemists quickly and easily draw chemical structures, reactions, and schematic diagrams, calculate chemical properties, and design professional reports and presentations.

ACD/ChemSketch includes:

- Structure mode for drawing chemical structures and calculating their properties (for more information, refer to Section 3).
- Draw mode or text and graphics processing (for more information, refer to Section 4).
- Additional modules that extend the ACD/ChemSketch possibilities (most of them should be purchased separately).

1.2 Additional Modules

There are additional ACD/Labs applications accessible through the ACD/ChemSketch interface, as single-click buttons or add-on applications. These applications, which are increasing in number with each upgrade, are available as additional options and should be considered as separate items. Please contact us or consult our Web site for more details on pricing and availability.

- **ACD/ChemBasic**—the special programming language that enables you to customize ACD/Labs software. ACD/ChemBasic is available as part of the ACD/ChemSketch freeware that you can download from [http://www.acdlabs.com/](http://www.acdlabs.com/). For examples on how ACD/ChemBasic can be used with ACD/ChemSketch, refer to Appendix C.

- **ACD/I-Lab**—the Internet-based service that allows you to get instant access to chemical databases and property-prediction programs. An account on ACD/I-Lab can be set up from [http://ilab.acdlabs.com/](http://ilab.acdlabs.com/). A 2-week demo period can be arranged for the ACD/I-Lab sessions where you can run test calculations using Java applets without purchasing software. ACD/ChemSketch can connect to ACD/I-Lab automatically if run on a PC with Internet connection (for more information, refer to Section 3.17).

- **ACD/Tautomers**—checks and generates the most reasonable tautomeric forms of organic chemical structures. This tool is included in both freeware and commercial versions of ACD/ChemSketch. For more information, refer to Section 3.12.3.
• **ACD/Dictionary**—looks up the molecular structure for common drug names—*Commercial version only!* This software module of ACD/ChemSketch contains more than 158,000 systematic and non-systematic names, registry numbers, and abbreviations along with the corresponding molecular structures of the most frequently used chemicals. The entries cover more than 220 therapeutic categories, and the inhibitors for more than 500 different enzymes are also available. For more information, refer to Section 3.13.6.

• **ACD/3D Viewer**—generates 3D representations of drawn chemical structures in a striking color display. This additional module is described in the separate *ACD/3D Viewer User’s Guide* (\DOCS\3D.PDF)

• **ACD/Name Freeware Add-On**—generates names for structures according to IUPAC Recommendations on Organic, Biochemical, and Inorganic Nomenclature. This tool is distributed as a free add-on to ACD/ChemSketch. For more information, refer to Section 3.12.16.

The following applications can be purchased in addition to ACD/ChemSketch:

• **ACD/Boiling Point and Vaporization**—calculates accurate (in most cases to ±10 degrees or better) boiling points at any pressure from 0.001 torr to 7600 torr for a structure as drawn in the ChemSketch window. This additional application is described in the separate *ACD/Boiling Point User’s Guide* located in the ACD/Labs documentation folder, \DOCS\BP.PDF.

• **ACD/Sigma**—estimates the Hammett-type or related parameters for different substituent groups as drawn in the ChemSketch window. This additional application is described in the separate *ACD/Sigma User’s Guide* located in the ACD/Labs documentation folder, \DOCS\SIGMA.PDF.

• **ACD/Name to Structure**—generates a molecular structure for almost any chemical name. ACD/Name to Structure processes the majority of the names of general organic compounds and many natural product derivatives according to IUPAC Recommendations on Organic, Biochemical, and Inorganic Nomenclature. This additional application is described in the separate *ACD/Name to Structure User’s Guide* located in the ACD/Labs documentation folder, \DOCS\NAMESTR.PDF.

### 1.3 What’s New?

ACD/ChemSketch includes some new enhanced features and options as compared to the previous version.

**In Version 12.01**

- Possibility to generate Standard InChI and InChI Key.
- Ability to generate structure(s) quickly from an InChI notation or a SMILES string contained in the Clipboard.
- Calculating and displaying monoisotopic mass values for ions of different types.

**In Version 12.00**

**General Capabilities**

- ACD/Dictionary has been expanded to over 30,000 well-known structures. Associated with these structures, there is over 165,000 corresponding chemical names and registry numbers.
- Possibility to set standard InChI options: to increase the role of InChI and InChI key as universal structure identifier, IUPAC decided to define standard InChI options that need to be used to generate standard InChI and InChI key for a structure.
Introduction

Interface Enhancements

- Application of the desired coloration theme to all of the ACD/Labs programs.
- Ability to expand the buttons of the currently running ACD/Labs programs over the Windows taskbar.
- The new interface controls for manipulating images and structure objects are made similar to those used by Microsoft Word, ChemDraw, and many other applications.

Structure Mode

- Customization of the atom numbers position: now atom numbers are located near the atom nodes by default that is more common for chemical drawings.
- Ability to copy all tautomeric forms generated by the tautomer verification tool in one click to the ChemSketch window.

1.4 Freeware Version

From April 1999 onward, ACD/Labs has been making ACD/ChemSketch available as freeware, through the Freeware link at our Web site:

http://www.acdlabs.com/resources/freeware/chemsketch/

Now version 12.0 of ACD/ChemSketch can be downloaded for free!

Important ACD/ChemSketch freeware should be installed in its own separate folder. This folder can contain other ACD/Labs freeware concurrently available but should not contain any purchased ACD/Labs software.

All of the limitations on the freeware and also the Frequently Asked Questions (FAQs) can be found on our Web site at http://www.acdlabs.com/resources/knowledgebase/faqs/chemsketch_freeware.php.
2. Interface Overview

2.1 Objectives

This chapter will familiarize you with the ChemSketch window and its basic elements. Information about minimum system requirements as well as installation instructions are provided in the Quick Installation Guide which is included in every shipment of ACD/Labs software.

2.2 Common Window Elements

When describing the program throughout this reference manual, some terms defining various parts of its interface are used. Below, you will find some general information on the interface arrangement.

At the very top of each window, there is a title bar that shows the name of the program, name of the current window and buttons controlling the size and position of the window (for more details, refer to the Section 2.3).

Right below the title bar, you will find the menu bar that contains the program menus. By clicking the menus, you can access the program commands.

Below the menu bar, you can see one or two toolbars containing buttons that you use for working in that window (note that toolbars of most of the ACD/Labs programs can be customized; for more information, refer to the Section 2.2.1). These toolbars are specific for each window and are referred to with different names (e.g., you can find General and Editing toolbars in the ChemSketch window).

Workspace is a changeable part of a window where you work (draw structures, view results of your manipulations, see the opened files and databases, etc.). The workspace may be divided into several subwindows each of which display a specific type of data.

Beneath the workspace, there is usually a status bar that displays information that may be useful for your work at the current moment, e.g., the name of the currently opened file, the position of the cursor in the workspace, etc.

If ACD/ChemSketch is run from another ACD/Labs program, at the very bottom of each window, the Window Switching bar incorporates buttons for switching between the program windows and for performing specific actions that result in switching to another window. For example, clicking Substructure Search will start the substructure search and as a result will automatically switch to the Database window displaying the search result.

Note When ACD/ChemSketch starts up, you will find many menu commands and toolbar buttons appear dimmed (inactive). They will be available as soon as you draw a structure in the workspace.
2.2.1 Toolbar Customization

Toolbars of most of the ACD/Labs programs can be customized using the toolbar shortcut menu (to display the menu, click **Show Buttons** or right-click a toolbar). The following options are available on this menu:

- **Toolbar buttons**—you can cancel the selection of a button to hide it on the toolbar.
- **Reset Toolbar**—selects all of the toolbar buttons on the shortcut menu.
- **Chevron Style**—adds **More Buttons** at the end of the toolbar if the buttons do not fit the toolbar.

**Note** A style specified for any toolbar will be applied to all of the toolbars within all the ACD/Labs programs.

2.3 Title Bar

At the very top of the window, there is a title bar that shows the name of the program, the name of the current window, the name and location of the currently open file (the default file name is NONAMEXX.SK2, where ‘XX’ is the ordinal number of a file starting from 00), and three small buttons controlling the size and position of the window. If the window does not fill the entire screen, dragging the title bar will move the window but will not change its size.

Click the program icon on the left side of the bar to view the commands controlling the window. Some of them are present on the title bar as the buttons:

<table>
<thead>
<tr>
<th>Command</th>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Restore</td>
<td></td>
<td>Returns the window to its previous size. Note that this option is available only if the window is maximized.</td>
</tr>
<tr>
<td>Move</td>
<td></td>
<td>Allows you to move the window using the arrow keys. Note that this command is available only if the window is not already maximized.</td>
</tr>
<tr>
<td>Size</td>
<td></td>
<td>Allows you to size the window using the arrow keys. Note that this command is available only if the window is not already maximized.</td>
</tr>
<tr>
<td>Minimize</td>
<td></td>
<td>Reduces the window to a button on the taskbar.</td>
</tr>
<tr>
<td>Maximize</td>
<td></td>
<td>Makes the window fill the entire screen. Note that this option is available only if the desktop or window is not already maximized.</td>
</tr>
<tr>
<td>Close</td>
<td></td>
<td>Closes all of the opened documents and quits the program. If you have made any changes and haven’t saved your work yet, the program prompts you to do so. <strong>Shortcut</strong>: ALT+F4</td>
</tr>
</tbody>
</table>
2.4 Color Palette

The Color palette is displayed horizontally below the workspace and allows you to change the color of the selected objects.

You can display/hide the Color palette by selecting/clearing the Palette check box in the Preferences dialog box (General tab) or by selecting Show Palette on the Options menu.

To display more colors, click More to the right of the palette.

To change the color of the selected objects, click the required color on the Color palette according to the following scheme:

- In the Structure mode, clicking the color box changes the color of selected atoms and right-clicking the color box changes the color of selected bonds.
- In the Draw mode, clicking the color box changes the fill color of selected objects, right-clicking the color box changes the pen color of the selected objects.

2.5 RSS News bar

RSS News bar is a line displayed above the status bar that lists the latest news from ACD/Labs, Reactive Reports, and any other RSS channels specified by the user.

Note You can display/hide the RSS News bar by selecting/clearing the RSS check box in the Preferences dialog box (General tab), or by selecting Show RSS on the Options menu.

2.5.1 RSS Channels Dialog Box

This dialog box allows you to add, remove RSS channels and set options of displaying news creeping line.
To display the dialog box, on the RSS News bar, click \[\text{Setup RSS}\].

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>RSS Channels</strong></td>
<td>Displays a list of RSS channels. Select the check boxes of the channels you want to be displayed. Note that ACD/Labs RSS Feed and Reactive People news cannot be switched off.</td>
</tr>
<tr>
<td>Add</td>
<td>Click this button to add the new URL to the RSS Channels list.</td>
</tr>
<tr>
<td>Delete</td>
<td>Click this button to delete the currently highlighted row of the required channel in the RSS Channels list. Note that you cannot delete Reactive People and ACD/Labs News channels.</td>
</tr>
<tr>
<td>Update Every...min.</td>
<td>In this box, specify the interval of information renewal (in the range from 1 to 120 minutes).</td>
</tr>
<tr>
<td>Scroll Items</td>
<td>Select this check box to set continuous scrolling of RSS News bar. If this check box is not selected, the bar is scrolled with pauses of several seconds.</td>
</tr>
<tr>
<td>Scroll Speed</td>
<td>Move the slider left or right to set the speed of scrolling.</td>
</tr>
<tr>
<td>Proxy...</td>
<td>Displays the HTTP Proxy Parameters dialog box. For more information, refer to Section 2.5.20.</td>
</tr>
<tr>
<td>Apply</td>
<td>Click this button to apply the specified settings without closing the dialog box.</td>
</tr>
</tbody>
</table>

### 2.5.2 HTTP Proxy Parameters Dialog Box

This dialog box allows you to specify parameters of a proxy server if the latter is required.

**Note**  A proxy server acts as an intermediary between your internal network (intranet) and the Internet, retrieving data from remote Web servers.

To display the dialog box, in the RSS Channels dialog box, click \[\text{Proxy...}\].
Interface Overview

This dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Use Default Proxy Settings</td>
<td>Select this check box if you want to use the default settings of the proxy server specified in Internet Explorer. When the check box is selected, all other areas of the dialog box are not available.</td>
</tr>
<tr>
<td>Use Proxy Server</td>
<td>In this area, select the check box and specify the required IP address and port number of the proxy server in your local network. When the check box is cleared, the Need authentication area below is not available.</td>
</tr>
<tr>
<td>Need authentication</td>
<td>In this area, select the check box and specify the proxy server access credentials in the Login and Password boxes.</td>
</tr>
<tr>
<td>Defaults</td>
<td>Click this button to populate fields of the dialog box with the default settings of the proxy server specified in Internet Explorer. The button is available only when the Use Default Proxy Settings check box is cleared.</td>
</tr>
</tbody>
</table>

2.6 Status Bar

The status bar is displayed horizontally at the very bottom of the ChemSketch window, below the Color palette. It contains a great deal of useful information:

<table>
<thead>
<tr>
<th>Element</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="ACD/I-Lab indicators" /></td>
<td>ACD/I-Lab indicators. For more information, refer to the technical documentation on ACD/I-Lab.</td>
</tr>
<tr>
<td><img src="image" alt="I-Lab Login" /></td>
<td>Allows you to login to ACD/I-Lab. For more information, refer to Section 3.17.</td>
</tr>
<tr>
<td>$877.50</td>
<td>Shows your current I-Lab balance.</td>
</tr>
<tr>
<td>NONAME01:SK2</td>
<td>Displays the name of the current document (also shown on the title bar).</td>
</tr>
</tbody>
</table>
### Element | Description
--- | ---
Modified | Indicates if the current document has been modified or not.
| | Displays the previous / next page in the current document (if any).
Page 1/1 | Shows the number of the current page / total number of pages in the document. Clicking this button displays the drop-down list of all the pages.
| | When the Header and Footer toolbar is on (refer to Section 3.11.7), this field is replaced by `Header/Footer`.
Fragments: 3 / Sel. Fragments: 2 | Shows either the total number of fragments in the workspace or the number of currently selected fragments.
| | Structure mode only
C8H10 | Shows the molecular formula of the selected fragment / structure (if any) or the overall number of elements currently present on the page (if no fragment or structure is selected).
| | Structure mode only
Property fields | Shows values of the physicochemical properties currently chosen from the `Properties` menu (see below) and automatically calculated for the drawn structure.
| | Structure mode only
Properties —New to 12.0! | Displays the menu with various physicochemical properties. You can view their values automatically calculated for selected structure (or, if no structure is selected, for all of the structures displayed) on the status bar by selecting the corresponding property names on this menu.
Grad: 1.2491 | Structure mode only
CANCEL | Shows the progress of the 3D optimization process and allows you to cancel it (for more information, refer to Section 3.12.4).

### 2.7 Structure and Draw Modes

In the ChemSketch window, there are two modes, Structure and Draw. You can switch between them by pressing SPACEBAR or using the buttons on the General toolbar:

In the Structure mode, you can draw chemical structures and reaction schemes while the Draw mode provides you with the tools for typing text and drawing various graphical objects. The interface elements in these modes differ.

For more information on these modes, refer to the chapters that follow.
3. Structure Mode

3.1 Objectives

This chapter will familiarize you with the features available in the Structure mode of ACD/ChemSketch. You will also get acquainted with all the parts of the ChemSketch window available in this mode and what they are aimed at.

To switch to the Structure mode, on the General toolbar, click Structure.

3.2 General Information

In the Structure mode, you can perform the following actions:

- Draw chemical structures using the buttons located on the different toolbars of the ChemSketch window.
- Instantly see elemental composition, formula, and formula weight of the drawn structure(s) as well as physicochemical properties of the currently selected structure on the status bar.
- Calculate the molar refractivity, molar volume, parachor, index of refraction, surface tension, density, and some other physicochemical properties for the selected structure, and then copy the results of calculation to the ChemSketch window.
- Find chemical structures according to their systematic or non-systematic names, therapeutic category or inhibited enzyme via the integrated ACD/Dictionary. You can also draw a structure and see all of its names, type of therapeutic category, and inhibited enzymes, which are listed in ACD/Dictionary—for the Commercial Version only
- Refer to the NMR and mass data for all of the isotopes of a chemical element selected in the Periodic Table of Elements dialog box.
- Look for the most favorable tautomeric forms of the drawn structure and automatically correct the structure by using the integrated Check Tautomeric Forms feature.
- Convert 2D structures into their 3D counterparts and view, measure, and handle them in virtual 3D space.
- Produce a cleaned-up version of a structure.
- Draw chemical reactions and label reaction arrows with specific experimental conditions. Associate atoms in reactant to product schemes with atom-atom mapping.
- Save drawn structures/reactions to an .SK2 file, load the file contents to the ChemSketch window, export/import structures/reactions to/from various file formats, and paste copied structures/reactions as ACD/ChemSketch-linked object to other MS Windows applications (e.g., to the MS Word text editor).
3.3 Screen

Below, you can see the ACD/ChemSketch screen with the Structure mode enabled. Names and positions of toolbars and other elements to be used throughout this manual are indicated.

<table>
<thead>
<tr>
<th>Interface Element</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Title bar</td>
<td>Shows the name of the program, the name and location of the currently open file, and buttons controlling the size and position of the window (for more information on the title bar, refer to Section 2.3).</td>
</tr>
<tr>
<td>Menu bar</td>
<td>Contains the program menus of commands intended for working in the Structure mode of the ChemSketch window (for a detailed description of each menu contents, refer to Sections 3.9–3.18.4).</td>
</tr>
<tr>
<td>General toolbar</td>
<td>Includes tools that are present in both Structure and Draw modes and will help you with tasks relevant to both modes such as: saving and opening .SK2 files, undoing/redoing operations, copying and pasting, zooming in and out, as well as inserting various templates (for more information, refer to Section 3.5).</td>
</tr>
</tbody>
</table>
### Interface Element | Description
--- | ---
ChemBasic toolbar | Includes additional tools that extend the functionality of ACD/ChemSketch. Note that the ChemBasic toolbar is present in both Structure and Draw modes only if you have the Goodies tools previously installed (for more information, refer to Appendix C).
Structure toolbar | For the Structure mode only
Contains tools for drawing and manipulating chemical structures and reactions (for more information, refer to Section 3.6).
Atoms toolbar | For the Structure mode only
Contains buttons representing atoms, as well as tools for changing atom properties (for more information, refer to Section 3.7).
References toolbar | Contains the Table of Radicals and various buttons representing ready-made radicals you take from the table (for more information, refer to Section 3.8). You can also access ACD/Dictionary from this toolbar—*for Commercial Version only*
Workspace | Displays currently active page of an opened ChemSketch document where you can draw and edit the required objects (structures, reactions, pictures).
Color Palette | Allows you to quickly color atoms and bonds in the selected chemical structures (for more information, refer to Section 2.4).
RSS News bar | Lists the latest news from ACD/Labs, Reactive Reports, and any other RSS channels specified by the user (for more information, refer to Section 2.5).
Status bar | Contains the following actual information: name of the open file, page number, molecular formula of the selected structure, etc. It also contains a button for automatic I-Lab access (for more information, refer to Section 2.6).

### 3.4 Menu Bar

Right below the title bar, you will find the menu bar that contains the program menus. By clicking the menus you can access the program commands.

For detailed information on the commands that are available from the menus of the ChemSketch window in the Structure mode, refer to Sections 3.9–3.18.4.

### 3.5 General Toolbar

In both Structure and Draw modes, below the menu bar, the General toolbar is displayed. The General toolbar contains buttons for opening and closing files, undoing and redoing actions, as well as cutting, copying, pasting, and zooming graphical objects in the workspace. Most of the buttons on this toolbar are shortcuts of the menu commands; the other buttons are tools that have no corresponding menu commands.
The table below gives the short description of all of the buttons available on the General toolbar:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
<th>Menu Command</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structure</td>
<td>Switches the ChemSketch window to the Structure mode. You can also press SPACEBAR to switch between the modes.</td>
<td></td>
</tr>
<tr>
<td>Draw</td>
<td>Switches the ChemSketch window to the Draw mode (for more information on this mode, refer to Section 4). You can also press SPACEBAR to switch between the modes.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Adds a new blank ChemSketch document (see Section 3.9.1).</td>
<td>New command (File menu).</td>
</tr>
<tr>
<td></td>
<td>Adds a new blank page to the end of current ChemSketch document (see Section 3.11.1).</td>
<td>New command (Pages menu).</td>
</tr>
<tr>
<td></td>
<td>Displays the Open dialog box where you can specify the name and location of an .SK2 file to be opened (see Section 3.9.2).</td>
<td>Open command (File menu).</td>
</tr>
<tr>
<td></td>
<td>Saves current ChemSketch document. When you are saving your work for the first time, the Save Document As dialog box prompts you to specify name and location of the .SK2 file to be created (see Sections 3.9.4–3.9.5).</td>
<td>Save or Save As command (File menu)</td>
</tr>
<tr>
<td></td>
<td>Displays the Print dialog box where you can specify the required settings for printing current ChemSketch document (see Section 3.9.12).</td>
<td>Print command (File menu)</td>
</tr>
<tr>
<td></td>
<td>Displays the Export dialog box where you can specify the name and location of an Adobe PDF file to which current ChemSketch document is to be exported (see Section 3.9.7)</td>
<td>Export command (File menu)</td>
</tr>
<tr>
<td></td>
<td>Cancels the last action (see Section 3.10.1).</td>
<td>Undo command (Edit menu)</td>
</tr>
<tr>
<td></td>
<td>Reverts the last canceled action (see Section 3.10.2).</td>
<td>Redo command (Edit menu)</td>
</tr>
<tr>
<td></td>
<td>Enables the Delete tool that allows you to remove specific objects in the workspace (see Section 3.5.1).</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Removes the selected object from the workspace and places it to the Clipboard (see Section 3.10.3).</td>
<td>Cut command (Edit menu)</td>
</tr>
<tr>
<td></td>
<td>Copies the selected object(s) to the Clipboard (see Section 3.10.4).</td>
<td>Copy command (Edit menu)</td>
</tr>
<tr>
<td></td>
<td>Allows you to insert the contents of the Clipboard into the workspace (see Section 3.10.5).</td>
<td>Paste &gt; Default command (Edit menu)</td>
</tr>
<tr>
<td></td>
<td>Magnifies the workspace display according to the pre-defined factor (see Section 3.5.2).</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Enables the Zoom Selection tool that allows you to magnify the display scale so that the selected area will fit into the workspace (see Section 3.5.2).</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Reduces the workspace display according to the pre-defined factor (see Section 3.5.3).</td>
<td></td>
</tr>
<tr>
<td>100%</td>
<td>In this box, click an arrow and choose the appropriate option or display scale value from the drop-down list, or enter the desired value (in percents), and then press ENTER (see Section 3.5.4).</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Sets the workspace display to 100% (see Section 3.5.4).</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Displays the current page scaled to the full width and height in the workspace.</td>
<td></td>
</tr>
</tbody>
</table>
### Button | Description | Menu Command
---|---|---
Displays the current page scaled to the full width in the workspace. | | 
Fits all of the objects on current ChemSketch page into the workspace. | | 
The zoom-in and zoom-out functions re-scale the display of the objects on the screen, but do not affect the actual size of the objects. To re-size objects, use the Select/Move/Resize tool (Draw mode) or the Select/Move/Resize tool (Structure mode). | 
Displays the Template Window dialog box that contains both the built-in and user-defined templates to simplify drawing structures and chemistry-related graphics such as molecular orbitals and laboratory glassware (see Section 3.13.1). | Template command (Templates menu) 
Displays the ACD/Search for Structure dialog box that allows you to search for the required structures in the specified folders without opening the files the folders can contain (see Section 3.12.25)—for Commercial version only! | Search for Structure command (Tools menu) 
Generates the name either for a selected single structure or structure (see Section 3.12.16) or for a two-component mixture (indicating proportion of the components in round brackets). | Generate > Name for Structure command (Tools menu) 
Click this button to generate structure(s) for a selected name either of a single compound or of a two-component mixture (with indicated proportion of the components given in round brackets) (see Section 3.12.6). Displays the ACD/Name to Structure dialog box that allows you to generate structures from names (see Section 3.12.17). | Generate > Structure from Name command (Tools menu) 
Generates the InChI notation for drawn structure(s) (see Section 3.12.22). | Generate > InChI for Structure command (Tools menu) 
Runs ACD/3D Viewer (see Section 3.5.5). | 
Closes an active ChemSketch document (see Section 3.9.3). | Close command (File menu) 

Optionally, the General toolbar can contain extra buttons corresponding to ACD/Labs add-ons currently registered in ACD/ChemSketch—for example, to ACD/Web Search Add-On. For more information on how to organize add-ons, refer to Section 3.14.7.

**Note** Toolbars of most of the ACD/Labs programs can be customized using the toolbar shortcut menu (for more information, refer to Section 2.2.1).

### 3.5.1 Delete Button

Using the **Delete** tool, you can remove objects drawn in the workspace. Note that the mouse pointer in this mode becomes an arrow labeled Del.

The **Delete** tool works differently in the Structure and Draw modes as described in the sections below.
3.5.1.1 Structure Mode

In this mode, you can delete chemical structures either totally or partly (fragments, single atoms, and bonds), as well as graphical objects.

**Important** To be able to select and delete in the Structure mode the objects created in the Draw mode, as well as reaction pluses and arrows, on the Structure tab of the Preferences dialog box, select the Select Graphics check box. For more information on this dialog box, refer to Section 3.14.1.2.

To delete an atom or a bond:
- With the Delete tool active, click an atom or a bond you want to delete.

The Delete tool removes the pointed atom along with the adjacent bonds. It never leaves individual atoms/groups in the workspace. However, you can retain parts of a structure: hold down CTRL and click a bound atom/group (for example, the central atom in isobutene). Only the atom/group you click disappears—all other atoms are retained.

The Delete tool erases the pointed bond. If an individual atom/group is left after the deletion process, it is also automatically removed. However, you can retain all single atoms/groups if you hold down CTRL when using the Delete tool.

To delete a structural fragment:
1. With the Delete tool active, drag over the structural fragment you want to delete so that the selection nodes appear.
2. Point to any of selection nodes so that they become black, and then click.

**Tip** To delete several fragments at once, hold down SHIFT while selecting them, then release SHIFT, point to any of the selection nodes so that they become black, and click.

To delete entire structure(s):
1. With the Delete tool active, drag over the structure(s) you want to delete so that the selection nodes appear.
2. Point to any of selection nodes so that they become black, and click.

**Tip** To delete selected objects, you can also use the Delete command (Edit menu). Note that this command is available only if there is a selection in the workspace.

3.5.1.2 Draw Mode

In this mode, you can delete chemical structures and graphical objects.

To delete an object:
- With the Delete tool active, point to the object you want to delete so that the selection rectangle appears around it, and then click.

To delete several objects at once:
1. With the Delete tool active, drag over the objects you want to delete so that the selection nodes appear around them.
2. Point to any selected object so that the selection rectangles appear around all of the selected objects, and click.

**Note** To delete a part of a structure, switch to the Structure mode, and follow the instructions given in the previous section.
3.5.2 Zoom In and Zoom Selection Buttons

Using these tools, you can magnify the workspace display in the following ways:

- Click the Zoom In button sequentially to enlarge the display of all present objects from their current scale up to the next scale preset (displayed in the adjacent Zoom box on the toolbar) and to center them in the workspace (if the objects have been previously selected).

- When you click the Zoom Selection button, the mouse pointer cursor turns into a magnifying glass. Select the area you want to see magnified by dragging over it. The selected area will be fit into the workspace.

  **Important** This function rescales the display of the objects on the screen, but does not affect the actual size of the objects. To resize objects, use the Select/Move tool, the Select/Rotate/Resize tool (Structure mode), or the Select/Move/Resize tool (Draw mode).

3.5.3 Zoom Out Button

Using the Zoom Out tool, you can reduce the display of the object(s) from the current magnification to a previous view or a pre-defined factor down to 10% scale by sequentially clicking the button.

  **Important** This function rescales the display of the objects on the screen, but does not affect the actual size of the objects. To resize objects, use the Select/Move tool, the Select/Rotate/Resize tool (Structure mode), or the Select/Move/Resize tool (Draw mode).

3.5.4 Zoom Box

In the Zoom box, you can manage the workspace display scale.

To set the desired display scale, use one of the following ways:

- Click the arrow button in the box, and choose the percentage of decrease or increase from the drop-down list of pre-defined options (refer to the table below); or

- Enter the desired percentage value directly in the box (the minimum available value is 10; the maximum is 500), and then press ENTER.

  **Important** This function rescales the display of the objects on the screen, but does not affect the actual size of the objects. To resize objects, use the Select/Move tool, the Select/Rotate/Resize tool (Structure mode), or the Select/Move/Resize tool (Draw mode).
In this box, you can select one of the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
<th>Button</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full Page</td>
<td>Displays the current page scaled to the full width and height in the workspace.</td>
<td></td>
</tr>
<tr>
<td>Page Width</td>
<td>Displays the current page scaled to the full width in the workspace.</td>
<td></td>
</tr>
<tr>
<td>Fit Selected</td>
<td>Fits the selected objects into the workspace.</td>
<td></td>
</tr>
<tr>
<td>Fit All</td>
<td>Fits all of the objects on the current ChemSketch page into the workspace.</td>
<td></td>
</tr>
<tr>
<td>Magnification scale</td>
<td>When selecting one of the magnification values (25%, 50%, 75%, 100%, 150%, 200%, or 400%), displays the current page scaled to this value.</td>
<td></td>
</tr>
</tbody>
</table>

### 3.5.5 3D Viewer Button

Using the 3D View tool, you can start ACD/3D Viewer that is a fast yet accurate 3D modeling and visualization program. It is fully integrated with ACD/ChemSketch, allowing you to draw 2D structures and quickly obtain their 3D representations in a striking 16 color display. For more information, refer to the ACD/3D Viewer User's Guide located in the ACD/Labs documentation folder, \DOCS\3D.PDF.

### 3.6 Structure Toolbar

Below the General toolbar, there is the Structure toolbar containing buttons for drawing chemical structures.

The table below lists all of the buttons available on the Structure toolbar and gives the short description for each of them:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="select-move-resize.png" alt="Select, Move, Resize" /></td>
<td>Allows you to select, move, and resize objects over the workspace (see Section 3.6.1).</td>
</tr>
<tr>
<td><img src="select-resize-rotate.png" alt="Select, Resize, Rotate" /></td>
<td>Allows you to select, resize, and rotate objects on the workspace (see Section 3.6.2).</td>
</tr>
<tr>
<td><img src="rotate.png" alt="Rotate" /></td>
<td>Allows you to rotate the selected structure or structural fragment in 3D (see Section 3.6.3).</td>
</tr>
<tr>
<td><img src="lasso-rectangle.png" alt="Lasso and Rectangle" /></td>
<td>Switches between two modes of selection: Lasso and Rectangle (see Section 3.6.4).</td>
</tr>
<tr>
<td><img src="discontinuous-bonds.png" alt="Discontinuous Bonds" /></td>
<td>Allows you to draw chemical bonds in a discontinuous manner (see Section 3.6.5).</td>
</tr>
<tr>
<td><img src="continuous-bonds.png" alt="Continuous Bonds" /></td>
<td>Allows you to draw chemical bonds in a continuous manner (see Section 3.6.6).</td>
</tr>
<tr>
<td><img src="atom-chains.png" alt="Atom Chains" /></td>
<td>Allows you to draw atom chains (see Section 3.6.7).</td>
</tr>
<tr>
<td><img src="stereo-toward.png" alt="Stereo Bonds Toward" /></td>
<td>Allows you to draw stereo bonds facing towards the viewer (see Section 3.6.8).</td>
</tr>
<tr>
<td><img src="stereo-away.png" alt="Stereo Bonds Away" /></td>
<td>Allows you to draw stereo bonds facing away from the viewer (see Section 3.6.9).</td>
</tr>
</tbody>
</table>
### Structure Mode

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Button" /></td>
<td>Allows you to draw various types of coordinating (non-covalent) bonds (see Section 3.6.10): <img src="image2.png" alt="Coordinating Bonds" /></td>
</tr>
<tr>
<td><img src="image3.png" alt="Button" /></td>
<td>Allows you to draw various types of special bonds (see Section 3.6.11): <img src="image4.png" alt="Special Bonds" /></td>
</tr>
<tr>
<td><img src="image5.png" alt="Button" /></td>
<td>Allows you to draw various types of delocalized bonds (see Section 3.6.12): <img src="image6.png" alt="Delocalized Bonds" /></td>
</tr>
<tr>
<td><img src="image7.png" alt="Button" /></td>
<td>Allows you to draw various types of Markush bonds (see Section 3.6.13): <img src="image8.png" alt="Markush Bonds" /></td>
</tr>
<tr>
<td><img src="image9.png" alt="Button" /></td>
<td>Allows you to draw reaction pluses (see Section 3.6.14).</td>
</tr>
<tr>
<td><img src="image10.png" alt="Button" /></td>
<td>Allows you to draw various types of reaction arrows (see Section 3.6.15): <img src="image11.png" alt="Reaction Arrows" /></td>
</tr>
<tr>
<td><img src="image12.png" alt="Button" /></td>
<td>Allows you to label reaction arrows (see Section 3.6.16).</td>
</tr>
<tr>
<td><img src="image13.png" alt="Button" /></td>
<td>Allows you to automatically calculate synthesis data for each reaction components (see Section 3.6.17).</td>
</tr>
<tr>
<td><img src="image14.png" alt="Button" /></td>
<td>Allows you to map a drawn reaction either manually or automatically (see Section 3.6.18).</td>
</tr>
<tr>
<td><img src="image15.png" alt="Button" /></td>
<td>Allows you to draw polymers (see Section 3.6.19).</td>
</tr>
<tr>
<td><img src="image16.png" alt="Button" /></td>
<td>Allows you to change the double bond arrangement, hydrogen position, bond intersection point, and connection point of an atom label (see Section 3.6.20).</td>
</tr>
<tr>
<td><img src="image17.png" alt="Button" /></td>
<td>Allows you to rotate chemical structure(s) or selected fragment(s) so that a chosen bond becomes horizontal (see Section 3.6.21).</td>
</tr>
<tr>
<td><img src="image18.png" alt="Button" /></td>
<td>Allows you to rotate chemical structure(s) or selected fragment(s) so that a chosen bond becomes vertical (see Section 3.6.22).</td>
</tr>
<tr>
<td><img src="image19.png" alt="Button" /></td>
<td>Allows you to flip chemical structure(s) or selected fragment(s) on the axis of a chosen bond (see Section 3.6.23).</td>
</tr>
<tr>
<td><img src="image20.png" alt="Button" /></td>
<td>Rotates chemical structure(s) or selected fragment(s) on its horizontal axis, giving its mirror reflection (see Section 3.6.24).</td>
</tr>
<tr>
<td><img src="image21.png" alt="Button" /></td>
<td>Rotates chemical structure(s) or selected fragment(s) on its vertical axis, giving its mirror reflection (see Section 3.6.25).</td>
</tr>
<tr>
<td><img src="image22.png" alt="Button" /></td>
<td>Allows you to create an instant template based on any structure or selected fragment, so that you can insert it anywhere in the workspace or attach it to another structure (see Section 3.6.26).</td>
</tr>
<tr>
<td><img src="image23.png" alt="Button" /></td>
<td>Redraws and resizes chemical structure(s) or selected fragment(s) in order to standardize all of the bond lengths and angles (see Section 3.12.2).</td>
</tr>
<tr>
<td><img src="image24.png" alt="Button" /></td>
<td>Checks and generates the most reasonable tautomeric forms of drawn organic structure (see Section 3.12.3).</td>
</tr>
<tr>
<td><img src="image25.png" alt="Button" /></td>
<td>Creates realistic 3-dimensional model(s) of planar (2D) chemical structure(s) (see Section 3.12.4).</td>
</tr>
<tr>
<td>Button</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td><img src="image1" alt="button" /></td>
<td>Calculates boiling point (BP), vapor pressure (VP), enthalpy of vaporization, and flash point for the selected structure (see Section 3.12.5).</td>
</tr>
<tr>
<td><img src="image2" alt="button" /></td>
<td>Calculates and displays monoisotopic masses for specified fragments of a structure (see Section 3.12.6).</td>
</tr>
<tr>
<td><img src="image3" alt="button" /></td>
<td>Calculates a set of Hammett Sigma ($\sigma$) electronic constants (e.g., inductive, resonance, meta-, para-, etc.) as well as steric and hydrophobic ones for drawn substituents (see Section 3.6.27).</td>
</tr>
</tbody>
</table>

**Note** Toolbars of most of the ACD/Labs programs can be customized using the toolbar shortcut menu (for more information, refer to Section 2.2.1).

### 3.6.1 Select/Move Button

Using the Select/Move tool (the mouse pointer changes to $\rightarrow$), you can select, move, and resize atoms, bonds, fragments, structures, and graphical objects. Note that this tool influences the actual size of the object; to change the scale of the object display in the workspace, use zooming tools (refer to Sections 3.5.2–3.5.4).

**Note** Clicking this button automatically enables currently set selection mode: Lasso ()$\square$ or Rectangle ()$\square$. For more information, refer to Section 3.6.4.

To be able to manipulate in the Structure mode the objects created in the Draw mode, as well as reaction pluses and arrows, on the Structure tab of the Preferences dialog box, select the Select Graphics check box. For more information on this dialog box, refer to Section 3.14.1.2.

**Table 1.** The table below summarizes the actions you can perform to select different objects:

<table>
<thead>
<tr>
<th>To select…</th>
<th>You should…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single atom or bond in the structure</td>
<td>Click any atom or bond in the required structure.</td>
</tr>
<tr>
<td>Single fragment or structure</td>
<td>Drag over the required fragment or structure. Note that you can previously set either Lasso or Rectangle selection mode (refer to Section 3.6.4).</td>
</tr>
<tr>
<td>Multiple structures or fragments one by one</td>
<td>Sequentially drag over the required fragments or structures while holding down SHIFT. Note that you can previously set either Lasso or Rectangle selection mode (refer to Section 3.6.4).</td>
</tr>
<tr>
<td>Entire structure at once</td>
<td>Click an empty space in the drawing area adjacent to, but not touching the structure you wish to select.</td>
</tr>
<tr>
<td>All structures in the workspace</td>
<td>Click an empty space in the drawing area away from any drawn structure. Note that all the structures become framed with nodes (handles) and their elements (atoms and bonds) are marked with hollow squares. Clicking again will deselect all of the structures.</td>
</tr>
<tr>
<td>Objects drawn in the Draw mode</td>
<td>Click the object once.</td>
</tr>
<tr>
<td>All objects drawn in the Structure and Draw modes</td>
<td>Press CTRL+A.</td>
</tr>
</tbody>
</table>

**Table 2.** The table below summarizes the actions you can perform to move selected objects:

<table>
<thead>
<tr>
<th>To move…</th>
<th>You should…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Object</td>
<td>Point to the object so that the gray rectangle appears around it (for graphics) or so that the hollow selection squares become black (for structures), and drag.</td>
</tr>
</tbody>
</table>
To move… | You should…
---|---
Object with leaving its copy behind | Point to the object so that the gray rectangle appears around it (for graphics) or so that the hollow selection squares become black (for structures), and drag while holding down CTRL.

Object with fixing its coordinates along one of the axes | Drag the object while holding down SHIFT. This will move the selected object strictly horizontally (vertically) without changing its initial coordinate position along the Y (X) axis.

| Note | If the Informative Cursor check box is selected on the General tab of the Preferences dialog box, the object’s shift coordinates are displayed near the mouse pointer. For more information, refer to Section 3.14.1.1.

If you want to move object with/without snapping it to grid in the workspace, select/deselect the Snap on Grid command on the Options menu (refer to Section 3.14.3). Clicking CTRL+SHIFT ignores the Snap on Grid command selection.

Table 3. The table below summarizes the actions you can perform to resize selected objects:

| To resize… | You should…
---|---
Object relative to one of its sides or corners | Point to the required selection handle so that the mouse pointer changes to a double-headed arrow (mouseenter, mouseleave, or mouseover), and drag.

- Dragging the top/bottom selection handles resizes the object’s height;
- dragging the left/right handles resizes the width; and
- dragging the corner handles resizes the object proportionally in all directions.

Object relative to its center | Hold down CTRL when dragging the selection handles as described above.

Object’s width or height at certain percent | Point to a side selection handle while holding down SHIFT, and drag.

The selected object will be resized by percent value multiple of 5.

Object so that the height and width change independently | Point to a corner selection handle while holding down SHIFT, and drag.

| Note | To view the percentage of resizing displayed near the mouse pointer, on the General tab of the Preferences dialog box, select the Informative Cursor check box. For more information, refer to Section 3.14.1.1.

If you want to resize object with/without snapping it to grid in the workspace, select/deselect the Snap on Grid command on the Options menu (refer to Section 3.14.3). Clicking CTRL+SHIFT ignores the Snap on Grid command selection.

If you double-click the selected structural fragment or the whole structure with this tool active, the Properties panel appears (for more information on options available in this panel, refer to Section 3.12.1). On this panel, you can change the style of the selected object.

| Tip | You can quickly switch between this tool and:
- The Draw Normal tool by pressing ESC;
- The Select/Rotate/Resize tool by right-clicking in the workspace.
3.6.2 Select/Rotate/Resize Button

Using the Select/Rotate/Resize tool (the mouse pointer changes to \( \text{\textcopyright} \)), you can select, rotate, and resize atoms, bonds, fragments, structures, and graphical objects. Note that this tool influences the actual size of the object; to change the scale of the object display in the workspace, use zooming tools (refer to Sections 3.5.2–3.5.4).

**Note**  To be able to manipulate in the Structure mode the objects created in the Draw mode, as well as reaction pluses and arrows, on the Structure tab of the Preferences dialog box, select the Select Graphics check box. For more information on this dialog box, refer to Section 3.14.1.2.

The actions you can perform to select the required objects on the ChemSketch page are described in Table 1 of the previous section.

**Table 4.** The table below summarizes the actions you can perform to rotate objects:

<table>
<thead>
<tr>
<th>To rotate…</th>
<th>You should…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unselected object</td>
<td>Drag the object by any of its elements. The object will be rotated around its center.</td>
</tr>
</tbody>
</table>
| Selected object around its center | Point to the object so that the mouse pointer changes to \( \text{\textcopyright} \), and drag.  
Prior to rotating, make sure that the object's action center is located correctly. To view the action center on an object, on Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), under Show, select Action Center. |
| Selected object around the specified point | 1. On Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), under Show, select Action Center.  
2. Define the center of rotation either by dragging the action center to the required location or by clicking the required location while holding down CTRL.  
3. Point to the object so that the mouse pointer changes to \( \text{\textcopyright} \), and drag. |
| Selected object in 15 degree increments | Point to the object so that the mouse pointer changes to \( \text{\textcopyright} \), and drag while holding down SHIFT. The selected object will be rotated around its action center at the required angle multiple of 15°. |

**Note**  To view the angle of rotation displayed near the mouse pointer, in the Preferences dialog box (General tab), select the Informative Cursor check box.

**Table 5.** The table below summarizes the actions you can perform to resize selected objects:

<table>
<thead>
<tr>
<th>To resize…</th>
<th>You should…</th>
</tr>
</thead>
</table>
| Object relative to one of its sides or corners | 1. On Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), under Show, clear Action Center.  
2. Point to the required selection handle so that the mouse pointer changes to a double-headed arrow (\( \text{\textcopyright} \), \( \text{\textcopyright} \), \( \text{\textcopyright} \), or \( \text{\textcopyright} \)), and drag.  
Dragging the top/bottom selection handles resizes the object's height; dragging the left/right handles resizes the width; and dragging the corner handles resizes the object proportionally in all directions. |
To resize… | You should…
---|---
Object relative to the specified point | 1. On the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), under Show, select Action Center.

2. Define the center of resizing either by dragging the action center of the selected object to the required location or by clicking the required location while holding down CTRL.

3. Point to the required selection handle so that the mouse pointer changes to a double-headed arrow (←, →, ↑, or ↓), and drag.

Dragging the top/bottom selection handles resizes the object’s height; dragging the left/right handles resizes the width; and dragging the corner handles resizes the object proportionally in all directions.

Object relative to its center | Point to the required selection handle while holding down CTRL so that the mouse pointer changes to a double-headed arrow (←, →, ↑, or ↓), and drag.

Dragging the top/bottom selection handles resizes the object’s height; dragging the left/right handles resizes the width; and dragging the corner handles resizes the object proportionally in all directions.

Object’s width or height at certain percent | Point to a side selection handle while holding down SHIFT, and drag. The selected object will be resized by percent value multiple of 5.

Object so that the height and width change independently | Point to a corner selection handle while holding down SHIFT, and drag.

**Note** To view the percentage of resizing displayed near the mouse pointer, on General tab of the Preferences dialog box, select the Informative Cursor check box. For more information, refer to Section 3.14.1.1.

You can quickly switch between this tool and the Select/Move tool by right-clicking in the workspace.

### 3.6.3 3D Rotation Button

Using the 3D Rotation tool (the mouse pointer is changed to 🔄), you can rotate structures or selected fragments in three dimensions:

- Point to any bond or atom so that it is surrounded with a gray rectangle, and drag.

**Note** Direction of rotation of the front atoms in the 3D-optimized structure (for more information, refer to Section 3.12.4) corresponds to the movement of the cursor. That is, dragging to the right makes the front atoms move to the right.

If you are using the up and down stereo bonds for defining the direction of bonds, you should do that on the "flat", non-3D-optimized structure and then start 3D optimization anew.

You can designate any bond as the axis of 3D-rotation by clicking it while holding down CTRL. The bond will change its color to green and will be highlighted with pink. To cancel this, click the bond once again while holding down CTRL.

**Tip** You can quickly switch from this tool to the Select/Move tool 🛹 by right-clicking in the workspace.
3.6.4 Lasso On/Off Button

Using this tool, you can switch between the Lasso / Rectangle modes of selecting objects:

- The Lasso Off tool selects objects with the rectangular selection box;
- The Lasso On tool selects objects with the lasso selection line.

Note that using the lasso allows you to select objects in a more specific and precise manner.

To choose between the selection modes, click the button. To select the required object on the screen, drag over it.

**Note** In most cases, clicking the Lasso On/Off button automatically enables the Select/Move tool.

3.6.5 Draw Normal Button

Using the Draw Normal tool (the mouse pointer changes to \( \text{\text{\text{\text{\text{\text{\text{\text{C}}}}}}}} \)), you can draw chemical bonds in a discontinuous manner where new chemical bonds can be drawn by clicking the first atom and dragging to the second one. This tool is enabled by default on after ACD/ChemSketch is loaded.

**Tip** You can quickly switch between this tool and the Draw Continuous tool by right-clicking in the workspace.

The table below summarizes the actions you can do with this tool:

<table>
<thead>
<tr>
<th>Action</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clicking in the workspace.</td>
<td>Draws an atom of the chemical element currently selected on the Atoms toolbar.</td>
</tr>
<tr>
<td>Clicking a non-bound atom of the same chemical element as the atom selected on the Atom toolbar.</td>
<td>Sprouts a single bond of a fixed length, with a terminal atom of the same chemical element as the selected one.</td>
</tr>
<tr>
<td>Clicking a terminal bound atom of the same chemical element as the atom selected on the Atom toolbar.</td>
<td>Sprouts a single bond of a fixed length at an angle of 120° to the existing bond, with a terminal atom of the same chemical element as the selected one.</td>
</tr>
<tr>
<td>Clicking a terminal bound atom of the same chemical element as the atom selected on the Atom toolbar while holding down CTRL.</td>
<td>Sprouts a single bond of a fixed length at an angle of 180° to the existing bond, with a terminal atom of the same chemical element as the selected one.</td>
</tr>
<tr>
<td>Clicking a non-terminal bound atom of the same chemical element as the atom selected on the Atom toolbar.</td>
<td>Sprouts a single bond of a fixed length as a bisecting line of the angle between existing bonds, with a terminal atom of the selected chemical element.</td>
</tr>
<tr>
<td>Clicking an atom of a chemical element different from the atom selected on the Atom toolbar.</td>
<td>Changes the drawn atom to the atom of chemical element selected on the Atom toolbar. Note that by clicking this atom for the second time you can sprout a single bond of a fixed length, with a terminal atom of the selected chemical element, exactly as described above in this table.</td>
</tr>
<tr>
<td>Clicking a bond.</td>
<td>Repetitively switches between available bond types: single, double, or triple.</td>
</tr>
</tbody>
</table>
### Action

<table>
<thead>
<tr>
<th>Action</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dragging.</td>
<td>Sprouts a single bond at any angle and of any length.</td>
</tr>
<tr>
<td></td>
<td>If the Fixed Bond Angle and Bond Length check boxes are selected on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), you can draw bonds of a length multiple of the specified value and at an angle multiple of 15°.</td>
</tr>
<tr>
<td></td>
<td>If the Snap on Grid command is selected on the Options menu (refer to Section 3.14.3) is selected, the drawing is constrained by the grid.</td>
</tr>
<tr>
<td>Dragging while holding down SHIFT.</td>
<td>Sprouts a single bond of a length multiple of the value specified in the Fixed area on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2) and at an angle multiple of 15° in case the Fixed Bond Angle and Bond Length check boxes are not selected on the Structure tab of the Preferences dialog box.</td>
</tr>
<tr>
<td></td>
<td>Otherwise, you will draw bonds at any angle and of any length.</td>
</tr>
<tr>
<td>Dragging while holding down CTRL+SHIFT.</td>
<td>Sprouts a single bond according to the grid.</td>
</tr>
<tr>
<td></td>
<td>If the Snap on Grid command is selected on the Options menu (refer to Section 3.14.3), the drawing is not constrained by the grid.</td>
</tr>
<tr>
<td>Right-clicking in the workspace.</td>
<td>Switches to the Draw Continuous tool.</td>
</tr>
</tbody>
</table>

#### 3.6.6 Draw Continuous Button

Using the Draw Continuous tool (the mouse pointer changes to ), you can draw chemical bonds in a continuous manner where new chemical bonds can only be drawn from the atom that is currently selected (i.e., highlighted with the black square). If none of atoms is selected, either click any atom to select it or click an empty workspace to insert a new atom in advance. Note that only one atom can be selected at a time in the workspace.

> **Tip** You can quickly switch between this tool and the Draw Normal tool by right-clicking in the workspace.

The table below summarizes the actions you can do with this tool:

<table>
<thead>
<tr>
<th>Action</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clicking in the workspace.</td>
<td>Draws an atom of the chemical element currently selected on the Atoms toolbar and highlights it.</td>
</tr>
<tr>
<td>Double-clicking in the workspace</td>
<td>Draws atoms of the chemical element selected on the Atoms toolbar and connects them with a single bond.</td>
</tr>
<tr>
<td>Clicking an existing atom.</td>
<td>Highlights the atom.</td>
</tr>
<tr>
<td>Clicking the highlighted atom.</td>
<td>Sprouts a single bond of a fixed length with a terminal atom of the chemical element currently selected on the Atoms toolbar.</td>
</tr>
<tr>
<td>Sequentially clicking two different atoms.</td>
<td>Connects the two atoms with a single bond.</td>
</tr>
<tr>
<td>Double-clicking a terminal bound atom.</td>
<td>Sprouts a single bond of a fixed length at an angle of 120° to the existing bond, with a terminal atom of the chemical element currently selected on the Atoms toolbar.</td>
</tr>
</tbody>
</table>
**Table of Actions and Descriptions**

<table>
<thead>
<tr>
<th>Action</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Double-clicking a terminal bound atom while holding down CTRL.</td>
<td>Sprouts a single bond of a fixed length at an angle of 180° to the existing bond, with a terminal atom of the chemical element currently selected on the Atoms toolbar.</td>
</tr>
<tr>
<td>Double-clicking a non-terminal bound atom.</td>
<td>Sprouts a single bond of a fixed length as a bisecting line of the angle between existing bonds, with a terminal atom of the chemical element currently selected on the Atoms toolbar.</td>
</tr>
<tr>
<td>Clicking a bond.</td>
<td>Repetitively switches between available bond types: single, double, or triple.</td>
</tr>
<tr>
<td>Dragging.</td>
<td>Sprouts a single bond at any angle and of any length.</td>
</tr>
<tr>
<td>Dragging while holding down SHIFT.</td>
<td>Sprouts a single bond of a length multiple of the value specified in the Fixed area on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2) and at an angle multiple of 15°.</td>
</tr>
<tr>
<td>Dragging while holding down CTRL+SHIFT.</td>
<td>Sprouts a single bond according to the grid.</td>
</tr>
<tr>
<td>Right-clicking in the workspace.</td>
<td>Switches to the Draw Normal tool.</td>
</tr>
</tbody>
</table>

### 3.6.7 Draw Chains Button

Using the Draw Chains tool (the mouse pointer changes to \(\text{\textbullet\text{-}\textbullet}\)), you can draw molecular chains.

To draw a long molecular chain, drag in the workspace with this tool active.

**Note** To view the number of chain members displayed by the cursor as you drag with this tool, on the General tab of the Preferences dialog box, select the Informative Cursor check box. For more information, refer to Section 3.14.1.1.

The table below summarizes the actions you can perform with this tool:

<table>
<thead>
<tr>
<th>Action</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clicking in the workspace</td>
<td>Draws an atom of the chemical element currently selected on the Atoms toolbar.</td>
</tr>
<tr>
<td>Clicking a separate atom</td>
<td>Sprouts a single bond of a fixed length, with a terminal atom of the chemical element currently selected on the Atoms toolbar.</td>
</tr>
</tbody>
</table>
### Action | Description
--- | ---
Clicking a terminal bound atom. | Sprouts a single bond of a fixed length at an angle of 120° to the existing bond, with a terminal atom of the chemical element currently selected on the Atoms toolbar.
Clicking a terminal bound atom while holding down CTRL. | Sprouts a single bond of a fixed length at an angle of 180° to the existing bond, with a terminal atom of the chemical element currently selected on the Atoms toolbar.
Clicking a non-terminal bound atom. | Sprouts a single bond of a fixed length as a bisecting line of the angle between existing bonds, with a terminal atom of the chemical element currently selected on the Atoms toolbar.
Clicking a bond. | Repetitively switches between available bond types: single, double, or triple.
Dragging. | Sprouts a chain. The atoms in the chain are bound at an angle of 120° to each other.
If the Fixed Bond Angle and Bond Length check boxes are selected on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), you can draw bonds of a length multiple of the specified value and at an angle multiple of 15°.
If the Snap on Grid command is selected on the Options menu (refer to Section 3.14.3), the drawing is constrained by the grid.
Dragging while holding down CTRL. | Sprouts a chain. The atoms in the chain are bound at an angle of 180° to each other.
If the Fixed Bond Angle and Bond Length check boxes are selected on the Structure tab of the Preferences dialog box, you can draw bonds of a length multiple of the specified value and at an angle multiple of 15°.
If the Snap on Grid command is selected on the Options menu (refer to Section 3.14.3) is selected, the drawing is constrained by the grid.
Dragging while holding down SHIFT. | Draws a chain at a fixed length and fixed angle of 15°.
If the Fixed Bond Angle and Bond Length check boxes are selected on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), you will draw bonds at any angle and of any length.
Dragging while holding down CTRL+SHIFT. | Draws a chain according to the grid.
If Snap on Grid from the Options menu is selected, the drawing is not constrained by the grid.
Pressing TAB when dragging | Flips the drawn chain relative to the axis of dragging direction.
Right-clicking in the workspace. | Switches to the Draw Normal tool.

### 3.6.8 Up Stereo Bonds Button

Using the Up Stereo Bonds tool (the mouse pointer changes to ), you can draw stereo bonds that are facing towards the viewer in a 3-dimensional representation of the drawn structure.
With this tool active, new chemical bonds can be drawn in the same manner as with the Draw tool (for more information, refer to Section 3.6.5) but there are some differences between these tools:

- When a new bond is placed between two atoms or is sprouted from one atom, it is a stereo bond facing toward the viewer.
- Clicking a stereo bond several times changes the direction of the bond but does not change its order (i.e., you cannot draw double and triple bonds with this tool).

To change any other bond to a stereo bond that is facing towards the viewer, activate this tool and then click the bond.

**Tip** You can quickly switch between this tool and the Down Stereo Bonds tool by right-clicking in the workspace.

### 3.6.9 Down Stereo Bonds Button

Using the Down Stereo Bonds tool (the mouse pointer changes to ), you can draw stereo bonds that are facing away from the viewer in a 3-dimensional representation of the drawn structure.

With this tool active, new chemical bonds can be drawn in the same manner as with the Draw tool (for more information, refer to Section 3.6.5), but there are some differences between these tools:

- When a new bond is placed between two atoms or is sprouted from one atom, it is a stereo bond facing away from the viewer.
- Clicking a stereo bond several times changes the direction of the bond but does not change its order (i.e., you cannot draw double and triple bonds with this tool).

To change any other bond to a stereo bond that is facing away from the viewer, activate this tool, and then click the bond.

**Tip** You can quickly switch between this tool and the Up Stereo Bonds tool by right-clicking in the workspace.

### 3.6.10 Coordinating Bonds Buttons

Using these tools, you can draw coordinating (non-covalent) bonds.

To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Structure toolbar.

The following tools are available on the panel:
With one of the **Coordinating Bonds** tool active, new chemical bonds are drawn in the same manner as with the **Draw Normal** tool (for more information, refer to Section 3.6.5), but there are some differences between these tools:

- When a new bond is placed between two atoms or is sprouted from one atom, it is a coordinating (non-covalent) bond.
- Clicking a coordinating bond changes the direction of the bond but does not change its order (i.e., you cannot draw double and triple bonds with this tool).

**Note** The number of coordinating bonds drawn on a given atom does not affect its valence or charge. The maximum number of coordinating bonds on an atom is defined by its coordinating number, which is set by default to 6 for non-metals and to 4, 6, 8, or 10 for metals.

To change any other bond to a coordinating bond, activate the required **Coordinating Bonds** tool by clicking the corresponding button, and then click the bond.

### 3.6.11 Special Bonds Buttons

Using these tools, you can draw various types of special bonds.

To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Structure toolbar.

The following tools are available on the panel:

![Special Bonds Tools](image)

With one of the special bonds active, new chemical bonds are drawn in the same manner as with the **Draw Normal** tool (for more information, refer to Section 3.6.5) but there are some differences between these tools:

- When a new bond is placed between two atoms or is sprouted from one atom, it is a special bond.
- Clicking a special bond does not change its order (i.e., you cannot draw double and triple bonds with this tool).

To change any other bond to a special bond, activate the required **Special Bonds** tool by clicking the corresponding button, and then click the bond.

**Tip** You can quickly switch from this tool to the **Draw Normal** tool by right-clicking in the workspace.

### 3.6.12 Solid / Dotted Delocalization Curve Buttons

Using these tools, you can either draw solid or dotted curves indicating the delocalized chemical bonds.
To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Structure toolbar.

The following tools are available on the panel:

![Solid Delocalization Curve](image1) ![Dotted Delocalization Curve](image2)

To insert the delocalization curve, select the fragment or the entire structure for which you want to insert a curve, and then click the desired **Delocalization Curve** button. If nothing is selected as you click the button, a warning message will appear asking if you wish to create the delocalization curve for the entire structure.

**Important** To apply this tool, the selected fragment should contain at least two bonds and no branchings. Otherwise, the corresponding warning message will appear.

Note that query, triple, and quadruple bonds are not allowed in delocalization.

After you apply this tool, an action center of the drawn curve is displayed. The center is not visible while printing. You can place it wherever you need by dragging. Any new bond can be regularly drawn from the center by clicking and dragging.

It is possible to drag an atom or bond in the modified fragment/structure along with its delocalization curve.

If necessary, you can change an atom in the modified fragment/structure—the curve is not removed in the process.

To delete the delocalization curve, select the action center by clicking it, and press DELETE. The curve will be also removed if you change the bond order to double/triple in the modified fragment/structure.

The charges or radicals present in the selected fragment/structure will be moved on the action center after you apply any of the **Delocalization Curve** tools to it.

**Tip** You can also set charge or radical signs to the action center manually by using the **Charges/Radicals** tools (for more information, refer to Section 3.7.6).

### 3.6.13 Markush Bond Buttons

Using these tools, you can attach various types of Markush bonds to an entire structure or a selected structural fragment. The resulting structure is the generic one (*i.e.*, it represents a group of corresponding structures) where the Markush bond denotes the variability in position of a substituent within the structure.

To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Structure toolbar.

The following tools are available on the panel:

![Markush Bond](image3) ![Markush Bond with Shadow](image4) ![Added or Removed Fragment with Shadow](image5) ![Added or Removed Fragment](image6)

To attach a Markush bond:

1. On the Atoms toolbar, click the atom required to be at the end of the Markush bond (or select...
2. Select the required structure in the workspace (if there is more than one structure drawn).

3. On the Structure toolbar, click the **Markush Bond** buttons.

   **Note**  If nothing is selected as you click the button, a warning message will appear asking if you wish to attach the Markush bond to the whole structure.

To visibly display the atoms a Markush bond refers to, use the **Markush Bond with Shadow** tool.

To draw the structures with the attached mass or formula difference values, instead of the added or removed structural fragments themselves, use either the **Added or Removed Fragment** or **Added or Removed Fragment with Shadow** tool.

As you select a structure and click the desired button, the Define Markush Mass Difference dialog box appears:

![Define Markush Mass Difference dialog box](image)

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Additional / Subtraction</td>
<td>In this area, select whether the difference value will be marked as added (Additional) or removed (Subtraction).</td>
</tr>
<tr>
<td>Mass</td>
<td>Select this option, and then, in the adjacent box, type a needed mass difference to attach the difference value as a Markush fragment.</td>
</tr>
<tr>
<td></td>
<td>For example, to describe a transformation of (N,N)-dimethyl-4-nitrosoaniline that resulted in a product with the formula weight less by 14 units than initial, select the <strong>Subtraction</strong> and <strong>Mass</strong> options, and then, in the adjacent box, type 14. The following scheme represents monodemethylation (the upper right structure of the product) or the oxygen atom removal from the nitroso group (the lower right structure of the product) of the reactant:</td>
</tr>
</tbody>
</table>

![Chemical structures](image)

Both product structures have formula weight 14 units less than the initial compound.
**Option**  | **Description**  
---|---
Fragment  | Select this option, and then, in the adjacent box, type a needed formula difference to attach the formula difference as a Markush fragment.

For example, the following Markush structure with the added oxygen fragment describes at least three hydroxylation products and amine oxide at the same time:

![Markush structure example](image)

**Note**  | If you wish to perform a substructure search for structures with a Markush bond, you should pay more attention to choosing atoms which you want to participate in Markush binding.

### 3.6.14 Reaction Plus Button

Using the **Reaction Plus** tool, you can draw a reaction plus sign.

To insert a plus:

- Select the tool, move the cursor to the place where you want a plus to be inserted, and click once.

Clicking the plus for the second time will delete it.

**Note**  | You can change the color and style of reaction pluses in the Preferences dialog box (**Reaction** tab). For more information on this dialog box, refer to Section 0.

To be able to move and rotate reaction pluses in the Structure mode, make sure that the **Select Graphics** check box is selected in the Preferences dialog box (**Structure** tab).
3.6.15 Reaction Arrow Buttons

Using these tools, you can draw various reaction arrows.

To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Structure toolbar.

The following tools are available on the panel:

To insert an arrow, choose the required tool on the panel, and then use one of the following ways:

• Click in the workspace to place an arrow of a fixed length; or
• Drag to draw an arrow of desired length.

Clicking the arrow for the second time with this tool (as you point to the arrow, the mouse pointer changes to \(\text{DEL}\)) will delete it.

Note You can change the color and style of reaction arrows on the Reaction tab of the Preferences dialog box (for more information, refer to Section 3.14.1.3).

To be able to move and rotate reaction arrows, make sure that the Select Graphics check box is selected on the Structure tab of the Preferences dialog box (for more information, refer to Section 3.14.1.2).

You can switch between the available Reaction Arrow tools by right-clicking in the workspace.

3.6.16 Reaction Arrow Labeling Button

Using the Reaction Arrow Labeling tool, you can insert labels that specify the appropriate reaction conditions.
To insert reaction conditions:
1. With this tool selected, click the reaction arrow.
2. In the Edit Reaction Conditions dialog box that appears, type your own comment, and then click OK.

Tip    You can also use several buttons from the toolbar on the right side of the dialog box.

This dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
<th>Shortcut</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Cut" /></td>
<td>Cuts the selected text and places it to the Clipboard.</td>
<td>CTRL+X</td>
</tr>
<tr>
<td><img src="image" alt="Copy" /></td>
<td>Copies the selection to the Clipboard.</td>
<td>CTRL+C</td>
</tr>
<tr>
<td><img src="image" alt="Paste" /></td>
<td>Inserts the contents of the Clipboard.</td>
<td>CTRL+V</td>
</tr>
<tr>
<td><img src="image" alt="Font Style" /></td>
<td>In this box, specify the appropriate font style.</td>
<td></td>
</tr>
<tr>
<td><img src="image" alt="Font Size" /></td>
<td>In this box, specify the size of the font.</td>
<td></td>
</tr>
<tr>
<td><img src="image" alt="Bold" /></td>
<td>Formats the selected text with bold.</td>
<td>CTRL+B</td>
</tr>
<tr>
<td><img src="image" alt="Italic" /></td>
<td>Formats the selected text with italic.</td>
<td>CTRL+I</td>
</tr>
<tr>
<td><img src="image" alt="Underline" /></td>
<td>Underlines the selected text.</td>
<td>CTRL+U</td>
</tr>
<tr>
<td><img src="image" alt="Superscript" /></td>
<td>Formats the selected text with superscript. The superscript tool is automatically enabled when you type a formula in any of the panes. For example, when typing H+, the hydrogen atom charge is turned into superscript.</td>
<td>CTRL+SHIFT+=</td>
</tr>
<tr>
<td><img src="image" alt="Subscript" /></td>
<td>Formats the selected text with subscript. The subscript tool is automatically enabled when you type a formula in any of the panes. For example, when typing H2O, the hydrogen atom number is turned into subscript.</td>
<td>CTRL+=</td>
</tr>
<tr>
<td><img src="image" alt="Align Left" /></td>
<td>Aligns the text left.</td>
<td>CTRL+L</td>
</tr>
<tr>
<td><img src="image" alt="Align Center" /></td>
<td>Centers the text.</td>
<td>CTRL+E</td>
</tr>
<tr>
<td><img src="image" alt="Align Right" /></td>
<td>Aligns the text right.</td>
<td>CTRL+R</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
<td>Shortcut</td>
</tr>
<tr>
<td>--------------</td>
<td>------------------------------------------------------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>Upper Pane</td>
<td>In this pane, specify the reaction conditions to be placed above the reaction arrow.</td>
<td></td>
</tr>
<tr>
<td>Lower Pane</td>
<td>In this pane, specify the reaction conditions to be placed below the reaction arrow.</td>
<td></td>
</tr>
<tr>
<td>hν</td>
<td>Inserts the Photon symbol (denoting an application of lighting).</td>
<td></td>
</tr>
<tr>
<td>Δ</td>
<td>Inserts the Delta symbol (denoting an application of heating).</td>
<td></td>
</tr>
<tr>
<td>°C</td>
<td>Inserts the Celsius symbol (denoting a measurement on the Celsius scale).</td>
<td></td>
</tr>
<tr>
<td>acid</td>
<td>Inserts acid (denoting an acidic reaction medium).</td>
<td></td>
</tr>
<tr>
<td>base</td>
<td>Inserts base (denoting a basic reaction medium).</td>
<td></td>
</tr>
</tbody>
</table>

**Note** If you export a reaction with the reaction conditions specified by the Reaction Arrow Labeling tool into an .RXN file, the conditions objects will be lost.

### 3.6.17 Reaction Calculator Button

Using the Reaction Calculator tool, you can automatically calculate synthesis data for each reaction components.

To calculate the data, with this tool selected, click the reaction arrow.

The Reaction Calculator dialog box that appears contains the Components table with the following columns: Reactant, Formula (molecular formula), FW (formula weight), K (stoichiometric coefficient)—these four columns are filled in automatically, n (quantity), C (concentration), m (mass), V (volume), d (density), as well as Yield (yield of products).

To provide automatic calculation of reaction data, the data is divided into two types—**independent** and **relative**. You can edit the independent data only. The relative data is automatically calculated on the basis of the editable data and cannot be edited.
To edit the independent data, double-click the corresponding cell directly within the **Components** table, and then type the data value. After you press ENTER, all of the relative data is automatically calculated.

**Note**  
To provide the calculation of mass and quantity, you need to type the density value.

The **Yield** data is always relative and its calculation is based on the component with the lowest amount.

To calculate yield, in the **m** (mass) column, double-click the cell corresponding to the product, type the proper value, and then press ENTER. You will see that the yield is calculated and the **Based on** notation appears in the **Yield** column for the row corresponding to the reactant with the lowest amount.

To display the summarized quantity of the reactants, select the **Show Total** check box under the **Components** table.

Clicking **OK** closes the **Reaction Calculator** dialog box and pastes the populated **Components** table in the ChemSketch page right below the reaction scheme.

### 3.6.18 Atom-Atom Map Button

Using the **Atom-Atom Map** tool, you can map a drawn reaction either manually or automatically. As you click the button, the **Map Tools** panel appears, and the Manual Mapping mode is enabled by default.

The panel contains the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Manual Mapping" /></td>
<td>Switches to the Manual Mapping mode where you can map atoms of the reactant to the corresponding atoms of the product manually by pointing to a chosen atom and dragging to its counterpart.</td>
</tr>
<tr>
<td><img src="image" alt="Select/Move" /></td>
<td>Click this button to work like using the <strong>Select/Move</strong> tool (for more information on this tool, refer to Section 3.6.1) except for ability to move objects.</td>
</tr>
</tbody>
</table>
### Structure Mode

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Auto Mapping" /></td>
<td>Switches to the Auto Mapping mode where you can map your reaction automatically. Note that you can use this tool to map one reaction at a time only. If there is more than one reaction in the workspace, you need to select one of them using the Select Reaction tool.</td>
</tr>
<tr>
<td><img src="image2.png" alt="Auto Mapping Cancel" /></td>
<td>Cancels the mapping of all of the reactions on the current page. To cancel the mapping of a certain reaction, first select it using the Select Reaction tool, and then click this button.</td>
</tr>
</tbody>
</table>

It is possible to perform both automatic and manual mapping for the same reaction. To distinguish between automatically generated and manually inserted numbers, select different colors for automatic and manual mapping:

- To define the color for manually inserted map numbers, on the Reaction tab of the Preferences dialog box (refer to Section 3.14.1.3), in the Manual Mapping Color box, set the appropriate color.
- For automatic mapping, on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), in the Auto/Manual Numbering Color box, set the appropriate color.

To close the Map tools panel, click ![Close](image3.png). Whenever you close the panel, you quit the mapping mode, and atom numbers are no longer visible.

**Tip** You can export the mapped reactions either as an MDL rxnfiles (.RXN) or as an ISIS/Sketch files (.SKC). For more information on the export formats, refer to Section 3.9.7.

### 3.6.19 Polymers Button

Using the Polymers button, you can turn fragment(s) of a drawn structure into monomeric unit(s) of a (co)polymer.

Clicking this button displays the Polymer panel where you can specify the settings of monomeric units:

The panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Index</strong></td>
<td>In this box, specify an index (number or letter) for a given monomeric unit of (co)polymer. As you select the desired fragment in a drawn structure, brackets of the defined style appear around the unit and index is placed at the lower right corner of the right bracket.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>--------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Connectivity</strong></td>
<td>In this box, select the way the monomeric units are connected to each other in (co)polymer: <strong>head-to-tail</strong>, <strong>head-to-head</strong>, or <strong>either/unknown</strong>. The default setting is head-to-tail, so the upper right corner of the right bracket is not specifically labeled, while choosing head-to-head or either/unknown type of (co)polymerization will produce the <strong>hh</strong> or <strong>eu</strong> label respectively.</td>
</tr>
<tr>
<td><strong>Style</strong></td>
<td>Select the way the monomeric unit will be marked: in brackets [], in parenthesis (), or in braces {}.</td>
</tr>
<tr>
<td><strong>Apply</strong></td>
<td>Applies the defined parameters to the selected monomeric unit in (co)polymer.</td>
</tr>
</tbody>
</table>

To draw a (co)polymer, follow the steps:

1. Draw structure of the monomer (real or implicit/hypothetical) you want to turn into a (co)polymer.
   - **Tip**: To create open-end structures, replace the terminal atoms in a drawn monomer with empty atoms using the Pseudo Atom tool (refer to Section 3.7.5).

2. On the Structure toolbar, click **Polymers**.

3. On the **Polymer** panel that appears, specify the required settings.

4. Select the fragment of the structure you want to turn into a monomeric unit either by clicking starting and ending bonds or by dragging. As soon as the fragment is selected, it turns into a monomeric unit of (co)polymer.

5. If required, repeat steps 3-4 to specify the other monomeric unit(s) until the desired polymer structure is set.

To close the **Polymer** panel:

- On the panel’s title bar, click **X**. This quits the Polymer mode.

To remove brackets from the structure:

1. Close the **Polymer** panel and click in the workspace to cancel selection (if any) of the monomeric unit.

2. On the General toolbar, select **Delete**, and then click any of the unit’s brackets.

### 3.6.20 Change Position Button

Using the **Change Position** tool, you can change the arrangement of a double bond in a structure or the display position of hydrogen atoms within a functional group, as well as control the bonds intersection point and specify the connection point of an atom label:

- **Double bond in a structure can be arranged either symmetrically or asymmetrically as shown below:**
  
  ![Symmetric](image1.png) ![Asymmetric](image2.png)

  - **Symmetric** (e.g., a double bond belonging to non-cyclic structure)
  - **Asymmetric** (e.g., a double bond belonging to cyclic structure where ring is drawn below the bond)

To switch between the three types, click repeatedly the bond in the structure.
• Hydrogens can be displayed around the central atom of a selected functional group in four positions:

\[
\begin{align*}
\text{H}_2\text{N} & \quad \text{N} & \quad \text{H}_2 \\
\text{H}_2 & \quad \text{N} & \quad \text{NH}_2 \\
\text{Left} & \quad \text{Bottom} & \quad \text{Top} & \quad \text{Right}
\end{align*}
\]

To switch between the various positions, click repeatedly the group.

• When bonds intersect, one of them is displayed as a background bond and another as a foreground bond.

To bring the background bond to the front, holding down SHIFT, point to the bond (the mouse pointer changes to \(\text{X}\)), and click it.

• Atom labels (functional group abbreviations and shorthand formulas) inserted with the **Edit Atom Label** tool (for more information, refer to Section 3.7.4) can be connected to the bond by any symbol of the label.

To change the connected symbol, holding down SHIFT, point to the label (the mouse pointer changes to \(\text{abc}\)), and click repeatedly the atom label. The label will shift left symbol-by-symbol. As the needed symbol becomes a connection point, stop clicking.

If you click the shorthand formula label without holding down SHIFT, the program will turn the label horizontally while keeping the connection point of it.

### 3.6.21 Set Bond Horizontally Button

Using the **Set Bond Horizontally** tool, you can turn a chemical structure or a selected fragment so that the desired bond is displayed horizontally in the workspace.

As you click the bond, it becomes horizontal, and the entire structure is rotated accordingly.

Clicking the horizontal bond repeatedly rotates the structure/fragment by 180° back and forth.

### 3.6.22 Set Bond Vertically Button

Using the **Set Bond Vertically** tool, you can turn a chemical structure or a selected fragment so that the desired bond is displayed vertically in the workspace.

As you click the bond, it becomes vertical, and the entire structure or a selected fragment is rotated accordingly.

Clicking the vertical bond repeatedly rotates the structure/fragment by 180° back and forth.

### 3.6.23 Flip on Bond Button

Using the **Flip on Bond** tool, you can flip a chemical structure or a selected fragment relative to the chosen bond.

Make this tool active and then click the required bond.

**Note** Applying this tool to the 3D-optimized structures may cause distortion of structures. Thus, it is recommended to use the **3D Rotation** tool instead.
3.6.24 Flip Top to Bottom Button

Using the Flip Top to Bottom tool, you can flip chemical structure(s) or a selected fragment relative to the horizontal axis.

**Important** Flipping structures having optical center(s) produces enantiomers.

Select the structure/fragment you want to rotate, and then click this button. If nothing is selected on the current page, clicking this button flips all of the drawn structures as a single object.

**Note** If the Select Graphics check box is selected on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), you can apply this tool to objects created in the Draw mode, as well as to reaction pluses and arrows.

3.6.25 Flip Left to Right Button

Using the Flip Left to Right tool, you can flip chemical structure(s) relative to the vertical axis.

**Important** Flipping structures having optical center produces enantiomers.

Select the structure/fragment you want to rotate, and then click this button. If nothing is selected on the current page, clicking this button flips all of the drawn structures as a single object.

**Note** If the Select Graphics check box is selected on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), you can apply this tool to objects created in the Draw mode, as well as to reaction pluses and arrows.

3.6.26 Instant Template Button

Using the Instant Template tool, you can create a current pattern from any structure or selected fragment so that you can insert it anywhere in the workspace or attach it to a structure.

To create an instant template, follow the steps:

1. Select a structural element which you want to reproduce. Note that to create a template of an entire structure, you don't need to select it.

2. On the Structure toolbar, click Instant Template.

3. Point to the selected structure/structural element and click. The outline of the structure/element becomes attached to the mouse pointer.

**Note** If you are going to use a template for attaching it to the already drawn structure, make sure that you click the atom or bond which is to be a connection point of the template. For example, if you are going to insert a structure fused with a specific bond, select the corresponding template by clicking the bond (not the atom).

You can flip the template outline in the workspace by pressing TAB.

4. Move the mouse pointer to the desired location in the workspace, and click to paste the template.

**Note** When you attach the template taken by an atom and click an atom in the drawn structure while holding down SHIFT, the template will be attached without a bond. Of the two atoms of different elements, the senior one will be used as the connection point.
You can use the same template as many times as you want until you choose any other button from the toolbar or right-click in the workspace. If you need the template later, choose it all over again with this tool.

3.6.27 Calculate Parameters of Substituent Button

Using the Calculate Parameters of Substituent tool, you can calculate Hammett Sigma (σ) electronic substituent constants of different types (e.g., inductive, resonance, meta-, para-, etc.), as well as steric constants (molar volume and molar refractivity) and a hydrophobic constant (the π constant of Hansch) for a selected substituent structure. This option is useful for correlation of different properties which depend on characteristics of substituents attached to a constant reaction center.

Clicking the Calculate Parameters of Substituent runs the ACD/Sigma module. This module should be purchased in addition to ACD/ChemSketch. For more details on electronic substituent constants calculation, refer to ACD/Sigma User’s Guide located in the ACD/Labs documentation folder, \DOCS\SIGMA.PDF.

3.7 Atoms Toolbar

The Atoms toolbar is displayed vertically to the left of the workspace. This toolbar contains buttons that can be used to quickly insert atoms of the corresponding elements into the drawing area and to change the atom properties.

The table below lists the tools available on the toolbar and the short description for each of them:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Periodic Table]</td>
<td>Displays the Periodic Table of Elements (see Section 3.13.5).</td>
</tr>
<tr>
<td>![Query Atom]</td>
<td>Enables the Query Atom tool that allows you to specify atoms for performing a substructure search (see Section 3.7.1):</td>
</tr>
<tr>
<td>![Query Bond]</td>
<td>Enables the Query Bond tool that allows you to specify bonds for performing a substructure search (see Section 3.7.2):</td>
</tr>
<tr>
<td>![Atoms]</td>
<td>Use these buttons to draw atoms of corresponding chemical element in the workspace (see Section 3.7.3).</td>
</tr>
<tr>
<td>![Edit Atom Label]</td>
<td>Enables the Edit Atom Label tool that allows you to insert or change atom labels (see Section 3.7.4).</td>
</tr>
<tr>
<td>![Radical]</td>
<td>This tool allows you to insert pseudo atoms or radical designation labels (see Section 3.7.5):</td>
</tr>
</tbody>
</table>
### Structure Mode

#### 3.7.1 Query Atom Buttons

Using these tools, you can specify the query atoms when performing a substructure search.

To display a drop-down panel with the tools, click the lower right triangle on the button that is currently displayed on the Atoms toolbar.

The following tools are available on the panel:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Atom specified with this tool may be any atom except hydrogen.</td>
</tr>
<tr>
<td>Q</td>
<td>Atom specified with this tool may be any atom except carbon or hydrogen.</td>
</tr>
<tr>
<td>Ho</td>
<td>No hydrogens can be attached to an atom specified with this tool.</td>
</tr>
<tr>
<td>L</td>
<td>Creates a list of atoms to be allowed.</td>
</tr>
<tr>
<td>NL</td>
<td>Creates a list of atoms to be excluded.</td>
</tr>
</tbody>
</table>

To specify query atoms for a substructure search, choose the required tool on the panel, and then click the atom of the structure which you want to be replaced with the query atom.

For more information on how to perform a substructure search, refer to online Help of the corresponding ACD/Labs program.

**Tip** You can switch between currently active Query Atom tool and the Any Bond tool by right-clicking in the workspace.

#### 3.7.2 Query Bond Buttons

Using these tools, you can specify the query bonds when performing a substructure search.

To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Atoms toolbar.
The following tools are available on the panel:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Any</strong></td>
<td>Bond specified with this tool can be any type of bond (single, double, triple, or aromatic).</td>
</tr>
<tr>
<td><strong>Ar</strong></td>
<td>Bond specified with this tool can only be aromatic.</td>
</tr>
<tr>
<td><strong>S/D</strong></td>
<td>Bond specified with this tool can only be single or double (i.e., not aromatic or triple).</td>
</tr>
<tr>
<td><strong>Rn</strong></td>
<td>Bond specified with this tool must be a part of a ring (i.e., cancels chains).</td>
</tr>
<tr>
<td><strong>Ch</strong></td>
<td>Bond specified with this tool must be a part of a chain (i.e., cancels ring).</td>
</tr>
</tbody>
</table>

To specify query bonds for a substructure search, choose the required tool on the panel, and then click the bond in the structure which you want to be replaced with the query one.

For more information on how to perform a substructure search, refer to the online Help of the corresponding ACD/Labs program.

**Tip** You can switch between currently active Query Bond tool and the Any Atom tool by right-clicking in the workspace.

### 3.7.3 Atom Buttons

Using the Atom tools, you can quickly insert atoms of required chemical elements into the workspace without opening the Periodic Table of Elements dialog box (for more information, refer to Section 3.13.5).

Click the required atom button on the Atoms toolbar, and perform one of the following actions:

- Click an empty space to draw atom of the chosen element: either a cation for a metal or a hydride for a non-metal.
- With the Draw Normal tool active, click any atom in the drawn structure to replace it with the chosen one, or click the same atom to sprout a new single bond.
- With the Draw Continuous tool active, click an atom twice to sprout a new single bond with the chosen terminal atom.
- With the Draw Chains tool active, draw chains constructed from atoms of the chosen chemical element.

For more information on the aforementioned tools, refer to Sections 3.6.5–0 correspondingly.

By default, Atoms toolbar contains buttons of the following chemical elements: carbon, hydrogen, nitrogen, oxygen, fluorine, sodium, silicon, phosphorus, sulfur, chlorine, potassium, and bromine.
When drawing structures, the following chemical elements can be selected by pressing keys on the keyboard. If the element has not yet been used, pressing the assigned key on the keyboard will add the corresponding atom button on the toolbar:

<table>
<thead>
<tr>
<th>Element</th>
<th>Shortcut key</th>
<th>Element</th>
<th>Shortcut key</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>C</td>
<td>Bromine</td>
<td>R</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H</td>
<td>Tungsten</td>
<td>W</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N</td>
<td>Tritium</td>
<td>T</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O</td>
<td>Yttrium</td>
<td>Y</td>
</tr>
<tr>
<td>Fluorine</td>
<td>F</td>
<td>Uranium</td>
<td>U</td>
</tr>
<tr>
<td>Phosphorus</td>
<td>P</td>
<td>Iodine</td>
<td>I</td>
</tr>
<tr>
<td>Sulfur</td>
<td>S</td>
<td>Deuterium</td>
<td>D</td>
</tr>
<tr>
<td>Chlorine</td>
<td>L</td>
<td>Vanadium</td>
<td>V</td>
</tr>
<tr>
<td>Potassium</td>
<td>K</td>
<td>Boron</td>
<td>B</td>
</tr>
</tbody>
</table>

In addition, you can add buttons of user-defined elements by choosing them from the Periodic Table of Elements:

- On the Atoms toolbar, click **Periodic Table of Elements** to display the **Periodic Table of Elements** dialog box where you can choose the user-defined element, and then click OK. The selected element will be placed on the Atoms toolbar as a new button.

**Note**  Up to five user-defined elements can be displayed on the toolbar simultaneously.

To remove all of the user-defined atoms from the Atoms toolbar, double-click the toolbar. In the message that appears, click **Yes**.

For non-metals, the inserted atom appears in its lowest valence as a hydride derivative, whereas for metals, the inserted atom appears in its common oxidation state as an ion.

You can change the atomic charge / oxidation state of an atom by using the **Increment(+) Charge** or **Decrement (–) Charge** buttons (for more information, refer to Section 3.7.6.1) or by drawing new chemical bonds from this atom. You can also change the atomic charge, valence, oxidation state, coordination number, and isotope number by clicking **Atom Chemical Properties** (for more information, refer to Section 3.7.7).
### 3.7.4 Edit Atom Label Button

Using the [Edit Atom Label](#) tool, you can either insert a label in the workspace, or replace any atom in a structure with a functional group abbreviation or a shortcut formula which then can be expanded (for more information, refer to Section 3.12.9).

To insert a label, click the [Edit Atom Label](#) tool and then click the needed atom or empty space. In the [Edit Label](#) dialog box that appears, specify the label to be inserted, and then click **Insert**.

To switch this tool off, right-click in the workspace; the [Draw Normal](#) tool will be enabled.

**Note**  You can change the connection point of the label by using the [Change Position](#) tool (for more information, refer to Section 3.6.20).

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
</table>
| **Format toolbar** | With these tools, you can format an input label by specifying its font type and style.  
  Note that you can conveniently input Greek letters by using the [Greek Font](#) tool. |
| **Label box**   | In this box, enter the label (functional group abbreviation or shorthand formula) you want to insert or choose the corresponding one from the Labels list below. Note that the three last used labels are saved in the list and are displayed with dark red font at the top (they cannot be deleted).  
  To save your label or delete the existing ones, use the corresponding buttons to the right. |
| **Labels list** | In this list, select the label you want to add to the ChemSketch document. |
| **Formula Style** | Select this check box if you want the shorthand formulas to be inserted using formula-specific subscript / superscript formatting. |
| **List**        | In this area, select the required option to specify the type of labels to be displayed: all of the available labels (All), just the standard built-in labels provided by the program (Standard), or custom labels you have previously created (User). |
### Option | Description
--- | ---
**Save** | Saves the label specified in the Label box. This label will be added to the list of User labels. The User labels are displayed in dark blue. Three labels that have been recently entered are saved to the list automatically. They are displayed in red and cannot be deleted.

**Delete** | Removes the selected label from the list. Note that if you try to remove standard built-in labels, the warning message appears. Three labels that have been recently entered are saved to the list automatically. They are displayed in red and cannot be deleted.

**Insert** | Replaces the selected atom / label with the specified label or inserts the label in the empty workspace of the ChemSketch page.

**Expand** | *For terminal atoms only*  
Expands the specified label (represents it as a structure). The atom label can be expanded only if it was entered in capitals. Also, only labels which replace the terminal atoms in a structure can be expanded.

The following symbols are accepted by this tool:

- ~ tilde negative charge
- + plus positive charge
- – minus single bond (can be omitted)
- = equal sign double bond
- % percent triple bond
- ( ) brackets enclose a group of atoms

You can find the conventions for label expanding in the EXPAND.TXT file located in the ACD/Labs installation folder (e.g., \ACD12 for version 12.0). The left column in this file contains notations supported by the Expand tool. It is not recommended to modify this file.

If ACD/ChemSketch cannot expand the current abbreviation, the corresponding message appears. You can also expand the inserted labels using the Expand Shorthand Formulae command (for more information, refer to Section 3.12.9).

### 3.7.5 Pseudo Atom and Radical Label Buttons

Using the **Pseudo Atom** and **Radical Labels** tools, you can replace atoms with radical labels or pseudo atoms.

To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Atoms toolbar:

The following tools are available on the panel:

To apply any of these tools, choose the required tool on the panel, and then click the atom which you want to be replaced with the label or pseudo atom.
Use the **Pseudo Atom** tool to create open-ended polymers and bent bonds. Bent bonds are ignored in calculations (treated as standard bonds).

**Tip**

To insert pseudo atoms, you can also:

1. With the **Select/Move** tool active, double-click a highlighted atom to display the corresponding **Properties** panel (refer to Section 3.12.1.2).
2. Click **Atom Symbol** and then, from the adjacent **Value** list, choose **Empty**.
3. Click **Apply**, and then close the panel.

You can switch between Radical Label tools by right-clicking in the workspace.

### 3.7.6 Charges/Radicals Buttons

Using these tools, you can change atomic charge / oxidation state of an atom or make radicals from the existing atoms.

To display a drop-down panel of the tools, click the lower right triangle on the button that is currently displayed on the Atoms toolbar.

The following tools are available on the panel:

![Charge/Radical Tools]

To apply any of these tools, choose the required tool on the panel, and then click the atom which you want to modify.

#### 3.7.6.1 Increment (+) Charge and Decrement (–) Charge Buttons

Use these tools **+** / **−** to change the charge of a chosen non-metal atom or both the charge and oxidation state of a chosen metal atom.

The atomic charge and/or oxidation state increase in increments or decrease in decrements according to the valid oxidation states for metals or the valid valences for non-metals.

**Note**

These tools only allow you to change the charge and/or oxidation state of an atom within certain limits. For non-metals, the charge can be changed from −4 to +4 in general, whereas for metals the charge can only be changed according to the allowed oxidation states given in the Periodic Table of Elements. To set any other charges and/or oxidation states, use the **Properties** panel or **Atom Chemical Properties** button (refer to Sections 3.12.1.2 and 3.7.7 correspondingly).

You can switch between the **Increment (+) Charge** **+** and **Decrement (–) Charge** **−** tools by right-clicking in the workspace.

#### 3.7.6.2 Radicals Buttons

Using the **Radical** **•** tool, you can create radicals from both neutral and charged molecules.

Clicking the atom repetitively brings it to one of the available states:

- Monoradical, for example CH₃⁻
- Singlet biradical, for example CH₂⁺
• Triplet biradical, for example \( \cdot CH_2^* \)

The **Positive Radical Ion** tool allows you to create positive radical ions, for example \( CH_4^+ \).

The **Negative Radical Ion** tool allows you to create negative radical ions, for example \( CH_4^- \).

You can switch between the Radical tools by right-clicking in the workspace.

### 3.7.7 Atom Chemical Properties Button

Using the **Atom Chemical Properties** tool, you can specify physicochemical properties for a drawn atom.

As you click the atom with this tool active, the **Atomic Properties** dialog box that appears where you can specify the required atom properties:

![Atomic Properties Dialog Box]

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Valence</td>
<td>In this box, enter the valence value (in a range from 0 to 8) or choose it from the drop-down list.</td>
</tr>
<tr>
<td>Charge</td>
<td>In this box, enter the charge value or choose it from the drop-down list. Note that you can also define radicals here.</td>
</tr>
<tr>
<td>Isotope</td>
<td>In this box, enter the isotopic mass value.</td>
</tr>
<tr>
<td>Numbering</td>
<td>In this box, specify a numerical or textual string to be used as a marking for the selected atom.</td>
</tr>
<tr>
<td>Keep non-typical visibilities</td>
<td>Select this check box if you want to keep previously specified visible characteristics (such as valence or isotope). This check box is available in case you have manually set some of the visible characteristics of the atom through the <strong>Properties</strong> panel (refer to Section 3.12.1).</td>
</tr>
</tbody>
</table>

Click this button to save the properties you have specified in this box and add the corresponding **Element Properties** button to the Atoms toolbar. Now, as you click the desired atom on the workspace with the created button active, the atom's properties will be changed accordingly.

Note that you can add as many user-defined buttons as you want. To remove all of the custom buttons from the Atom toolbar, double-click the toolbar. In the message that appears, click **Yes**.

**Note** To change the style (font size, color, etc.) of atom properties' labels, use the **Properties** panel (refer to Section 3.12.1).
3.7.8 Manual Numbering Button

Using the Manual Numbering tool, you can number atoms in the drawn structure(s) manually. Clicking this button displays the Manual Numbering dialog box where you can specify the numbering format:

![Manual Numbering dialog box](image)

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Text Before</td>
<td>In this box, type the text to be inserted before the number.</td>
</tr>
<tr>
<td>Number</td>
<td>From the list of available numbering types, choose the required one.</td>
</tr>
<tr>
<td>Text After</td>
<td>In this box, type the text to be inserted after the number.</td>
</tr>
<tr>
<td>Start At</td>
<td>In this box, specify the value from which the numbering should be started.</td>
</tr>
<tr>
<td>OK</td>
<td>Closes the dialog box and enables the Manual Numbering tool with the specified options.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Closes the dialog box and enables the Manual Numbering tool with the default options.</td>
</tr>
</tbody>
</table>

After the format is set, click OK. Note that cursor becomes 

Click the desired atom in the workspace. The specified starting number will be assigned to it. Subsequent clicking other atoms in the workspace will continue numbering.

To stop numbering and disable the Manual Numbering tool, click any other button of the program.

To edit the numbering format, right-click in the workspace with the tool still active and specify new settings in the Manual Numbering dialog box.

**Note** You can specify the color of atom numbers in the Auto/Manual Numbering box on the Structure tab of the Preferences dialog box. For more information on this dialog box, refer to Section 3.14.1.2.

To change the style (font size, color, etc.) of the atom number labels, use the Properties panel. For more information on this panel, refer to Section 3.12.1.
3.8 References Toolbar

The References toolbar is displayed vertically to the right of the workspace. This toolbar contains buttons for quick and accurate creating of structures with the help of templates.

The toolbar contains the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Commercial version only!]</td>
<td>Displays ACD/Dictionary. For more information, refer to Section 3.13.6.</td>
</tr>
<tr>
<td>![Table of Radicals]</td>
<td>Displays the Table of Radicals panel containing the most frequently needed templates of radicals for a quick drawing of structures. For more information, refer to Section 3.13.4.</td>
</tr>
<tr>
<td>Shortcut buttons for radicals</td>
<td>Click the desired button, and then click in the workspace to draw the structural fragment(s) separately or attached to a previously drawn structure. These shortcut buttons appear on the toolbar after you select corresponding templates from the Table of Radicals at least once. You can add up to twelve buttons to the References toolbar. To remove the user-defined buttons from the toolbar, double-click the toolbar, and, in the message box that appears, click Yes.</td>
</tr>
</tbody>
</table>

Note To customize the toolbar contents, right-click it or click [ ] to display the shortcut menu (for more information, refer to Section 2.2.1). As you choose Reset Toolbar from the menu, the following default set of twelve templates will be available as buttons: benzene, cyclohexane, cyclopentane, t-butyl, i-propyl, acetyl, carboxyl, benzoyl, nitro, acetoxy, sulfo, and phosphono.

3.9 File Menu

This menu contains commands allowing you to load and save files, import and export files to other formats, print your work, and set printer and page formats. At the end of the menu, there is a quick-access list of 10 last loaded files.

3.9.1 New

This command creates a new blank ChemSketch document which immediately becomes active.

You do not need to execute the New command after starting ACD/ChemSketch. The program starts with a blank document, named NONAME00.SK2, active in the workspace. Subsequent new documents are named NONAME01.SK2, NONAME02.SK2, etc., until you save them with a new filename.

If you have several open documents, you can have only one document visible at a time—you cannot tile or cascade multiple document windows. All the other open files remain open but are no longer active.

To make any ChemSketch document active, choose its name from the Documents menu (for more information, refer to Section 3.15).

Note ACD/ChemSketch allows you to have up to ten documents open at once. If you have ten documents open, the New command becomes unavailable until at least one of the documents is closed.
Shortcuts:

General toolbar:  
Keyboard:  CTRL+N

3.9.2 Open

This command displays the Open Document dialog box where you can specify the name and location of a file that you want to load.

The following formats are supported:
- ChemSketch 2.0 Document (.SK2)
- MDL Mofile (.MOL)
- MDL Extended (V3000) Mofile (.MOL)
- ISIS/Sketch (.SKC)
- MDL RXNfile (.RXN)
- ChemSketch 1.0 (.MST, .RPT)
- CambridgeSoft ChemDraw (.CHM, .CDX)
- Windows Metafile (.WMF)

As soon as you open the document, its name is displayed on the status bar.

Note ACD/ChemSketch allows you to have up to ten documents open at once. If you have ten documents open, the Open command becomes unavailable until at least one of the documents is closed.

Shortcuts:

Keyboard:  CTRL+O
General toolbar

3.9.3 Close

This command closes the active document. If you made changes since the last time you opened or saved this document, ACD/ChemSketch prompts you to save your work. If this is the last of the open documents, ACD/ChemSketch automatically creates a new blank NONAME##.SK2 document and displays it in the workspace.

Tip To close all of the currently open documents, from the Documents menu, choose Close All.

Shortcuts:

Keyboard:  CTRL+W
General toolbar

---

* You can import objects from the ISIS/Sketch BIN files of any version but some new features may be missing for the files of the versions earlier than 2.0.
† You can import objects from the CS ChemDraw files of any versions later than 3.0.
‡ While importing Windows Metafiles, note that the bitmaps from the imported file will not be placed into ACD/ChemSketch.
3.9.4 Save

This command allows you to save the active document as a ChemSketch 2.0 Document (.SK2) file. If you are saving your work for the first time, the Save Document As dialog box appears prompting you to specify the file name and location.

Tip If you want to change the name or location of an existing file, from the File menu, choose Save As. To save all of the open documents at once, from the File menu, choose Save All.

Shortcuts:
- Keyboard: CTRL+S
- General toolbar

3.9.5 Save As

This command displays the Save Document As dialog box where you can specify a new name, location, and format of the file to which the currently open ChemSketch document is to be saved.

The following formats are supported:
- ChemSketch 2.0 Document (SK2)
- MDL Molfie (.MOL)
- MDL Extended (V3000) Molfie (.MOL)
- ISIS/Sketch (.SKC)
- MDL RXNfile (.RXN)
- CambridgeSoft ChemDraw (.CHM, .CDX)
- CML file (.CML)
- Adobe Portable Document Format (.PDF)
- Windows Metafile (.WMF)
- Windows Bitmap (.BMP, .DIB)
- Paintbrush (.PCX)
- TIFF Bitmap (.TIF)
- GIF Bitmap (.GIF)
- Portable Network Graphics (.PNG)

If the BMP, DIB, TIFF, or PNG format is selected, the dialog box includes the Options button. Click it to display the Windows Bitmaps Export Options, TIFF Export Options, or Portable Network Graphics Export Options dialog box correspondingly (refer to the section that follows) where you can set the required image resolution.

Tip If you want to save a file with the same name and to where it is currently located, from the File menu, choose Save. To save all of the open documents at once, from the File menu, choose Save All.

Shortcut:
- Keyboard: CTRL+SHIFT+S
3.9.5.1 Windows Bitmaps Export Options, TIFF Export Options, and Portable Network Graphics Export Options Dialog Boxes

These dialog boxes allow you to set the required image resolution for the active file you are working with.

| Note | Since all three dialog boxes are similar, their description is located in one topic. |

To display any of the dialog boxes, in the **Save Document As** or **Export** dialog box, from the **Save as type** drop-down list, choose *Windows Bitmaps (*.bmp, *.dib)*, *TIFF Bitmaps (*.tif)*, or *Portable Network Graphics (*.png)* correspondingly, and then click **Options**.

To set the image resolution, click the arrow button in the **Image Resolution** box, then select the required value (in dots per inch) from the list of available ones, and click **OK**.

3.9.6 Save All

This command saves all of the open documents (up to ten may be open at once) as .SK2 files. When you are saving your work for the first time, the **Save Document As** dialog box prompts you to specify the name and location for each open file. If any of the documents have been saved before, the existing names and locations are used.

| Tip | If you want to change the name or location of an existing file, from the **File** menu, choose **Save As**. To save only the current document, from the **File** menu, choose **Save**. |

**Shortcut:**

Keyboard: SHIFT+ F12

3.9.7 Export

This command displays the **Export** dialog box where you can specify the name, location, and format of file to which contents of the active document are to be exported.

The following formats are supported:

- MDL Molfile (.MOL)
- MDL Extended Molfile (.MOL)
- ISIS/Sketch (.SKC)
- MDL RXNfile (.RXN)
- CS ChemDraw (.CHM, .CDX)
- CML file (.CML)
- Adobe Portable Document Format (.PDF)
- Windows Metafile (.WMF)
- Windows Bitmap (.BMP, .DIB)
- Paintbrush (.PCX)
- TIFF Bitmap (.TIF)
- GIF Bitmap (.GIF)
- Portable Network Graphics (.PNG)
If the BMP, DIB, TIFF, or PNG format is selected, the dialog box includes the Options... button. Click it to display the Windows Bitmaps Export Options, TIFF Export Options, or Portable Network Graphics Export Options dialog box correspondingly (refer to Section 3.9.5.1), where you can set the required resolution.

3.9.8 Import

This command displays the Import dialog box where you can specify the name, location, and format of the file whose contents are to be added to the active document.

The following formats are supported:

- MDL Molfiles (.MOL)
- ISIS/Sketch (.SKC)*
- MDL RXNfile (.RXN)
- ChemSketch 1.0 (.MST, .RPT)
- CS ChemDraw (.CHM, .CDX)†
- Windows Metafile (.WMF)‡

The imported structures retain their original design and chemical significance. You can change and manipulate the imported structures, save them to a new file, print, insert them into other Windows applications, and calculate their chemical properties.

Some of the imported structures may have the size that the system can consider non-feasible. If this is the case, the Import Warning dialog box appears. To rescale the structure, click Yes.

3.9.9 Run ChemBasic

This command displays the Run Program dialog box where you can specify the name and location of a ChemBasic Program file (.BAS) written in ACD/ChemBasic language. As you click OK, the program will be run. You can create such programs yourself or use the ones available for free as goodies (for more information, refer to Appendix C) from our Web site.

ACD/ChemBasic programs may have shortcut buttons which can be placed on a toolbar with the help of the ChemBasic Organizer command (Options menu). For more information, refer to Section 3.14.8.

3.9.10 Forms Manager

This command displays the Forms Manager dialog box where you can design input forms for ACD/ChemBasic programs.

For more information on ACD/ChemBasic and ACD/Forms Manager, refer to the ACD/ChemBasic Tutorial (CHEMBAS.PDF) and ACD/Forms Manager User’s Guide (FORMSMAN.PDF) located in the ACD/Labs documentation folder, \DOCS.

* You can import objects from the ISIS/Sketch BIN files of any version, but for the files of the versions later than 2.0 some new features may be missing.
† You can import objects from the CS ChemDraw files of any versions later than 3.0.
‡ While importing Windows Metafiles, note that the bitmaps from the imported file will not be placed into ACD/ChemSketch.
3.9.11 Page Setup

This command displays the Page Setup dialog box where you can specify page settings either for the whole document or for the current page.

The dialog box contains three tabbed pages described in the following sections and the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apply To</td>
<td>In this box, you can choose whether to apply the settings specified in the dialog box to the whole document (Whole Document) or to the current page of the open document only (Current Page). If there is the only page in the document, this option is not available.</td>
</tr>
<tr>
<td>Preview area</td>
<td>Shows the results of the specified settings.</td>
</tr>
<tr>
<td>Set Default</td>
<td>Saves the currently specified paper size, orientation, and margins as default.</td>
</tr>
<tr>
<td>Restore Default</td>
<td>Changes the current settings to the last accepted default settings. If no defaults have been recently set, this button has no effect.</td>
</tr>
</tbody>
</table>
3.9.11.1 Page Setup Dialog Box: Size & Orientation Tab

On this tab, you can specify the paper format and orientation of the page(s), either landscape or portrait.

The tab contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Format</td>
<td>In this box, specify the paper size available for your printer. As you choose any standard paper format, the Width and Height boxes display the corresponding values. As you enter your own values of width and/or height, the Format box displays Custom Size.</td>
</tr>
<tr>
<td>Width</td>
<td>This box displays the width* of the currently set paper format. As you enter your own value, the Format box displays Custom Size.</td>
</tr>
<tr>
<td>Height</td>
<td>This box displays the height* of the currently set paper format. As you enter your own value, the Format box displays Custom Size.</td>
</tr>
<tr>
<td>Portrait</td>
<td>Select this option to print the document so that the short edge of the paper is horizontal. Refer to the Preview area to see what the page will look like.</td>
</tr>
<tr>
<td>Landscape</td>
<td>Select this option to print the document so that the long edge of the paper is horizontal. Refer to the Preview area to see what the page will look like.</td>
</tr>
<tr>
<td>Restore From Printer</td>
<td>Changes the page configuration to the current printer settings (paper size and orientation only).</td>
</tr>
</tbody>
</table>

* Units of measurement in these boxes correspond to those set in the Preferences dialog box (Options menu). To enter the value in points/inches/millimeters/centimeters type the values and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The values will be recalculated into the corresponding units of measurement.
3.9.11.2 Page Setup Dialog Box: Margins Tab

On this tab, you can set margins for the open ChemSketch document.

**Note** 
Margins are shown on the ChemSketch pages as a dotted-line *rectangle*. Do not confuse them with the nonprintable region dotted *lines* (i.e., minimum margins that are supported by the system's default printer) displayed along the page as well.

To display the margins/printable area, select the **Page Margins/Printable Area** check box in the **Preferences** dialog box (**General** tab). For more information on this dialog box, refer to Section 3.14.1.1.

![Page Setup Dialog Box](image)

On this tab, in the appropriate boxes, set the distance* between the left/top/right/bottom edge of the paper and the corresponding line of the margin in the ChemSketch.

3.9.11.3 Page Setup Dialog Box: Poster Tab

On this tab, you can set the number of pages your poster will consist of.

![Page Setup Dialog Box](image)

On this tab, set the length width and height for the virtual page size.
The tab contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Width Calculation</strong></td>
<td>In this box, specify the number of separate pages (the size page dimensions is specified on the Size &amp; Orientation tab) the poster will horizontally include. Note that the maximal number of pages depends on the paper format chosen. The calculated poster size will be displayed in the Virtual Page Size area.</td>
</tr>
<tr>
<td><strong>Height Calculation</strong></td>
<td>In this box, specify the number of separate pages (the page size is specified on the Size &amp; Orientation tab) the poster will vertically include. Note that the maximal number of pages depends on the paper format chosen. The calculated poster size will be displayed in the Virtual Page Size area.</td>
</tr>
<tr>
<td><strong>Virtual Page Size</strong></td>
<td>This area displays the calculated virtual size of a poster: Post size = page size × number of pages – sum of nonprintable regions. Nonprintable regions mean the minimum margins between the adjacent pages that are supported by the system's default printer. Do not confuse nonprintable region dotted lines with the dotted-line rectangle of the ChemSketch margins (for more information, refer to the previous section) that can be displayed on the page as well.</td>
</tr>
</tbody>
</table>

**3.9.12 Print**

This command displays the Print dialog box where you can specify the pages of the active document to be printed, the number of printed copies, and the printer to use. For proper printing of your work, make sure that your Microsoft Windows environment and your printer are properly configured and connected. See your Microsoft Windows User's Guide for details.

| Note | When you start printing the colored page (for more information, refer to Section 3.11.6), a message box appears asking if you want to print the page with the set background color. If you choose No, the set background color will be ignored and the page will remain white. Be careful when canceling background color printing: if you have, for example, a black background and the structures drawn in white, the structures will not be visible on the printout if you cancel background color. |

**Shortcuts:**

<table>
<thead>
<tr>
<th>Keyboard</th>
<th>General toolbar</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTRL+P</td>
<td></td>
</tr>
</tbody>
</table>

**3.9.13 Print Preview**

This command switches the ChemSketch window to the Print Preview mode that displays each page as it will look on the printout. You can view multiple pages at a time, and magnify or reduce the visible size of the pages on the screen.

In this mode, the Top toolbar of the window consists of the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Displays the Print dialog box where you can specify the required settings for printing current ChemSketch document (see the previous section).</td>
</tr>
<tr>
<td></td>
<td>Magnifies the visible size of the pages on the screen to get a close-up view of the document. You can also zoom in by pressing PLUS SIGN (+) on the numeric keypad.</td>
</tr>
<tr>
<td>Button</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td><img src="image" alt="Zoom Out" /></td>
<td>Reduces the visible size of the pages on the screen to see more of the page (multiple pages) at a reduced size. You can also zoom out by pressing the MINUS SIGN (−) on the numeric keypad.</td>
</tr>
<tr>
<td><img src="image" alt="One Page" /></td>
<td>Displays only one page of the current document at once. You can also display one page by pressing ASTERISK (*) on the numeric keypad.</td>
</tr>
<tr>
<td><img src="image" alt="First Page" /></td>
<td>Displays the first page of the current document.</td>
</tr>
<tr>
<td><img src="image" alt="Previous Page" /></td>
<td>Displays the previous page of the current document (if any).</td>
</tr>
<tr>
<td><img src="image" alt="Next Page" /></td>
<td>Displays the next page of the current document (if any).</td>
</tr>
<tr>
<td><img src="image" alt="Last Page" /></td>
<td>Displays the last page of the current document (if any).</td>
</tr>
<tr>
<td><img src="image" alt="Close" /></td>
<td>Quits the Print Preview mode and returns the ChemSketch window to the previous view of the document.</td>
</tr>
</tbody>
</table>
3.9.14 Properties

This command displays the Document Properties dialog box where you can set attributes of the active ACD/ChemSketch document. Specifying the attributes will help you to track the data later on.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Title</td>
<td>In this box, enter the title you want to use when searching for the file.</td>
</tr>
<tr>
<td>Subject</td>
<td>In this box, enter the subject of the file. Use this property to group similar files together, so you can search for all files that have the same subject.</td>
</tr>
<tr>
<td>Author</td>
<td>In this box, enter the name of the file author. By default, this box contains your system logon name.</td>
</tr>
<tr>
<td>Organization</td>
<td>In this box, enter your company name.</td>
</tr>
<tr>
<td>Comments</td>
<td>In this box, enter the comments for your file.</td>
</tr>
<tr>
<td>Set as Default Properties</td>
<td>Select this check box if you want the information specified in this dialog box to be automatically inserted into the properties for all newly created ChemSketch documents.</td>
</tr>
<tr>
<td>Statistics</td>
<td>Displays the fully qualified pathname of the file, the dates when the document was created and modified, and the file size.</td>
</tr>
</tbody>
</table>
3.9.15 Send > As Is / As PDF

Use these commands to send the current document by e-mail either as a ChemSketch 2.0 Document or Adobe Portable Document Format file.

When you choose the appropriate command, your default e-mail client starts, and a new message is created with the current document attached (either as an .SK2 or .PDF file). Note that this command does not work properly if no default mail client is set.

If you have opened a saved document and have edited it without saving the changes, the attached document will have the same name as the source file but will contain all of the changes you have made up to the moment of the e-mail sending.

If you have opened a new document and have not saved it yet, ACD/ChemSketch will give it a default name NONAME01 (02, 03, etc.).

**Note** This command is not available if a new document is currently open and has not been edited yet.

3.9.16 File Associations

This command displays the File Associations dialog box where you can assign certain file formats to ACD/ChemSketch. If all of the supported file types have been already associated with the program, the corresponding message will be displayed.

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Available Formats</td>
<td>This box contains the formats that can be associated with the program. Select the check boxes of the formats that are to be associated with ACD/ChemSketch. The Associated with area below shows the application to which the currently highlighted format is linked.</td>
</tr>
<tr>
<td>Always perform check when starting the program</td>
<td>If this check box is selected, each time ACD/ChemSketch is started, it will check the system for the formats supported by your version that are not associated with it yet. If there are any, this dialog box will appear at the startup.</td>
</tr>
</tbody>
</table>
### Option  Description

<table>
<thead>
<tr>
<th><strong>Select All</strong></th>
<th>Click this button to select all of the file formats in the Available Formats box.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unselect All</strong></td>
<td>Click this button to cancel the selection of all the file formats in the Available Formats box.</td>
</tr>
<tr>
<td><strong>Yes</strong></td>
<td>Click this button to close the dialog box applying the specified settings.</td>
</tr>
<tr>
<td><strong>No</strong></td>
<td>Click this button to close the dialog box without applying the specified settings.</td>
</tr>
</tbody>
</table>

If you open the File Associations dialog box under Windows 2000/XP/Vista but have no rights to change file associations, a warning message appears. Contact your system administrator to resolve the problem.

Note that you can change file association through Windows Explorer:

1. Right-click the required file, on the shortcut menu, point to Open With, and select Choose Program.
2. In the Open With dialog box that appears, select the application that should be used to open the files of given format.
3. Select the Always use the selected program to open this kind of file check box, and click OK.

#### 3.9.17 Exit

This command quits ACD/ChemSketch. The program will prompt you to save your work unless you have just done so.

| Note | If you have other programs from the ACD/Labs package running, you won't quit them with this command. To close all of the programs, from the ACD/Labs menu, choose Exit All. |

**Shortcuts:**

- **Keyboard:** ALT+X
- **Mouse:** double-click the program icon on the title bar (refer to Section 2.3).

#### 3.9.18 Recent Files

Use these submenu commands to display the recently opened files.

You can display the file opened this day, the day before, within the last 7, 14, 30 days, or 12 months. To clear the History, on the History submenu commands, choose Clear History.

| Note | If you save a document in a format that is not supported by the Import command of ACD/ChemSketch, this file will not be displayed in the list of recently opened files. |
3.10 Edit Menu

The commands located on this menu allow you to manage actions with graphics (cut, copy, paste, etc.) in the open ACD/ChemSketch document.

3.10.1 Undo

This command cancels the last action performed. This command can be used up to 50 times in sequence so that you can restore almost any previous stage of your work.

Note To reverse the effect of the Undo command, from the Edit menu, choose Redo.

Shortcuts:
Keyboard: CTRL+Z or ALT+BACKSPACE
General toolbar: 

3.10.2 Redo

This command cancels the action performed by the last Undo command. This feature can be used sequentially up to 50 times so that you can restore almost any edit made to your work.

Note To reverse the effect of the Redo command, from the Edit menu, choose Undo.

The Redo command can be used only once for each corresponding Undo command.

Shortcuts:
Keyboard: CTRL+Y or SHIFT+ALT+BACKSPACE
General toolbar: 

3.10.3 Cut

This command removes the selected objects from the workspace and places them to the Clipboard. Once the objects are on the Clipboard, you can paste them to other Microsoft Windows applications, as well as to different documents within ACD/ChemSketch or other parts of the same document.

Note When pasting structures cut from ACD/ChemSketch to another application (e.g., Microsoft Excel), they may be placed as a set of numbers and figures (as an MDL Molfile). To place the structures as graphics, use the Paste Special feature of the application you are pasting to. Among the paste options, choose either the ACD ChemSketch Object or Picture option. The former inserts the structure as an OLE object thus allowing you to edit the inserted structure via ACD/ChemSketch by double-clicking the object.

Shortcuts:
Keyboard: CTRL+X
General toolbar: 

3.10.4 Copy

This command copies the selected objects to the Clipboard. Once the objects are on the Clipboard, you can paste the selection to other Microsoft Windows applications, as well as to different documents within ACD/ChemSketch or other parts of the same document.

**Note**  When pasting structures copied from ACD/ChemSketch to another application (e.g., Microsoft Excel), they may be placed as a set of numbers and figures (as an MDL Molfile). To place the structures as graphics, use the Paste Special feature of the application you are pasting to. Among the paste options, choose either the ACD ChemSketch Object or Picture option. The former inserts the structure as an OLE object thus allowing you to edit the inserted structure via ACD/ChemSketch by double-clicking the object.

Shortcuts:

- Keyboard: CTRL+C
- General toolbar: 

3.10.5 Paste > Default

This command pastes the last object added to the Clipboard. Once this command is selected, the mouse pointer with the attached outline of the Clipboard object appears. Click the desired location to place the object into the active ChemSketch document.

**Note**  If the object has been placed onto the Clipboard from an external application (not ACD/ChemSketch), it will be pasted by default as an embedded object and can be edited in the application it has been taken from. To paste the object in specific Clipboard formats, on the Edit menu, point to Paste, and then choose Special.

Shortcuts:

- Keyboard: CTRL+V
- General toolbar: 

3.10.6 Paste > In Place

This command pastes a copy of the Clipboard contents to the place the copy was taken from. If the object is copied / cut from any external application (not ACD/ChemSketch), it will be pasted in the left upper corner of the page.

**Note**  To paste the object at arbitrary place in the workspace, on the Edit menu, point to Paste, and then choose Default.

Shortcut:

- Keyboard: CTRL+SHIFT+V
3.10.7 Paste > Special

This command pastes objects from the Clipboard in a specific format. As you choose this command, the Paste Special dialog box with the Clipboard formats available for the current contents of the Clipboard appears. Select the needed format and click OK. The Clipboard contents appear as an outline attached to the mouse pointer. Click in the desired location to paste the object.

To edit the object pasted in this way, double-click it. If the object has been created in an external application (e.g., MS Excel), the corresponding application will be started (if available on your computer) where you can edit the object. As you close the application, the edited object will be updated in the ChemSketch window.

Note To insert an object created within another application or to link to another application and create an object without leaving ACD/ChemSketch, from the Edit menu, choose Insert Object.

Shortcut: Keyboard: CTRL+SHIFT+E

3.10.8 Paste > Structure

This command pastes chemical structure(s) from the Clipboard. The Clipboard may contain:

- Chemical structure(s) created with in the external applications (for example, in ISIS/Draw). In this case, the command, unlike the Paste > Special one, places such structure(s) not as a picture but as chemical structure(s) so that you can edit them in the Structure mode. Note that some structures created in third-party applications may be pasted incorrectly due to limitations of this command.

—OR—

- InChI notation or SMILES string. In this case, the structure(s) will be automatically generated from the string copied (as in the Generate > Structure from InChI and Generate > Structure from SMILES commands). For more information, refer to Sections 3.12.24 and 3.12.21 correspondingly.—New to 12.0!

As you select this command, click in the workspace to place the structure. If the Clipboard does not contain the proper information, the error message appears.

Shortcut: Keyboard: CTRL+SHIFT+U

3.10.9 Paste > Table

This command pastes the Clipboard contents to the workspace as a table. It allows you to paste tables that were not created in ACD/ChemSketch (e.g., MS Excel tables or MS Word tables) and then edit them as usual ChemSketch objects. Unlike the Paste > Special command, this command places table(s) created with other applications not as a picture or embedded object but as a ChemSketch table so that you can edit it in the Draw mode.

As you choose this command, the Clipboard contents appear as an outline attached to the mouse pointer. Click the desired location to paste the copied objects.

Note To insert in your ChemSketch document an object created with another application or to link to another application and create an object without leaving ACD/ChemSketch, from the Edit menu, choose Insert Object.
3.10.10 Delete

This command erases all of the selected objects from the current page without placing them on the Clipboard. If you want to delete specific objects only, use the Delete tool on the General toolbar (for more information, refer to Section 3.5.1.)

**Note** You can retrieve the deleted objects by using the Undo command.

**Shortcut:**
Keyboard: DELETE

3.10.11 Select All

This command selects all of the objects on the current ChemSketch page. To cancel the selection of objects, click an empty space. To cancel the selection of a single object, click it while holding down SHIFT. For more details on how to select/unselect individual objects in the Structure mode, refer to Sections 3.6.1 and 3.6.2.

**Note** If the Select Graphics check box is cleared on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), the objects created in the Draw mode cannot be selected in the Structure mode.

**Shortcut:**
Keyboard: CTRL+A

3.10.12 Insert Object

This command embeds an object created with another application. This command allows you either to create a new object (e.g., create a spreadsheet, picture, database, etc.) or to insert a previously created object into your drawing.

To insert an object, follow the steps:
1. Choose this command. The Insert Object dialog box with the list of the supported object types appears.
2. Select the desired type and click OK. The application associated with this type of objects will be opened (if available and properly installed).
3. In the application, create new or open an existing file.
4. Quit the application to return to ACD/ChemSketch. The object is embedded within the upper left corner of the dotted-line rectangle of margins (refer to Section 3.9.11.2) on the ChemSketch page.

**Note** To edit the embedded object, from the Edit menu, choose Edit Object or double-click the object.

3.10.13 Edit Object

This command allows you to edit the selected object of a specific type that was inserted into the ChemSketch window in one of the following ways:

- With the Insert Object command (see Section 3.10.12);
- With the Paste > Special command (see Section 3.10.7);
• With the Paste > Default or Paste > In Place command (see Sections 3.10.5 and 3.10.6) in case the object was previously copied to the Clipboard in some application.

As you select the object and choose this command, the application associated with the type of objects is started. Note that the command’s name has been changed from Edit Object to Edit <Object Type> Object. After making the necessary changes, quit the application to turn back to ACD/ChemSketch where the object is automatically updated.

**Note**  
You have to operate in the Draw mode to select and edit the majority of the inserted objects, including spreadsheets and pictures.

**Shortcut:**
- **Mouse:** Double-click the object to be edited.

### 3.11 Pages Menu

The commands located on this menu allow you to create, rename, or delete pages, browse through multipage document, and manage header/footer for the pages in your document.

#### 3.11.1 New

This command adds a new blank page to the end of the ChemSketch document and makes the page active.

**Note**  
One document can contain up to 100 pages.

**Shortcut:**
- **General toolbar:**

#### 3.11.2 Insert

This command adds a new blank page before the current page of the ChemSketch document and makes the page active.

**Note**  
One document can contain up to 100 pages.

**Shortcut:**
- **Keyboard:** SHIFT+F3

#### 3.11.3 Change Order

This command displays the Change Order of Pages dialog box where you can view the current page number and enter a new number for the page in your ChemSketch document. As you click OK, the other pages are reordered accordingly. Note that this command is not available if a one-page document is currently open.

**Tip**  
You can also use the Reorder Pages goody for rearrangement the ChemSketch pages. For more information, refer to Appendix C.
3.11.4 Delete

This command removes the current page and its contents from the current ChemSketch document. After a page has been deleted, the remaining pages in the document are renumbered.

ACD/ChemSketch will not ask you to confirm the deletion. Though, the removed page can be recovered with the Undo command until you quit ACD/ChemSketch.

Shortcut:
Keyboard: SHIFT+F4

3.11.5 Rename

This command displays the Rename Page dialog box where you can rename the current page of a ChemSketch document. In the Page Name box, type a new name for the current page. Click OK.

Assigned page names can be viewed on the status bar when you click the Page list:

Tip You can use the Insert Page Numbers / Annotations goody for page annotation. For more information, refer to Appendix C.

3.11.6 Color

This command displays the Page Color dialog box where you can specify the background color of the current page. Choose the color from the palette and click OK. This command both sets the color of your display and affects the color of the page on the printout.

Note When you start printing the colored page, a message box appears asking if you want to print the page with the set background color. If you choose No, the set background color will be ignored and the page will remain white. Be careful when canceling background color printing: if you have, for example, a black background and the structures drawn with white, structures will not be visible on the printout if you cancel background color.
3.11.7 Header and Footer > Edit

This command switches the program to the Draw mode and displays the Header and Footer toolbar that allows you to edit headers/footers for the pages in your ChemSketch document:

![Header and Footer toolbar](Image)

**Note**
Headers and footers can consist of both text and graphics. As in other applications, header appears at the top of a page while footer appears at the bottom.

By default, the header (footer) field objects are inserted within the upper (lower) left corner of the dotted-line rectangle of margins (refer to Section 3.9.11.2) on the ChemSketch page. Use the corresponding tools from the toolbar to align them right, center, or left.

The toolbar includes the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Insert AutoText</td>
<td>Click this button to insert automatically updated header or footer items in your document. From the drop-down list that appears as you click this button, choose the pre-defined item you want to insert into a header/footer field object. The information is placed in the header/footer as tags containing braces and macro elements. The macro elements denote the following:</td>
</tr>
<tr>
<td></td>
<td>$N—page numbers</td>
</tr>
<tr>
<td></td>
<td>$S—total page numbers</td>
</tr>
<tr>
<td></td>
<td>$A—author’s name</td>
</tr>
<tr>
<td></td>
<td>$O—organization name</td>
</tr>
<tr>
<td></td>
<td>$L—document title</td>
</tr>
<tr>
<td></td>
<td>$J—document subject</td>
</tr>
<tr>
<td></td>
<td>$F—file name</td>
</tr>
<tr>
<td></td>
<td>$P—path with file name</td>
</tr>
<tr>
<td></td>
<td>$T—time</td>
</tr>
<tr>
<td></td>
<td>$D—date</td>
</tr>
</tbody>
</table>

As the header/footer is formatted and you close the Header and Footer toolbar, the program runs the macro replacement process. The author’s name, organization name, document title, and document subject are inserted from the settings in the **Document Properties** dialog box (refer to Section 3.9.14).

To avoid mistakes, do not try to insert one macro set into another. Do not modify the information within braces; the program inserts it by default.

- Inserts page numbers that are automatically updated when you add or delete pages.
- Inserts a time field that is automatically updated so that the current time is displayed when you open or print the file.
- Inserts a date field that is automatically updated so that the current date is displayed when you open or print the file.
- Moves the insertion point from left to right within the header and footer fields thus aligning it right, center, and left. Click this button as many times as required to occupy the desired position.
- Moves the insertion point from right to left within the header and footer fields thus aligning it left, center, and right. Click this button as many times as required to occupy the desired position.
- Moves the insertion point to the header.
- Moves the insertion point to the footer.
- Displays the **Open Document** dialog box where you can specify the name and location of any previously saved ChemSketch Header/Footer file (.HFP) to be loaded into the current document.
<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Button" /></td>
<td>Displays the <strong>Save Document As</strong> dialog box where you can specify the name and location of a ChemSketch Header/Footer file (.HFP) to which the current footer and header are to be saved.</td>
</tr>
<tr>
<td><img src="image" alt="Button" /></td>
<td>Closes the Header and Footer toolbar and applies the specified settings.</td>
</tr>
</tbody>
</table>

### Tip
You can use this feature to insert a background picture for your document. When the Edit Header/Footer toolbar is on, draw or insert the picture and place it in the required position on the page. When you leave the header/footer editing mode, the picture will become a background for your drawings for all the pages in the current document.

#### 3.11.8 Header and Footer > Load

This command displays the **Open Document** dialog box where you can specify the name and location of any previously saved ChemSketch Header/Footer file (.HFP) to be loaded into the current document.

**Shortcut:**

Header and Footer toolbar: ![Button](image)

#### 3.11.9 Header and Footer > Save

This command saves the header and footer of the current document to a specific ChemSketch Header/Footer file (.HFP), so that you can load it for other documents afterwards.

If you save the header and footer for the first time, the **Save Document As** dialog box appears (refer to the section that follows).

**Shortcut:**

Header and Footer toolbar: ![Button](image)

#### 3.11.10 Header and Footer > Save As

This command displays the **Save Document As** dialog box where you can specify the name and location of a ChemSketch Header/Footer file (.HFP) to which the header and footer of the current document are to be saved.

#### 3.11.11 Header and Footer > Set As Default

This command displays the **Set Header/Footer Page as Default** dialog box where you can specify contents of a ChemSketch Header/Footer file (.HFP) whose header and footer are currently active to be the default ones, that is, they will automatically be inserted in all newly created documents.

To define the default header and footer, click **Set Current as Default**. If you have not saved your header and footer into a file yet, the program will prompt you to do so. As soon as the file is saved, it is defined as the default one.

To cancel the default header and footer, click **Clear Default**.
3.11.12 Header and Footer > Clear

This command removes both the header and footer from the current document.

3.11.13 Header and Footer > Show

This command toggles the display of headers and footers in the ChemSketch document.

Note: This command is selected by default.

3.11.14 Previous

This command displays the previous page of the ChemSketch document.

Note: This command is disabled if you have opened one-page document.

You can also click the Page list [Page 64/65] on the status bar (for more information, refer to Section 2.6) to quickly switch to the required page.

Shortcuts:

Keyboard: PAGE UP
Status bar:  

3.11.15 Next

This command displays the next page of the ChemSketch document.

Note: This command is disabled if you have opened one-page document.

You can also click the Page list [Page 64/65] on the status bar (for more information, refer to Section 2.6) to quickly switch to the required page.

Shortcuts:

Keyboard: PAGE DOWN
Status bar:  

3.11.16 First

This command displays the first page of the ChemSketch document.

Note: This command is disabled if you have opened one-page document.

You can also click Page list [Page 64/65] on the status bar (for more information, refer to Section 2.6) to quickly switch to the required page.

Shortcut:

Keyboard: CTRL+HOME
3.11.17 Last

This command displays the last page of the ChemSketch document.

**Note** This command is disabled if you have opened one-page document.

You can also click the Page list on the status bar (for more information, refer to Section 2.6) to quickly switch to the required page.

**Shortcut:**

Keyboard: CTRL+END

3.12 Tools Menu

The commands located on this menu allow you to refine a created structure and to determine its properties.

3.12.1 Structure Properties

This command displays the **Properties** panel where you can specify the graphic representation of chemical drawings created in the Structure mode.

**Tip** You can also open this panel by double-clicking element of a drawn structure (either atom, bond, or selected fragment) with the **Select/Move** tool active.

The panel contains four tabbed pages described in the following sections and the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
</table>
| **Current Style** | This area contains a drop-down list of the existing styles, as well as buttons used for managing the user-defined styles.  
To load an existing style, click the arrow and choose the style from the list. To apply it to the selection, click **Apply**.  
To name a user-defined style, set the required options in the panel, click in this box, type the name of the style, and click **Save**.  
To delete a user-defined style, find it in the list and click **Del**. |
| **Apply**       | Applies the specified style settings to the selected structural fragments or structures. |
| **Set Default** | Saves the specified style settings as default, *i.e.*, the default style will be applied to all}
Option | Description
--- | ---
 | the newly drawn structures automatically.

**Update From**
Allows you to copy style attributes from the drawn structure to the panel. Note that the mouse pointer becomes an arrow labeled From. Click a structure to update its style settings to this panel.

**Restore Default**
Restores settings of current default style on the panel.

**Shortcuts:**

- **Keyboard:** ALT+SHIFT+S
- **Mouse:** double-click an atom, bond, or selected fragment

### 3.12.1.1 Properties Panel: Common Tab

On this tab, you can specify common style settings for the selected structural fragments or entire structures.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Show Carbons</strong></td>
<td>In this area, select the required check box(es) to control whether all of the carbons (All) or terminal carbons (Terminal) only should be displayed. If none of the check boxes is selected, no carbons will be displayed in the selected structure.</td>
</tr>
<tr>
<td><strong>Hide Zero Charge</strong></td>
<td>This check box controls whether the zero charges should be displayed.*</td>
</tr>
<tr>
<td><strong>Cross Out Invalid Atom</strong></td>
<td>This check box controls whether the invalid atoms should be crossed out. If you select this check box, the invalid atoms will be automatically crossed out with X.</td>
</tr>
</tbody>
</table>

* If several objects are selected on the ChemSketch page, the check box of an attribute can be: cleared, i.e., this attribute will not be applied to the selected objects; selected, i.e., this attribute will be applied to the selected objects; dimmed (if this attribute differs for the selected objects), i.e., this attribute will not be changed for the selected objects.
### Option | Description
--- | ---
**Size Calculation** | In this area, you can specify the atom symbol size and bond length **. Note that if the Auto check box is selected, the bond length will be automatically calculated to fit the entered atom symbol size and vice versa.

**Atom Style** | In this area, specify the font type, style, and color for atom labels. If the selected atoms are of mixed style, the Own button is enabled.

**Bond Style** | In this area, set the bond thickness** and color.

### 3.12.1.2 Properties Panel: Atom Tab

On this tab, you can specify the style settings for label(s) of the selected atom(s) / functional group(s).

![Attributes toolbar](image)

Each label comprises a set of attributes. To change settings for any of them, click the corresponding button on the Attributes toolbar:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Atom symbol" /></td>
<td>When this tool is selected, the settings are applied to the <strong>atom symbol</strong> (except for non-explicit hydrogens) attribute.</td>
</tr>
<tr>
<td><img src="image" alt="Non-explicit hydrogen" /></td>
<td>When this tool is selected, the settings are applied to the <strong>non-explicit hydrogen</strong> attribute.</td>
</tr>
<tr>
<td><img src="image" alt="Hydrogen index" /></td>
<td>When this tool is selected, the settings are applied to the <strong>hydrogen index</strong> attribute.</td>
</tr>
<tr>
<td><img src="image" alt="Charge" /></td>
<td>When this tool is selected, the settings are applied to the <strong>charge</strong> attribute.</td>
</tr>
<tr>
<td><img src="image" alt="Valence" /></td>
<td>When this tool is selected, the settings are applied to the <strong>valence</strong> attribute.</td>
</tr>
<tr>
<td><img src="image" alt="Isotope" /></td>
<td>When this tool is selected, the settings are applied to the <strong>isotope</strong> attribute.</td>
</tr>
<tr>
<td><img src="image" alt="Numbering" /></td>
<td>When this tool is selected, the settings are applied to the <strong>numbering</strong> attribute.</td>
</tr>
</tbody>
</table>

To apply the same style settings to several kinds of atom attributes at a time, hold down SHIFT and click the required buttons on the Attributes toolbar.

As you make changes on the tab, you can preview the label appearance in the preview area.

**Tip** If some of the changes made to the current attribute(s) are not displayed in the preview area at once, press ENTER.

The tab also contains the following options:

**Units of measurement in these boxes correspond to those set in the Preferences dialog box (Options menu).** To enter the value in points/inches/millimeters/centimeters, type the values and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The values will be recalculated into the corresponding units of measurement.

---

**Units of measurement in these boxes correspond to those set in the Preferences dialog box (Options menu).** To enter the value in points/inches/millimeters/centimeters, type the values and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The values will be recalculated into the corresponding units of measurement.
### Option Description

<table>
<thead>
<tr>
<th>Font Type</th>
<th>In this box, specify the font type to be applied to the attribute(s) currently selected on the Attributes toolbar.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Font Size</td>
<td>In this box, specify the font size to be applied to the attribute(s) currently selected on the Attributes toolbar.</td>
</tr>
<tr>
<td>Font Style</td>
<td>In this area, specify the font style (bold / italic / bold italic) to be applied to the attribute(s) currently selected on the Attributes toolbar. If the Own button is enabled, it means that the current attribute has mixed formatting in the selection.</td>
</tr>
<tr>
<td>Color</td>
<td>In this box, specify the color for the attribute(s) currently selected on the Attributes toolbar.</td>
</tr>
</tbody>
</table>

**Show**

*Except for the hydrogen index and charge attributes*

Select this check box to show the selected attribute in the structure.*

**Value**

*Except for the hydrogen index attribute*

In this box, choose among the values available for the selected attribute.

For the atom symbol attribute, if you choose Empty, no atom symbol will be inserted in the workspace.

For the non-explicit hydrogen attribute, you can specify the position of the hydrogen in a functional group: Auto, Right, Left, Bottom, or Top relative to the central atom symbol.

Note that to make this box appear on the panel, you should previously select one atom/group only.

**Y**

*Except for the atom symbol and non-explicit hydrogen attributes*

In this box, set the Y-coordinate** of the corresponding attribute relative to the central atom symbol.

**X**

*For the numbering attribute*

In this box, set the position of the numbering attribute relative to the atom label along the X-axis.

Note that the coordinate can have a negative value.*

**After H**

*For the charge and valence attributes*

Select this check box to place the charge / valence superscript attribute in the functional group after the non-explicit hydrogen.* If this check box is cleared, the charge/valence attribute will be located near the atom symbol itself.

**Soft**

*For the charge attribute*

Select this check box to make the charge ‘soft’. The ‘soft’ charge disappears after the charged atom is connected to a bond. If this check box is cleared, the specified charge will remain when any connections are made to the charged atom.

Note that if you increase or decrease the atom charge using one of the Increment (+) or Decrement (–) Charge tools on the Atoms toolbar, the charges are set as ‘soft’.*

---

* If several objects are selected on the ChemSketch page, the check box of an attribute can be: cleared, i.e., this attribute will not be applied to the selected objects; selected, i.e., this attribute will be applied to the selected objects; dimmed (if this attribute differs for the selected objects), i.e., this attribute will not be changed for the selected objects.

**Units of measurement in these boxes correspond to those set in the Preferences dialog box (Options menu). To enter the value in points/inches/millimeters/centimeters, type the values and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The values will be recalculated into the corresponding units of measurement.*
Option | Description
---|---
Center | For the numbering attribute
—New to 12.0! This check box controls the location of the atom numbers: if it is cleared, atom numbers are positioned near the atom nodes that is more common for chemical drawings:

![Chemical structure](image1)

If the check box is selected, atom numbers are displayed in place of hidden atoms:

![Chemical structure](image2)

### 3.12.1.3 Properties Panel: Bond Tab

On this tab, you can specify the style settings for the selected bond(s).

Each type of bond has specific display parameters. To change settings for any of them, click the corresponding button on the Bond Types toolbar:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image3" alt="Single bond button" /></td>
<td>When this tool is selected, the settings are applied to the single bond type.</td>
</tr>
<tr>
<td><img src="image4" alt="Double bond button" /></td>
<td>When this tool is selected, the settings are applied to the double bond type.</td>
</tr>
<tr>
<td><img src="image5" alt="Triple bond button" /></td>
<td>When this tool is selected, the settings are applied to the triple bond type.</td>
</tr>
<tr>
<td><img src="image6" alt="Up stereo bond button" /></td>
<td>When this tool is selected, the settings are applied to the up stereo bond type.</td>
</tr>
<tr>
<td><img src="image7" alt="Down stereo bond button" /></td>
<td>When this tool is selected, the settings are applied to the down stereo bond type.</td>
</tr>
<tr>
<td><img src="image8" alt="Coordinating bond button" /></td>
<td>When this tool is selected, the settings are applied to the coordinating bond type.</td>
</tr>
<tr>
<td><img src="image9" alt="Undefined bond button" /></td>
<td>When this tool is selected, the settings are applied to the undefined bond type.</td>
</tr>
</tbody>
</table>

To apply the same style settings to several types of bonds at a time, hold down SHIFT and click the required buttons on the Bond Types toolbar.

As you make changes on the tab, you can preview the bond appearance in the preview area.

**Tip** If some of the changes made to the current type(s) are not displayed in the preview area at once, press ENTER.
The tab also contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>In this box, specify the line thickness</strong> to be used for the corresponding type of bond.</td>
<td></td>
</tr>
<tr>
<td><strong>In this box, specify the color for the bond lines of the type currently selected on the Bond Types toolbar.</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Between</strong></td>
<td><strong>For the double and triple bond types</strong></td>
</tr>
<tr>
<td>In this box, specify the distance between the lines in the bond.</td>
<td></td>
</tr>
<tr>
<td><strong>Shift</strong></td>
<td><strong>For the double bond type</strong></td>
</tr>
<tr>
<td>In this box, specify the shift (i.e., difference in length) between the lines when the bond is defined as asymmetric.</td>
<td></td>
</tr>
<tr>
<td><strong>For the triple bond type</strong></td>
<td>In this box, specify the difference between the central line length and the length of other two lines in a bond.</td>
</tr>
<tr>
<td><strong>Pos.</strong></td>
<td><strong>For the double bond type</strong></td>
</tr>
<tr>
<td>In this box, specify the position of two lines in a double bond relative to each other. You can see the specified position in the preview area.</td>
<td></td>
</tr>
<tr>
<td><strong>Width</strong></td>
<td><strong>For the up stereo, down stereo, and undefined bond types</strong></td>
</tr>
<tr>
<td>In this box, specify the thickness of the wider end for up / down stereo bonds, or the width of sections for undefined bonds.</td>
<td></td>
</tr>
<tr>
<td><strong>Step</strong></td>
<td><strong>For the down stereo and undefined bond types</strong></td>
</tr>
<tr>
<td>In this box, specify the step between the sections representing down stereo and undefined bonds.</td>
<td></td>
</tr>
<tr>
<td><strong>H.</strong></td>
<td><strong>For the coordinated bond type</strong></td>
</tr>
<tr>
<td>In these boxes, specify the length and width of the arrowhead for coordinating bond.</td>
<td></td>
</tr>
</tbody>
</table>

### 3.12.1.4 Properties Panel: Special Tab

On this tab, you can specify the style settings for the Markush bond shadow.

The tab contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Show</strong></td>
<td>Select this check box to show the Markush bond shadow in the structure.</td>
</tr>
<tr>
<td><strong>Click this button to shadow the Markush bond in a solid color. You can specify the fill color in the adjacent Color box that appears.</strong></td>
<td></td>
</tr>
</tbody>
</table>

*Units of measurement in these boxes correspond to those set in the Preferences dialog box (Options menu). To enter the value in points/inches/millimeters/centimeters, type the values and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The values will be recalculated into the corresponding units of measurement.*
3.12.2 Clean Structure

This command redraws and resizes selected chemical structure or selected fragment to standardize all bond lengths and angles. If there is more than one structure in the current page and none of them is selected, all of the structures will be standardized ("cleaned").

The "cleaning" function standardizes the bond lengths and angles while minimally changing the relative dislocations of all the inter-bonded atoms and fragments in the drawn structure. To define the way of structure representation ("clean method"), on Clean tab of the Preferences dialog box (for more information, refer to Section 3.14.1.4), select the required checkboxes.

If the results are not satisfactory, click Undo on the General toolbar to cancel the changes made, change the mutual dislocations of the selected atoms or fragments with the Select/Move or Select/Rotate/Resize tools, and then apply the Clean Structure command once again.

Shortcuts:

Structure toolbar: 
Keyboard: F9

3.12.3 Check Tautomeric Forms

This command checks and generates possible tautomeric forms of selected organic structure.

As soon as the forms are generated according to the rules of ACD/Tautomers algorithm (for more information, refer to the section that follows), the Check Tautomeric Forms dialog box appears displaying suggested tautomeric structures.

Note: If the drawn structure is the major tautomeric form itself, selecting this command displays the corresponding message.
The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Information field</td>
<td>Displays information on the number of generated tautomeric forms.</td>
</tr>
<tr>
<td>Structure area</td>
<td>Displays the drawn chemical structure as the dialog box is open. As you click the Next and Previous buttons below, this area displays the suggested tautomeric forms.</td>
</tr>
<tr>
<td>Replace</td>
<td>Replaces the drawn structure with the structure currently displayed in the Structure area.</td>
</tr>
<tr>
<td>Copy</td>
<td>Copies the currently displayed tautomeric form to the ChemSketch window. Note that the outline of the structure becomes attached to the mouse pointer. As you click in the workspace, the structure is inserted and the Select/Move tool becomes active again.</td>
</tr>
<tr>
<td>Copy All</td>
<td>Copies all of the generated tautomeric forms to the ChemSketch window. Note that the outline of the collection of structures becomes attached to the mouse pointer. As you click in the workspace, the structures are inserted and the Select/Move tool becomes active again.</td>
</tr>
</tbody>
</table>

Shortcuts:
- Structure toolbar: ![Structure toolbar icon]
- Keyboard: CTRL+SHIFT+T

3.12.3.1 ACD/Tautomers Algorithm

The ACD/Tautomers algorithm recognizes and takes into account most of the known types of tautomeric equilibrium such as:
- Aldehydes, ketones, thiaoaldehydes, thiolketones—enoles, thioenoles;
- Imines—enamines;
• Oximes—nitroso compounds;
• Nitro compounds—acetyl form of nitro compounds;
• Tautomeric equilibria of oxy-, amino- and thio- substituted and nonsubstituted 5- and 6-member heteroaromatics.

In most cases, the influence of the electron-withdrawing groups on the tautomeric equilibrium is taken into account as well.

The following major types of known tautomeric equilibrium are not taken into account in the current ACD/Tautomers algorithm:
• Ring—chain equilibria;
• Equilibria involving any changes in the atomic valence;
• Equilibria that are too slow without a catalyst.

The ACD/Tautomer algorithm does not proceed with the following classes of chemical structures:
• Structures containing metal atoms;
• Structures containing charged atoms, other than the derivatives of nitrogen (+) bonded to oxygen (–);
• Structures containing elements in their non-typical valence;
• Structures with coordinating bonds;
• Structures containing more than 255 atoms.

The current ACD/Tautomers algorithm provides only the suggested tautomeric forms, but not necessarily the correct ones. The possibility of the alternative tautomeric forms should always be carefully considered, if the drawn organic structure contains two or more double or triple bonds conjugated with or attached to oxygen, nitrogen, sulfur, or other heteroatoms. Consult other sources of information to make a final decision.

### 3.12.4 3D Structure Optimization

This command creates a realistic 3-dimensional model of a planar (2D) chemical structure.

| Note | This command can be applied to a single selected structure at a time. |

After the 3D optimization is complete:

• The model becomes available for 3D rotation (the mouse pointer changes to ) if the Switch to 3D-Rotation Mode check box is selected in the Structure tab of the Preferences dialog box (for more information on the dialog box, refer to Section 3.14.1.2). If this check box is cleared, you should manually switch to the 3D Rotation mode by clicking 3D Rotation on the Structure toolbar.

• All hydrogen atoms are explicitly shown on the model if the Add Hydrogens check box is selected on the Structure tab of the Preferences dialog box (for more information on the dialog box, refer to Section 3.14.1.2).

The 3D optimization is based on modified molecular mechanics which take into account bond stretching, angle bending, internal rotation, and Van der Waals non-bonded interactions. Modifications include minor simplification of potential functions and enforcement of the minimization scheme by additional heuristic algorithms for dealing with "bad" starting conformations. The 3D optimization algorithm is a proprietary version of molecular mechanics with the force field initially based on CHARMM parametrization (refer to B.R. Brooks, R.E. Bruccoleri, B.D. Olafson, D.J. States, S. Swaminathan, and M. Karplus. CHARMM: A program for macromolecular energy, minimization, and dynamics calculations. *J. Comput. Chem.* 4, 187–217
The modifications involve some simplification and were intended to increase the stability and speed of computation.

Important 3D optimizer is NOT a full-scale molecular mechanics engine. Its design aims to reliably reproduce reasonable conformations from (possibly very unreasonable) 2D drawings, rather than to precisely optimize 3D structures.

Occasionally, the 3D optimization produces a molecular conformation different from what you have expected. It is the very essence of the conformational analysis that structures typically have many possible conformations. The optimizer finds only one, and it is not necessarily the one you have expected. For example, you probably expect a cyclohexane fragment to be a chair, but the optimizer may generate twist-boat, which is also one of its suitable conformations (indeed, in many structures this fragment exists in a twisted form). To obtain another conformation, move some atoms in the resultant 3D structure to make the initial structure closer to the final conformation, and then optimize the structure once again.

Initial stereo configuration may occasionally change to an opposite one during optimization while you try to obtain a specific enantiomer for a structure with chiral centers. To solve the problem, it is usually enough to draw all four substituents of the chiral center and use both Up Stereo Bonds and Down Stereo Bonds tools to define the required direction of bonds in the initial 2D structure. If it doesn't work, you can move the atoms manually in the resulted 3D structure and optimize the structure once again. In any case, we recommend that you click No in the 3D Structure Optimization dialog box prompting you to remove hydrogens before starting the optimization.

You may wish to perform actual conformational analysis of your structure using a special molecular mechanics or quantum chemistry geometry optimization package. 3D structure optimized by means of ACD/ChemSketch may serve as input data in this case.

Note ACD/ChemSketch can optimize structures containing atoms from hydrogen to xenon with standard valence state and bonding states.

If you use up and down stereo bonds to define stereochemical configurations, you should do that on the “flat”, non-3D-optimized structure. Note that the stereo bonds on 3D structure can be ambiguous.

Shortcuts:
Structure toolbar:  
Keyboard:  CTRL+SHIFT+3

3.12.5 Calculate Boiling Point

This command displays the ACD/Boiling Point dialog box containing the boiling point (BP), vapor pressure (VP), enthalpy of vaporization, and flash point data calculated for selected structure.

Note The ACD/Boiling Point module can be purchased in addition to ACD/ChemSketch. For more information on available modules, refer to Section 1.2.

For more details on the ACD/Boiling Point dialog box options, refer to the ACD/Boiling Point User's Guide located in the ACD/Labs documentation folder, \DOCS\BP.PDF.

Shortcuts:
Structure toolbar:  
Keyboard:  CTRL+SHIFT+B
3.12.6 MassSpec Scissors

This command calculates and displays monoisotopic masses for specified fragments of a structure:

- Select bond(s) connecting the fragments for which you want to calculate monoisotopic masses, and then choose this command. Monoisotopic mass values will appear near the fragments along with the corresponding molecular formulas.

\[\text{C}_4\text{H}_3\]
51.0235 Da

\[\text{C}_4\text{H}_3\text{O}\]
67.0184 Da

Tip
To calculate monoisotopic mass for a single fragment, select it, and then choose the Monoisotopic Mass command from the Calculate submenu (Tools menu).

If three and more adjacent bonds are selected simultaneously, the warning message appears informing you that all of the selected bonds will be broken as a result of this operation. Click OK to continue the process anyway or Cancel to cancel it.

Shortcut:
Structure toolbar:

3.12.7 Show Aromaticity

This command transforms conjugated double bonds into delocalized double bonds in aromatic rings of a selected structure(s) or fragment(s). If no selection is made, the transformation is applied to aromatic rings of all the structures on current page.

Shortcut:
Keyboard: CTRL+SHIFT+A

3.12.8 Hide Aromaticity

This command transforms delocalized double bonds into the conjugated double bonds in aromatic rings of a selected structure(s) or fragment(s). If no selection is made, the transformation is applied to aromatic rings of all structures on current page.

Shortcut:
Keyboard: CTRL+SHIFT+H
3.12.9 Expand Shorthand Formulae

This command expands a label based on the shorthand formula that was inserted with the help of the Edit Atom Label tool (for more information, refer to Section 3.7.4):

- Select either the label you want to expand or the whole structure containing such label(s), and choose this command. The shorthand formula will be substituted by an explicitly drawn structural fragment.

If no label/structure is selected, this command affects all of the drawn structures on current page.

The following symbols are acceptable by this tool:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>~</td>
<td>tilde negative charge</td>
</tr>
<tr>
<td>+</td>
<td>plus positive charge</td>
</tr>
<tr>
<td>−</td>
<td>minus single bond (can be omitted)</td>
</tr>
<tr>
<td>=</td>
<td>equal sign double bond</td>
</tr>
<tr>
<td>%</td>
<td>percent triple bond</td>
</tr>
<tr>
<td>(</td>
<td>brackets embrace a group of atoms</td>
</tr>
</tbody>
</table>

**Note**
You can find conventions for label expanding in the EXPAND.TXT file located in the ACD/Labs installation folder (e.g., \ACD12 for version 12.0). The left column in this file contains notations supported by the Expand Shorthand Formulae command. It is not recommended to modify this file.

If ACD/ChemSketch cannot expand the current abbreviation, the corresponding message appears. You can also expand the inserted labels using the Expand tool of the Edit Label dialog box (for more information, refer to Section 3.7.4).

**Shortcut:**
Keyboard: CTRL+SHIFT+F

3.12.10 Add Explicit Hydrogens

This command adds explicit hydrogens to the selected fragment or structure. If there is no selection in the workspace, explicit hydrogens are added to all of the structures drawn on current ChemSketch page.

**Note**
If you choose to create a realistic 3-dimensional model of a drawn “flat” structure using the 3D Structure Optimization tool (for more information, refer to Section 3.12.4), you are prompted to remove explicit hydrogens before the 3D optimization.

Even if you choose Yes in the message box, the hydrogens will still remain in the 3D optimized structure if the Add Hydrogens option is selected on the Structure tab of the Preferences dialog box (for more information, refer to Section 3.14.1.2).
3.12.11 Remove Explicit Hydrogens

This command hides explicit hydrogens from the selected fragment or structure. If there is no selection in the workspace, explicit hydrogens will be removed from all of the drawn structures on current ChemSketch page.

Shortcut:
Keyboard: CTRL+SHIFT+Y

3.12.12 Bring Bond(s) to Front

This command brings selected background bond(s) to foreground.

If the Enable check box of the Bond Intersections area is selected on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), when drawing a bond, ACD/ChemSketch automatically creates gap(s) in the existing bond(s) the new one is drawn across. The gapped bond is considered as the background bond, while the continuous one is considered to be in the foreground.

Tip
You can also bring background bond to foreground using the Change Position tool (refer to Section 3.6.20).

Shortcut:
Keyboard: CTRL+F

3.12.13 Send Bond(s) to Back

This command brings selected foreground bond(s) to background (see the bond conventions in the previous section).

Tip
You also draw back a foreground bond using the Change Position tool (for more information, refer to Section 3.6.20).

Shortcut:
Keyboard: CTRL+K
3.12.14 Auto Renumbering

This command automatically numbers atoms of the selected structure or fragment. If there are no selected structures or fragments in the workspace, all of the atoms currently drawn in the workspace are numbered.

**Note** To edit atom numbers, use the Manual Numbering or Atom Chemical Properties tools (for more information, refer to Sections 3.7.8 and 3.7.7 correspondingly). To change the style (font size, color, etc.) of atom numbers, use the Properties panel (refer to Section 3.12.1).

**Shortcut:**
Keyboard: CTRL+SHIFT+N

3.12.15 Clear Numbering

This command removes atom numbering from the selected structure or fragment. If there are no selected structures or fragments in the workspace, atom numbering will be removed in all of the structures drawn in the workspace.

**Note** To insert or edit atom numbers, use the Auto Renumbering command (refer to Section 3.6.14) or the Manual Numbering and Atom Chemical Properties tools (for more information, refer to Sections 3.7.8 and 3.7.7 correspondingly). To change the style (font size, color, etc.) of atom numbers, use the Properties panel (refer to Section 3.12.1).

**Shortcut:**
Keyboard: CTRL+SHIFT+L

3.12.16 Generate > Name for Structure

This command generates IUPAC systematic name(s) for the drawn structure(s). Note that this command is available both in the Structure and Draw modes.

**Note** The name generation preferences specified either in ACD/Name or in any ACD/Labs database program affect the result of the name generation in ACD/ChemSketch.

To obtain name for a single structure, select it, and then choose this command. The generated name will be inserted under the structure as a text string.
To generate a name for a two-component mixture, select the required structures (no more than two types of different ones), and choose this command. The generated name for the mixture (with indicated proportion of the components given in round brackets) will appear under the lower structure as a text string in one line:

![Diagram of two structures: 2-methylbuta-1,3-diene - buta-1,3-diene (2:1)]

**Note** If only a single structure is drawn in the workspace, you do not have to select it.

If only two types of different structures are simultaneously present and not selected, the program will consider them a two-component mixture of corresponding proportion.

ACD/Name Freeware is distributed as a free add-on to ACD/ChemSketch. It has the following restrictions as compared to the commercial version: structures to be named can contain no more than 50 atoms (H, C, N, P, O, S, F, Cl, Br, I, Li, Na, or K) and no more than 3 cycles in any polycyclic part.

To get more information on the commercial version of ACD/Name software, visit our Web site at [http://www.acdlabs.com/products/draw_nom/nom/name/](http://www.acdlabs.com/products/draw_nom/nom/name/).

**Shortcuts:**

- **Keyboard:** CTRL+SHIFT+I
- **General toolbar:** ![Diagram icon]
3.12.17 Generate > Structure from Name

This command starts the ACD/Name to Structure module that generates structures from systematic chemical names created according to IUPAC Recommendations on Nomenclature of Organic Chemistry, Chemical Abstract Service (CAS) inverted names, trivial and trade names, registry numbers and abbreviations. Note that the ACD/Name to Structure module should be purchased in addition to ACD/ChemSketch. For detailed description on how to work with this module, refer to the ACD/Name to Structure User’s Guide located in ACD/Labs documentation folder (\DOCS\NAMESTR.PDF).

As you choose this command, the ACD/Name to Structure dialog box appears:

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>In this box, enter the name of the structure to be generated or choose the desired name from the drop-down list that includes the names for which the structure generation process has been run before (to display the list, click ).</td>
</tr>
<tr>
<td>Warning(s)</td>
<td>This field displays the possible errors and warning messages occurring in the process of structure generation. Note that the system may generate the optimal structure in spite of the warning messages.</td>
</tr>
<tr>
<td>Structure</td>
<td>Displays the generated structure. If the system generates several structures for one name (e.g., pentanedithioic acid), the structures are placed into separate tabbed pages. To view the structure, click the corresponding tab.</td>
</tr>
</tbody>
</table>
### Option Description

| Prompting(s) | This field displays the proposal on the next action to be performed or informs you if any error occurs while generating the structure. |
| Run | Starts the structure generation process for the name specified in the Name box. |
| Copy | Places the generated structure into the ChemSketch window. |
| Options... | Displays the ACD/Name to Structure Options dialog box where you can set preferences for the structure generation process (for more information, refer to Section 3.12.17.1). |
| About... | Displays information about your copy of the ACD/Labs package, including the version number, the copyright, and user registration information. This also contains information on how to contact ACD/Labs. Moreover, by clicking the License ID button, you can see your license ID number(s)—you will need the ID number(s) in case our technical support is required. |

### Shortcuts:

- **Keyboard**: CTRL+SHIFT+G
- **General toolbar**: ![Icon]
3.12.17.1 ACD/Name to Structure Options Dialog Box

In this dialog box, you can adjust settings for structure generation.

To display the dialog box, in the ACD/Name to Structure dialog box, click Options.

![ACD/Name to Structure Options Dialog Box]

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numbering</td>
<td>In this area, you can set the following options for numbering of atoms:</td>
</tr>
<tr>
<td></td>
<td>If the Show Numbering in Dialog check box is selected, the atoms numbering</td>
</tr>
<tr>
<td></td>
<td>will be displayed in the ACD/Name to Structure dialog box.</td>
</tr>
<tr>
<td></td>
<td>If the Copy to Editor with Numbering check box is selected, the atoms</td>
</tr>
<tr>
<td></td>
<td>numbering will be displayed on the structure when it is placed to the ChemSketch</td>
</tr>
<tr>
<td></td>
<td>page. Note that if the generated structure is taken from ACD/Dictionary,</td>
</tr>
<tr>
<td></td>
<td>numbering will not be displayed regardless of the options selected.</td>
</tr>
<tr>
<td>Warnings</td>
<td>In this area, you can choose among the following actions the program will</td>
</tr>
<tr>
<td></td>
<td>execute in case of warnings:</td>
</tr>
<tr>
<td></td>
<td>If the Ignore Warnings option is selected, the program will generate structure(s)</td>
</tr>
<tr>
<td></td>
<td>without displaying any warnings.</td>
</tr>
<tr>
<td></td>
<td>If the Report Warnings option is selected, the generated structure(s) will</td>
</tr>
<tr>
<td></td>
<td>be displayed together with warnings on its (their) reliability.</td>
</tr>
<tr>
<td></td>
<td>Select the Stop on Warnings option to stop the structure generation process</td>
</tr>
<tr>
<td></td>
<td>if any problems occur. As a result, the corresponding warnings will be</td>
</tr>
<tr>
<td></td>
<td>displayed without any structure(s).</td>
</tr>
<tr>
<td></td>
<td>If the structure is found in ACD/Dictionary, it is displayed along with the</td>
</tr>
<tr>
<td></td>
<td>corresponding warning.</td>
</tr>
<tr>
<td>Mark Undefined</td>
<td>If this check box is selected, the program will generate structure(s) with</td>
</tr>
</tbody>
</table>
### 3.12.18 Generate > Stereo Descriptors

This command determines stereo descriptors for double bonds, chiral, and pseudo chiral centers in selected structure(s).

**Note** The command is available in both Structure and Draw modes.

Select the required structure(s) and choose this command. Stereo descriptors will appear near the corresponding chiral center or double bond:

- \[ \text{S and R describe a chiral center configuration.} \]
- \[ \text{E and Z describe a double-bound configuration.} \]
- \[ \text{Small r and s describe configurations of pseudo chiral centers.} \]

**Note** If no selection is made in the workspace, stereo descriptors are automatically generated on current page for all structures which have stereo centers or double bonds for with Z/E or R/S isomerism.

When generating stereo descriptors for 3D-optimized structures, the program takes into account the actual X-, Y-, and Z-coordinates, while the stereo bonds are ignored.

When generating stereo descriptors, the program ignores the direction of the bond that depends on the way of drawing only (whether it points upwards or downwards). However, it differentiates between the up and down stereo bonds.

**Note** To change color of stereo descriptors, on the Structure tab of the Preferences dialog box (refer to Section 3.14.1.2), in the Auto/Manual Numbering Color box, set the appropriate color.

To generate special stereo descriptors for prochiral centers and mark the incorrectly defined stereochemical configurations, prior to using this command, select corresponding check boxes in the Stereo Options dialog box (for more information, refer to the following section).
3.12.19 Generate > Stereo Descriptors Options

This command displays the Stereo Options dialog box where you can specify options for determining stereo descriptors (for more information, refer to the previous section) in order to avoid mistakes in structure representation.

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Take into Account Stereo Wedges</td>
<td>If this check box is selected, the &quot;up&quot; and &quot;down&quot; wedges which specify</td>
</tr>
<tr>
<td>Stereocenters</td>
<td>stereo centers will be analyzed with regard to their directions</td>
</tr>
<tr>
<td>Direction</td>
<td>(depending to which atom a narrow end is attached).</td>
</tr>
<tr>
<td></td>
<td>If this check box is not selected, the sign (&quot;up&quot; or &quot;down&quot;) of the stereo</td>
</tr>
<tr>
<td></td>
<td>wedge doesn't depend on the direction.</td>
</tr>
<tr>
<td>Mark Undefined Chiral Centers</td>
<td>Select this check box to define prochiral centers.</td>
</tr>
<tr>
<td></td>
<td>These centers will be marked with the asterisk sign (*).</td>
</tr>
<tr>
<td>Mark Incorrectly Defined Stereo</td>
<td>Select this check box to mark atoms with an incorrectly defined stereochemical</td>
</tr>
<tr>
<td></td>
<td>configuration. They will be signed with a question mark (?).</td>
</tr>
</tbody>
</table>

After applying the Generate > Stereo Descriptors command (for more information, refer to the previous section), the prochiral centers will be marked with the asterisk sign (*), atoms with the incorrectly defined stereochemical configuration will be signed with the question mark (?):

![Chemical Structure Image]

3.12.20 Generate > SMILES Notation

This command generates SMILES (Simplified Molecular Input Line Entry Specification) string for the selected structure(s) displayed in the ChemSketch window.

**Note** This command is available in both Structure and Draw modes.

If none of the displayed structures is selected, the SMILES strings will appear for all of the structures displayed.
3.12.21 Generate > Structure from SMILES

This command displays the Generate Structure from SMILES dialog box where you can enter the source SMILES (Simplified Molecular Input Line Entry Specification) string from which chemical structure(s) will be generated.

**Note** This command is available in both Structure and Draw modes.

As you click OK in the dialog box, an outline of the generated structure(s) appears attached to the mouse pointer. Click in the workspace to place the structure(s) at the appropriate location. You can flip the outline orientation by pressing TAB.

**Tip** You can also generate structures from the existing SMILES strings. Select the required string and choose this command. The structure(s) will be placed below the string.

You can quickly paste the structure generated from SMILES with the Paste > Structure command in case the Clipboard contains a SMILES string (for more information, refer to Section 3.10.8).—New to 12.0!

3.12.22 Generate > InChI for Structure

This command generates the standard and non-standard InChI notation for a drawn structure.

**Note** This command is available in both Structure and Draw modes.

If none of the displayed structures is selected, InChI will appear for all of the structures displayed. More information about InChIs is available on the IUPAC website at www.iupac.org/inchi.

**Shortcut:**

General toolbar:  

3.12.23 Generate > InChI Options

This command displays the InChI Options dialog box where you can specify preferences for the generation of InChIs.
The dialog box contains the following options:

**Option** | **Description**
--- | ---
**Generate** | In this area, you can choose among the following InChI items to be generated:
  **InChI String** | Select this check box to generate InChI string.
  If neither InChI AuxInfo nor InChI Key check box is selected, the InChI String option is selected by default.
  **InChI AuxInfo** | Select this check box to generate the auxiliary information for creating structure(s) based on InChI string. It describes in a specific way the atom connections, numbers and coordinates.
  Note that auxiliary information can be different for the same structure, it depends on the structure-drawing order.
  **InChI Key** | Select this check box to generate InChI key.
  InChI key is a character signature based on a hash code of the InChI string. A hash code is a fixed length-condensed digital representation of a variable length character string. The length of InChI key is always 25 characters, including separator.
  Note that you cannot generate structure from InChI key.
  **Generate Standard InChI and InChI Key** | Select this check box to generate standard InChI and InChI key items for selected structure(s).
  InChI and InChI key may differ depending on specified InChI options. To increase a role of InChI and InChI key as universal structure identifier, IUPAC decided to define general InChI options required for generating standard InChI and InChI key for a structure.
  These default options include:
  - Mobile hydrogen perception;
  - Absolute stereochemical configuration;
  - Narrow end of wedge points to stereocenter.
  Note that standard and non-standard InChI and InChI Key have some differences.
  **Structure Options** | In this area, you can choose among the following options:
### Mobile H Perception
Select this check box to take possible tautomerism into account when generating structure(s) thus generating the favourite tautomer form.

Clear this check box to include the information on the specific tautomer into the InChI notation.

**EXAMPLE:** Source structure is

![3,4-dihydro-2H-pyrrol-5-amine](image)

If the check box is selected:

\[
\text{InChI=1/C4H8N2/c5-4-2-1-3-6-4/h1-3H2,(H2,5,6)}
\]

If the check box is cleared:

\[
\text{InChI=1/C4H8N2/c5-4-2-1-3-6-4/h1-3H2,(H2,5,6)/h/h5H2}
\]

### Include Bonds to Metal
Select this check box to include information about bonds between metal and other atoms. Otherwise, such information will be ignored.

### Stereo Options
In this area, you can choose whether to take into account stereochemical configurations in the drawn structure or not and how to treat them.

**Ignore**
Select the required option to include corresponding configurational information (except for **Ignore**) in the InChI string.

**EXAMPLE:** Source structure is

![2R,3S]-pentane-2,3-diol](image)

If the **Ignore** option is selected:

\[
\text{InChI=1/C5H12O2/c1-3-5(7)4(2)6/h4-7H,3H2,1-2H3}
\]

If the **Absolute** option is selected:

\[
\text{InChI=1/C5H12O2/c1-3-5(7)4(2)6/h4-7H,3H2,1-2H3/t4-,5+/m1/s1}
\]

If the **Relative** option is selected:

\[
\text{InChI=1/C5H12O2/c1-3-5(7)4(2)6/h4-7H,3H2,1-2H3/t4-,5+/s2}
\]

If the **Racemic** option is selected:

\[
\text{InChI=1/C5H12O2/c1-3-5(7)4(2)6/h4-7H,3H2,1-2H3/t4-,5+/s3}
\]
<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
</table>
| Narrow End of Wedge Points to Stereocenter | If the check box is selected, only a narrow end of a stereo bond between two stereocenters will be taken into account, and only one stereocenter will be defined in generated InChI string.  
If the check box is cleared, the program treats a stereo bond between two stereocenters as belonging to both stereocenters and having the same sense for both of them.  
EXAMPLE: Source structure is ![Chemical Structure Image](image)  
(2R,3S)-pentane-2,3-diol  
If the check box is selected:  
InChI=1/C5H12O2/c1-3-5(7)4(2)6/h4-7H,3H2,1-2H3/t4-,5?/m1/s1  
If the check box is cleared:  
InChI=1/C5H12O2/c1-3-5(7)4(2)6/h4-7H,3H2,1-2H3/t4-,5-/m1/s1 |

 Displays the short reference information about the IUPAC International Chemical Identifier (InChI™).

More information about InChI is available on the IUPAC website at [www.iupac.org/inchi](http://www.iupac.org/inchi).

### 3.12.24 Generate > Structure from InChI

This command displays the Generate Structure from InChI dialog box where you can enter the InChI (IUPAC International Chemical Identifier) string from which chemical structure(s) will be generated.

<table>
<thead>
<tr>
<th>Note</th>
<th>This command is available in both Structure and Draw modes.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tip</td>
<td>You can also generate structures from InChI notations selected in the ChemSketch window by choosing this command. The structures will be placed below the string. You can quickly paste the structure generated from InChI with the Paste &gt; Structure command in case the Clipboard contains an InChI notation (for more information, refer to Section 3.10.8).—New to 12.0!</td>
</tr>
</tbody>
</table>

More information about InChIs is available on the IUPAC website at [www.iupac.org/inchi](http://www.iupac.org/inchi).

### 3.12.25 Search for Structure

*Commercial version only!*

This command displays the ACD/Search for Structure window where you can search for selected chemical structure(s) in a variety of file formats without opening the files.

The following formats are supported:
- ACD/ChemSketch 2.0 Document (.SK2)
- MDL Molfile (.MOL)
- MDL SDfile (.SDF)
- ISIS/Sketch (.SKC)
- CambridgeSoft ChemDraw (.CHM; .CDX)
- Adobe Portable Document Format (.PDF) (created with ACD/Labs software)
- MDL RXNfiles (.RXN)
- Microsoft Word Document (.DOC)
- Microsoft Excel Document (.XLS)
- Microsoft PowerPoint Document (.PPT)
- Portable Network Graphics (.PNG)
- ACD/SpecManager Database (.NDB; .ND5; .ND8; .ND9)
- ACD/ChemFolder Database (.CFD)
- ACD/HNMR User Database (.HUD)
- ACD/CNMR User Database (.CUD)
- ACD/C+HNMR Predictors User Database (.NMRUDB)
- ACD/XNMR (X = F, P, N) Database (.XDB)
- ACD/PhysChem User Database (.PCD)
- ACD/LogP User Database (.LUD; .LU8)
- ACD/pKₐ User Database (.PUD)
- ACD/Solubility User Database (.SUD)
- ACD/ChromGenius User Database (.CGB)
- ACD/C+HNMR Predictor Internal Database (.INT)
- ACD/LogP Internal Database (.INT)
- ACD/pKₐ Internal Database (.INT)
- ACD/Solubility Internal Database (.INT)
The window contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Title bar</strong></td>
<td>Shows the name of the program and buttons controlling the size and position of the window (for more information on the title bar, refer to Section 2.3).</td>
</tr>
<tr>
<td><strong>Search Pattern</strong></td>
<td>Displays the structure(s) to search for in the files specified in the Look In area.</td>
</tr>
<tr>
<td><strong>Look In</strong></td>
<td>Select the check boxes against those folders that you want to search through. If you select the check box against a disk, all of the folders on this disk will be searched.</td>
</tr>
<tr>
<td><strong>File Formats box</strong></td>
<td>In this box, you can specify the mask for the files to be searched through. You can either type it manually or click the Browse button to the right of the box. In the Look Through Files dialog box that appears, choose the formats to be included into the search and set the file mask. For more details on this dialog box options, refer to Section 3.12.25.1.</td>
</tr>
<tr>
<td><strong>Preview</strong></td>
<td>This area displays the structure found by your query in the file currently highlighted in the Search Results list (only the structure rather than the entire page or the entire document). Click Open to display the shown structure either in ACD/ChemSketch or in any other selected application (depending on the option selected on the Open tab of the Search Options dialog box). For more information, refer to Section 3.12.25.1.</td>
</tr>
<tr>
<td><strong>Search Results</strong></td>
<td>This area displays the list of files where the query structure has been found. You can double-click pathname of any file from the list to open it either in ACD/ChemSketch or in any other selected application (depending on the option selected on the Open tab of the Search Options dialog box (for more information, refer to Section 3.12.25.2).</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>-------------</td>
</tr>
<tr>
<td>Search</td>
<td>Starts searching. As you initiate the search, the button is replaced by the Stop button which allows you to interrupt the search process and display the search results obtained so far.</td>
</tr>
<tr>
<td>Options...</td>
<td>Displays the Search Options dialog box where you can specify search conditions (for more information, refer to Section 3.12.25.2).</td>
</tr>
<tr>
<td>Load...</td>
<td>Displays the Load Search Results dialog box where you can specify the name and location of a previously saved ACD/Search for Structure file (.SSF) containing search data.</td>
</tr>
<tr>
<td>Save...</td>
<td>Displays the Save Search dialog box where you can specify the name and location of the ACD/Search for Structure file (.SSF) the search data are to be saved to. The file will include the structure(s) to be searched, the folder and the file mask settings, as well as the search results (if any).</td>
</tr>
</tbody>
</table>

**Status bar**

Contains the following information:
- Files Processed: 276
- Entries Found: 13
- Structures Compared: 8236
- Search Complete
- Search Saved
- Search Results Loaded
- Search Cancelled

- **Close** Closes the window. Before the ACD/Search for Structure window is closed, the program prompts you to save the changes to the search settings.
- **About** Displays information about your copy of ACD/Labs package, including the version number, the copyright, and user registration information. This also contains information on how to contact ACD/Labs. Moreover, by clicking the License ID button you can see your license ID number(s)—you will need the ID number(s) in case our technical support is required.

As the (set of) structure(s) is found, it can be viewed and placed either into the ChemSketch window or to the other applications.

If there are any results displayed in the Search Results box, and you want to start a new search, a message appears prompting you to confirm whether to perform a new search or not.

**Shortcuts:**

- Keyboard: CTRL+SHIFT+C
- General toolbar: ![License ID button]

### 3.12.25.1 Look Through Files Dialog Box

In this dialog box, you can select the formats of files to be searched through and set the file mask for each format.

To display the dialog box, in the File Formats box of the ACD/Search for Structure window, click [Browse button].
The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>List of Formats</td>
<td>Displays the formats (with the specified mask in broken brackets) supported by the ACD/Search for Structure module. To add a format to the list of files to be searched through, select the corresponding check box.</td>
</tr>
<tr>
<td>Change Mask...</td>
<td>Select the format you want to set a mask for, and then click this button to display the Change File Mask dialog box. Restrict your search through the files of the selected format to certain names by defining their mask(s)—for example, enter but* to search only the files whose names start with &quot;but&quot;. You can specify several masks separated by a comma. Note that you don’t need to type extensions because the mask will be applied to the selected file format only.</td>
</tr>
<tr>
<td>Clear Mask</td>
<td>Clears the mask(s) set for searching through the files of the format selected in the list. After that, all files of the corresponding format will be searched through.</td>
</tr>
<tr>
<td>Select All</td>
<td>Selects all of the file check boxes in the list. In this case, files of all types will be searched through. The masks specified for the formats will be taken into account.</td>
</tr>
<tr>
<td>Unselect All</td>
<td>Clears all of the check boxes in the list.</td>
</tr>
</tbody>
</table>

Note: For PDF format, you can search through the files generated by means of ACD/ChemSketch only—all other files are ignored.

### 3.12.25.2 Search Options Dialog Box

**Commercial version only**

In this dialog box, you can define the preferences for searching.

To display the dialog box, in the ACD/Search for Structure window, click **Options** (for more information on the window, refer to Section 3.12.25).
The dialog box contains two tabbed pages. To switch between them, click the corresponding tab.

**General tab**

On the **General** tab, you can specify the desired type of structural search and the amount of query structure occurrences to be searched in every file.

The tabbed page contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Search Type</strong></td>
<td>In this area, choose the type of structural search you want to be performed through files of specified formats:</td>
</tr>
<tr>
<td><strong>Exact Search</strong></td>
<td>Select this option to search for structures exactly matching the one(s) displayed in the <strong>Search Pattern</strong> box of the ACD/Search for Structure window.</td>
</tr>
<tr>
<td><strong>SubStructure Search</strong></td>
<td>Select this option to search for structures containing the one(s) displayed in the <strong>Search Pattern</strong> box of the ACD/Search for Structure window as their structural fragment(s). Note that you can use the Query Atom and Query Bond tools to define the search pattern (for more information, refer to Section 3.7.1–3.7.2).</td>
</tr>
<tr>
<td><strong>Similarity Search</strong></td>
<td>Select this option to search for structures similar to the one(s) displayed in the <strong>Search Pattern</strong> box of the ACD/Search for Structure window. To specify the settings for structural similarity, click the adjacent <strong>Options...</strong> button. In the <strong>Similarity Search Options</strong> dialog box that appears, you can choose among the following similarity coefficients: <strong>Tanimoto</strong>, <strong>Dice</strong>, <strong>Cosine</strong>, <strong>Based on Hamming Distance</strong>, <strong>Based on Euclidean Distance</strong>. For more information on the dialog box, refer to Section 3.12.25.3.</td>
</tr>
<tr>
<td><strong>Prompt to Save Changes</strong></td>
<td>If this check box is selected, each time you close the ACD/Search for Structure window, the program prompts you to save results of the last search to an ACD/Search for Structure file (.SSF) if you have not done so.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>------------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Search Within File</strong></td>
<td>In this area, you can define when the search within every specific file should be stopped:</td>
</tr>
<tr>
<td><strong>Until First Occurrence</strong></td>
<td>If you select this option, the program will stop searching within a specific file as soon as at least one matching structure is found in this file, and then the program will proceed with searching through the next file.</td>
</tr>
<tr>
<td><strong>All Occurrences</strong></td>
<td>If this option is selected, the program will find all occurrences of the query structure in each file and will display each found structure as a separate string in the Search Results box.</td>
</tr>
<tr>
<td><strong>Preview Cache Size</strong></td>
<td>In this box, you can specify the number of pages to be stored in cache. To speed up the display of the found structures, the pages displayed last in the Preview box are stored in cache and if you later view the same page, its display is taken from cache.</td>
</tr>
</tbody>
</table>

**Open Tab**

On the Open tab, you can specify applications to be used for loading files of different formats as you click Open in the Preview box of the ACD/Search for Structure window.

![Image of Search Options]

The tabbed page contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>List of Formats</strong></td>
<td>Displays the file formats that are currently supported by ACD/ChemSketch.</td>
</tr>
<tr>
<td><strong>Action</strong></td>
<td>In this area, specify which application should be used to open files of the selected format:</td>
</tr>
<tr>
<td><strong>Start Associated Program</strong></td>
<td>If this option is selected, the files of the selected format will be opened in the program currently associated with that format in the Windows system. When you select a format name in the list, the pathname of the associated application indicated below this option is changed accordingly.</td>
</tr>
<tr>
<td><strong>Start Another Program</strong></td>
<td>If this option is selected, you can specify the program (EXE file) that should be used to open the corresponding files (this does not affect the Windows file registration settings).</td>
</tr>
<tr>
<td><strong>Open in</strong></td>
<td>If this option is selected, the found structure will be placed into the</td>
</tr>
</tbody>
</table>
### 3.12.25.3 Similarity Search Options Dialog Box

*Commercial version only*

In this dialog box, you can specify settings for searching structures similar to the one(s) currently selected in the ChemSketch window.

To display the dialog box, in the **Search Options** dialog box, click **Options...** (for more information on the window, refer to Section 3.12.25.2).

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Select Similarity Coefficient</strong></td>
<td>Displays the list of similarity coefficients that can be applied during the similarity search. To apply the desired coefficient, select its check box.</td>
</tr>
<tr>
<td><strong>Show with Coefficient &gt;=</strong></td>
<td>In this box, specify the similarity coefficient that will serve as a filter for the found structures. During the similarity search, the program generates similarity coefficients for each structure; the structures having coefficients more than or equal to the value specified in this box will be announced as hits for your query.</td>
</tr>
</tbody>
</table>

### 3.12.26 Calculate > <Property Name>

This set of commands allows you to calculate one of the physicochemical properties for the currently selected structure or fragment.

---

**Note**  For more details on each property, refer to Appendix B.

The following `<Property Name>` commands properties are available on the menu:

- Molecular Formula
- Formula Weight
- Composition
- Molar Refractivity
• Molar Volume
• Parachor
• Index of Refraction
• Surface Tension
• Density
• Dielectric Constant
• Polarizability
• Monoisotopic, Nominal, and Average Mass
• $M^+$
• $M^-$
• $[M+H]^+$
• $[M+H]^-$
• $[M-H]^+$
• $[M-H]^-$

After you choose one of the commands, the corresponding property is calculated for the structure, and the Calculation Results dialog box appears displaying the data value.

To place the results of calculation in the ChemSketch window near the structure:

• In the dialog box, click Copy to Editor. Note that the window is automatically switched to the Draw mode.

If there are several structures drawn in the workspace and none is selected, the property is calculated for all of the structures (treating them as one composite structure), if possible. If it is failed to calculate a property, the value displayed in the dialog box will be Not available.

Tip
You can choose one of the properties to be instantly displayed on the status bar for the selected structure (for more information, refer to Section 2.6).

3.12.27 Calculate > All Properties

This command allows you to calculate all of the available physicochemical properties for the currently selected structure or fragment.

After you choose the command, the properties are calculated for the structure, and the results are listed in the Calculation Results dialog box that appears.

Among the results of calculation, you can specify the data to be placed by the structure:

• Holding down CTRL, click the desired properties in the list to select them, and then click Copy to Editor. Note that the window is automatically switched to the Draw mode.

3.12.28 Calculate > Select Properties to Calculate

This command allows you to define the physicochemical properties to be calculated by choosing the Calculate > Selected Properties command (for more information, refer to the section that follows).

As you choose this command, the Select Properties to Calculate dialog box appears:
The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Properties</strong></td>
<td>This box lists the names of all available physicochemical properties. To define the properties to be calculated, select the check boxes adjacent to the required property names.</td>
</tr>
<tr>
<td><strong>Select All</strong></td>
<td>Selects check boxes for all of the property names in the list.</td>
</tr>
<tr>
<td><strong>Unselect All</strong></td>
<td>Clears check boxes for all the property names in the list.</td>
</tr>
</tbody>
</table>

### 3.12.29 Calculate > Selected Properties

This command calculates the physicochemical properties selected in the Select Properties to Calculate dialog box (for more information, refer to the previous section) for the currently selected structure or fragment.

After you choose the command, the properties are calculated for the structure, and the results are listed in the Calculation Results dialog box that appears.

Among the results of calculation, you can specify the data to be placed by the structure:

- Holding down CTRL, click the desired properties in the list to select them, and then click **Copy to Editor**. Note that the window is automatically switched to the Draw mode.
3.13 Templates Menu

The commands located on this menu allow you to insert predefined, standard structures and graphical objects into your drawing and/or to create your own templates of commonly used structures or graphical objects.

3.13.1 Template Window

This command allows you to place any template unit into the ChemSketch page. Templates can contain structures and structural fragments as well as graphical objects.

Choosing this command displays the **Template Window** dialog box that includes the contents of available templates, either standard (built-in) or custom (user-defined).

![Template Window Dialog Box](image)

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Structure</strong></td>
<td>Click the desired button to choose either the Draw or Structure mode. This mode will be activated when you place the selected template structure / object on the ChemSketch page. Note that auto switching of the program to the Structure mode is not applicable for graphical objects—they will always be pasted in the Draw mode.</td>
</tr>
<tr>
<td><strong>Template box</strong></td>
<td>This box contains names of all template sets listed in the <strong>Template Organizer</strong> (for more information, refer to Section 3.13.2). To load a template set to the Preview area, select its name from the list.</td>
</tr>
<tr>
<td><strong>Page box</strong></td>
<td>In this box, you can choose the desired page of a multi-page template set.</td>
</tr>
</tbody>
</table>
### Option

<table>
<thead>
<tr>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Click these buttons to browse to the previous / next page to page within the multi-page template set.</td>
</tr>
<tr>
<td>Displays the <strong>User Template Window Organizer</strong> dialog box where you can manage template sets (for more information, refer to Section 3.13.2).</td>
</tr>
</tbody>
</table>
| This area contains tabs of the template sets currently available in the Preview area. To activate any of the sets, click the corresponding tab. The area is divided horizontally in two parts:  
  - The upper part displays the list of "fixed" template sets, *i.e.*, the sets whose names are displayed in this area every time you open the dialog box. You can specify up to 10 "fixed" template sets by selecting them in the **User Template Window Organizer** dialog box (for more information, refer to Section 3.13.2).  
  - The lower part displays the list of template sets that have been recently chosen from the Template box at the top of the window. If you use some sets frequently and want them to be available in the dialog box every time you open it, place them into the "fixed" list above by selecting names of the template sets in the **User Template Window Organizer** dialog box (for more information, refer to Section 3.13.2). |
| Displays the contents of the currently selected template set. |

---

**To insert a template chemical structure/graphical object in the ChemSketch page:**

1. In the **Template Window** dialog box, click **Structure** or **Draw** to indicate which drawing mode is to be active when you place the selected template on the ChemSketch page.
   
   **Note**  
   Automatic switching of the program to the Structure mode is not applicable for graphical objects—they will always be pasted in the Draw mode.

2. Load a necessary template set to the Preview area.
   
   **Tip**  
   If there is more than one page in the set, switch to a desired page by clicking the **Previous Page** and **Next Page** buttons.

3. Click a template item. The program closes the dialog box and switches the ChemSketch window to the previously selected drawing mode (depending on which button is selected on the Template toolbar), a template outline being attached to the mouse pointer.
   
   **Important**  
   If you are going to use a template of a chemical structure to attach it to the already drawn structure, make sure that you select the template by clicking the most proper **atom** or **bond**. For example, if you are going to insert a structure fused with a specific bond, select the corresponding template by clicking the bond (not the atom).

4. Click in the workspace to paste the copied template item. Every time you click, you place another instance of the structure/graphical object in the workspace.
   
   **Note**  
   If the item is a structure or fragment, it attempts to attach itself to the appropriate location as you move it over an existing structure; simply click to place it at the insertion point.

---

To cancel operating with a selected template, use one of the following ways:

- Click any button on any toolbar of the ChemSketch window; or
- Right-click in the workspace.
In the latter case, the corresponding Select/Move tool is enabled on the Structure toolbar (depending on the currently active drawing mode).

**Tip** You can flip the template outline by pressing TAB.

When inserting template of a chemical structure, the atom of the template will replace the atom you click (template will be attached without creating a bond) if you click an atom of the drawn structure while holding down SHIFT.

**Shortcuts:**

Keyboard: F5

General toolbar:

3.13.2 Template Organizer

This command displays the **User Template Window Organizer** dialog box where you can manage the standard (built-in) and custom (user-defined) template sets: create a template set, change the name of the SK2 file associated with a template set, and remove, rename, and modify the set’s contents.

**Tip** This dialog box can also be displayed by clicking **Organizer** in the **Template Organizer** dialog box (for more information, refer to the previous section).
The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Templates</td>
<td>This box lists the names of available template sets, depending on the option selected to the right of it:</td>
</tr>
<tr>
<td>Standard</td>
<td>If this option is selected, the names of standard (built-in) template sets are only displayed in the box.</td>
</tr>
<tr>
<td>User</td>
<td>If this option is selected, the names of custom (user-defined) template sets are only displayed in the box.</td>
</tr>
<tr>
<td>All</td>
<td>If this option is selected, the names of both standard and custom template sets are displayed in the box.</td>
</tr>
</tbody>
</table>

The names with selected check boxes are included into the list of "fixed" template sets in the Template Tabs area of the Template Window dialog box, i.e., the sets whose names are displayed in this area every time you open the dialog box. Note that only ten template sets can be placed as "fixed" at a time.

| Fixed / Available | This area displays the number of templates placed to the Template Window dialog box (Fixed) and the number of templates which can be added thereto (Available). Note that there can be up to 10 "fixed" templates placed simultaneously. |

| New...         | Displays the Create User Template dialog box where you can specify the name and location of the file to be used as a template set and enter name for the new set. As you click OK, the template set will be added to the Templates box. |
| Modify...      | Choose the name of a template set from the list and click this button to display the Modify Template dialog box where you can edit the template set name and a file serving as a template. |
| Remove         | Removes highlighted name of a template set from the list. Note that this action removes only the reference to the corresponding ACD/ChemSketch document, but not the file itself. |
| Open Document  | Loads the ACD/ChemSketch document associated with the highlighted name of a template set into the ChemSketch page for editing. |
| c:\acd\template\amnacid.sk2 | This field displays the location of the ACD/ChemSketch document associated with the name of a template set highlighted in the list. |

Note that the only difference between the template and standard ACD/ChemSketch files is the fact that you can find the template file in the User Template Window Organizer dialog box. In fact, it is the same as a regular document with the extension .SK2. By saving files this way there are several advantages:

- Your .SK2 files scattered over different locations will be gathered in the Template Window Organizer.
- You can assign a name to the template that is more descriptive than what the real file name is. This will better reflect the contents of the document and allow you to find the document quickly. Besides, you can quickly find the desired document by previewing its contents in the Preview area of the Template Window dialog box (for more information, refer to Section 3.13.1).

3.13.3 Save User Template

This command allows you to save the current ACD/ChemSketch document as a user template. If your document has not been saved before, the Save Document As dialog box appears where you can specify the name and location of the .SK2 file to be used as a template set. As soon as
you save the document, the **Save User Template** dialog box appears where you should specify the name for the new template set to be associated with your ACD/ChemSketch document.

As soon as the document is saved as a template set, a new tab with its name is added to the lower part of the Template Tabs area of the **Template Window** dialog box, as well as to the list of user template sets of the **Template Organizer** dialog box (for more information, refer to Sections 3.13.1 and 3.13.2, respectively).

### 3.13.4 Table of Radicals

This command displays the **Table of Radicals** panel containing the most frequently needed templates of radicals for a quick drawing of chemical structures.

When you point to a radical button, the corresponding structural fragment appears in the Preview area.

**Note**  The R-symbol in the radical structure denotes the position of attachment to other structures in the workspace of the ChemSketch window.

To choose a radical for drawing, click the required radical button. The **Table of Radicals** will be closed, and the radical’s outline will be attached to the mouse pointer:

- To insert a separate structure based on a chosen radical, click in the blank part of the workspace. Note that the R-symbol will be substituted by hydrogen atom in this case.
- To create a bond between a drawn structure and a chosen radical, click any atom in the structure.
- To replace an atom of a drawn structure with an atom neighboring to the R-symbol in a chosen radical template (*i.e.*, the radical will be attached without a bond), click the atom in the structure while holding down SHIFT.
Tip You can flip the template outline by pressing TAB. You can use the template as many times as you want until you right-click in the workspace to cancel this mode and switch to the Select/Move mode.

When a template of radical is chosen from the Table of Radicals, the corresponding button is automatically added to the References toolbar (for more information, refer to Section 3.8).

To remove all of the radical buttons from the References toolbar, double-click an empty space on the toolbar, and then, in the warning message that appears, click Yes.

Shortcuts:

Keyboard: F6

References toolbar: 

3.13.5 Periodic Table

This command displays the Periodic Table of Elements dialog box. This dialog box allows you to choose a new element for drawing and view the detailed information (symbol, name, atomic number, density, mass, typical valence or oxidation states and electron configuration) on it.
Note that depending on the state of the Change Navigation Mode button the work with this dialog box is slightly different:

### State of the Change Navigation Mode button

<table>
<thead>
<tr>
<th>Action</th>
<th>pulled position</th>
<th>pushed position</th>
</tr>
</thead>
<tbody>
<tr>
<td>To highlight an element and display the photo and detailed information about it</td>
<td>point to the desired element</td>
<td>click the desired element</td>
</tr>
<tr>
<td>To be able to insert the selected element into the workspace</td>
<td>click the desired element</td>
<td>click OK</td>
</tr>
</tbody>
</table>

You can do one of the following with the chosen element:

- Click an empty space to insert the atom at the insertion point.
- Point to any atom in the workspace and drag it to an empty place on the screen. A new bond appears with the chosen atom at the end.
- With the Draw Normal tool (for more information, refer to Section 3.6.5), click any atom in the drawing area to replace it with the chosen atom.
- With the Draw Continuous tool (for more information, refer to Section 3.6.6), double-click an atom to sprout a new single bond with the chosen atom.

Periodic Table of Elements contains images of all stable chemical elements in their natural form. To display the photo of an element, in the Periodic Table of Elements, click Show Photos of an Element, and then point to or click the required element (depending on the position of the Change Navigation Mode button).

**Tip**

To keep the photo of an element upon all of the windows, the Always on Top button should be in pushed position.

Periodic Table of Elements is expanded with tabs that include the following data:

- **General** tab: general data about an element;
- **NMR** tab: isotope, spin number, abundance, magnetic moment, magnetogyric ratio, quadrupole moment, frequency, and receptivity;
- **Mass** tab: isotope, abundance, and exact mass;
- **Coloration** tab: options allowing you to apply the coloration of four different schemes (Classic, Aggregative States, Metals/Non-metals, or Radioactivity) or discard the coloration at all.

If the tabs are not visible, click Show/Hide Extra Data. The tabs are displayed by default.

When an atom is taken from the Periodic Table of Elements dialog box, its button is automatically added on the Atoms toolbar (for more information, refer to Section 3.7). To remove the user-selected atoms from the Atoms toolbar and return to the original default set, double-click an empty space on the toolbar, and then click Yes in the message that appears.

**Note**

For non-metals, the inserted atom appears in its lowest valence state as a hydride derivative, whereas for metals, the inserted atom appears in its lowest oxidation state as an ion.

**Shortcuts:**

Keyboard: F7

Atoms toolbar: 

---

**Structure Mode**

ACD/ChemSketch Reference Manual 110
3.13.6 Dictionary

Commercial version only!

This command displays the ACD/Dictionary dialog box.

ACD/Dictionary is a program from ACD/Labs which allows you to find chemical structures according to their systematic or non-systematic names (as well as according to the parts of name), therapeutic category or inhibited enzymes, and registry numbers. You can copy these structures to other ACD/Labs programs and to Windows applications.

If there is structure(s) drawn or selected in the workspace and the Auto Search Structure option is selected in a shortcut menu (to display the menu, click an icon on the title bar), choosing this command will display the dialog box asking for whether you want to search for the drawn structure in the dictionary.

Note The ACD/Dictionary module is only included in the commercial version of ACD/ChemSketch and is not available with the freeware.

For more details on the functionality of the ACD/Dictionary, refer to ACD/Dictionary User’s Guide located in the ACD/Labs documentation folder (\DOCS\DICT.PDF).

Shortcuts:

Keyboard: F8
References toolbar: 

ACD/ChemSketch Reference Manual 111
3.14 Options Menu

These menu commands allow you to set on-screen viewing options: adjust the view of the cursor, border, on-screen grid, and color palette. They also allow you to change angles, bond length, and 3D optimization features.

3.14.1 Preferences

This command displays the Preferences dialog box where you can set preferences for functionality in ACD/ChemSketch.
3.14.1.1 Preferences Dialog Box: General Tab

On this tab, you can define settings common for both Structure and Draw mode:

![Preferences Dialog Box: General Tab]

The tab contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>View</td>
<td>In this area, you can specify the objects to be displayed: The <strong>Ruler</strong> check box switches on/off the display of the ruler. The rulers are useful for determining the size and position of objects. The <strong>RSS</strong> check box switches on/off the display of the RSS News bar. For more information on the RSS options, refer to Section 2.5.1. The <strong>Guides</strong> check box switches on/off the display of the guide lines that appear on both rulers indicating the cursor position, thus its coordinates can be accurately identified. Note that this option is available if the <strong>Ruler</strong> check box is selected. The <strong>Palette</strong> check box switches on/off the display of the Color palette (refer to Section 2.4). In the <strong>Measurement Units</strong> box, specify the units to be used for measurements in all dialog boxes.</td>
</tr>
</tbody>
</table>

---

"ACD/ChemSketch Reference Manual" 113
<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Borders</td>
<td>Select the <strong>Printable Area</strong> check box to display the dotted lines showing the borders of the printable area. Note that the margins of the printable area vary depending on the printer. Select the <strong>Page Margins</strong> check box to display the dotted lines showing the margins of the page. You can set the margins in the <em>Page Setup</em> dialog box (<em>File</em> menu).</td>
</tr>
<tr>
<td>Highlight Color</td>
<td>In this box, you can specify the color to be used for highlighting when you point to structure elements and drawing objects.</td>
</tr>
<tr>
<td>Grid</td>
<td>Allows you to specify the way the grid should be arranged: in the form of rectangles vertically hexagonally horizontally hexagonally</td>
</tr>
<tr>
<td>Visible</td>
<td>This check box controls whether to show or hide the grid. This is also controlled by the <strong>Show Grid</strong> command (<em>Options</em> menu).</td>
</tr>
<tr>
<td>Snap on Grid</td>
<td>If this check box is selected, objects &quot;stick to&quot; (become automatically aligned with) the grid (either visible or not) when you move or create them. This is also controlled by the <strong>Snap On Grid</strong> command (<em>Options</em> menu). Note that if this option is enabled, the <strong>Fixed Bond Length</strong> and <strong>Bond Angle</strong> features (<em>Structure</em> tab) are ignored.</td>
</tr>
<tr>
<td>Horizontal Step / Vertical Step</td>
<td>In the <strong>Horizontal Step</strong> box, you can specify the horizontal distance* between the grid points of the rectangular or horizontally hexagonal grid. In the <strong>Vertical Step</strong> box, you can specify the vertical distance between points for rectangular or vertically hexagonal grid.*</td>
</tr>
<tr>
<td>Keep Draw Tool Active</td>
<td>If this check box is selected, any of the drawing tools from the Drawing toolbar (except the <strong>Text</strong> tool) remains enabled until you click or right-click in the workspace. If this check box is cleared, the <strong>Select/Move/Resize</strong> tool becomes active every time after you have used a tool.</td>
</tr>
<tr>
<td>Informative Cursor</td>
<td>Controls whether to show or hide the informative cursor. This is a cursor showing the percentage of resizing, the new object’s coordinates when moving and rotating, the number of atoms in the chain when drawing the atom chains, etc.</td>
</tr>
<tr>
<td>Use Antialiasing</td>
<td>Select this check box to automatically remove the aliasing of drawn lines and curves.</td>
</tr>
<tr>
<td>Directories</td>
<td>In this area, you can specify the name of folders where some configuration information will be stored. In the <strong>Private</strong> box, you can specify the folder for recording the configuration of ChemSketch program (TEMPLATE.CFG and QRSTYLES.STL files). In the <strong>Default</strong> box, you can specify the folder which you want to become current for the first time when you open the <strong>Save As</strong>, <strong>Open</strong>, <strong>Import</strong>, or <strong>Export</strong> dialog boxes in current session.</td>
</tr>
</tbody>
</table>
3.14.1.2 Preferences Dialog Box: Structure Tab

On the **Structure** tab, you can define the preferences for the structures’ display and drawing.

The tab contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fixed</strong></td>
<td>In the <strong>Fixed</strong> area, you can control the structure drawing. If the <strong>Bond Angle</strong> check box is selected, you will be able to draw bonds at an angle multiple to 15°. If the <strong>Bond Length</strong> check box is selected, you will be able to draw bonds of a length multiple to the value specified in the adjacent box. If you find any of these check boxes unavailable, it can mean that the <strong>Snap on Grid</strong> check box is selected on the <strong>General</strong> tab of this dialog box. To make the check boxes in the <strong>Fixed</strong> area available, clear the <strong>Snap on Grid</strong> check box.</td>
</tr>
<tr>
<td><strong>Action Center</strong></td>
<td>Select this check box to view the special sign showing the center of rotation or resizing when you use the <strong>Select/Rotate/Resize</strong> tool. This will help you see the point relative to which the objects are resized or rotated.</td>
</tr>
<tr>
<td><strong>Template Shadow</strong></td>
<td>If this check box is selected, the shadow of the template structure will be displayed near the cursor when you use the <strong>Instant Template</strong> tool or use templates from the <strong>Table of Radicals</strong> or <strong>Template Window</strong>.</td>
</tr>
<tr>
<td><strong>Hidden Atoms</strong></td>
<td>If this check box is selected, the hidden atoms will be displayed when you point to them on the structure.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>-----------------------------</td>
<td>-----------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Proportional Resize</strong></td>
<td>If this check box is selected, the atom labels are resized in proportion to the bonds when the structure is resized. If it is not, the atom labels remain unchanged when the structure is resized.</td>
</tr>
<tr>
<td><strong>Wireframe 3D Rotation</strong></td>
<td>If this check box is selected, all of the bonds, single as well as the others, will be viewed as single bonds while 3D-rotating. If you want to view the structure as it was drawn (with all bond types remaining unchanged) while 3D-rotating, clear this check box.</td>
</tr>
<tr>
<td><strong>Select Graphics</strong></td>
<td>If this check box is selected, in the Structure mode, it is possible to select, move, and resize objects created in the Draw mode (text, shapes, arrows, etc.), as well as reaction plus and arrows. If this check box is cleared, you can only manipulate structures in the Structure mode.</td>
</tr>
<tr>
<td><strong>Auto-Select Bonds</strong></td>
<td>If this check box is selected, as you hold down SHIFT and click two atoms or bonds with the Select/Move tool or Select/Rotate/Resize tool active, the bond between them is also selected. If this check box is cleared, you can select atoms or bonds by holding down SHIFT and clicking them separately (so that it is possible to leave a bond unselected if its neighbors are selected). Besides, if you hold down SHIFT and click a selected bond, the neighbors remain selected.</td>
</tr>
<tr>
<td><strong>Auto-Stick Atoms</strong></td>
<td>Select this check box if you want atoms or bonds to be automatically stuck either in the Move or Template modes (refer to Sections 3.6.1 and 3.6.26), or when you paste a structure from the Clipboard. Note that one atom sticks to the cursor in any mode. The mode is inverted by pressing CTRL and vice versa.</td>
</tr>
<tr>
<td><strong>Bond Intersections</strong></td>
<td>In the Bond Intersection area, you can control the intersection point of bonds. If you select the Enable check box, ACD/ChemSketch automatically makes a kind of gap in the background bond (drawn first of the two intersecting bonds). You can specify the size of a gap in the background bond in the White Space box.</td>
</tr>
<tr>
<td><strong>3D-Optimization</strong></td>
<td>In this area, select the Switch to 3D-Rotation Mode check box if you want the 3D Rotation tool (refer to Section 3.6.3) to be automatically enabled after the 3D optimization is complete. Select the Add Hydrogens check box if you want the hydrogens to be added to the structure after the 3D optimization is complete. For more details on the 3D Optimization tool, refer to Section 3.12.4.</td>
</tr>
<tr>
<td><strong>Markush Shadow</strong></td>
<td>In this area, you can adjust the options for Markush bonds. These options are especially useful if some of the atoms in a structure participate in two or three Markush bindings. You can select the color and shading for atoms participating in a primary (created first), secondary (created second), and tertiary (created third) Markush binding. To make the Markush shadow available in other ACD/Labs software, e.g., in all databases, select the Show in Other ACD Software check box.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>-------------------------------</td>
<td>-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Keep Stereo Configuration on</strong></td>
<td>In this area, select the <strong>Clean</strong> check box to keep the configuration of stereo centers unchanged when applying the <strong>Clean Structure</strong> command. For example:</td>
</tr>
<tr>
<td></td>
<td><img src="image" alt="The Clean check box is selected" /> <img src="image" alt="The Clean check box is cleared" /></td>
</tr>
<tr>
<td></td>
<td>Select the <strong>Flips</strong> check box to keep the configuration of stereo centers unchanged when using the <strong>Flip on Bond</strong>, <strong>Flip Top to Bottom</strong>, or <strong>Flip Left to Right</strong> tools. For example, when you apply the <strong>Flip Left to Right</strong> tool, the following result will be obtained:</td>
</tr>
<tr>
<td></td>
<td><img src="image" alt="The Flips check box is selected" /> <img src="image" alt="The Flips check box is cleared" /></td>
</tr>
<tr>
<td><strong>Auto/Manual Numbering Color</strong></td>
<td>In this box, you can specify the color of atom numbers inserted either manually or automatically. For the details on atom numbering, refer to Sections 3.12.14 and 3.7.8.</td>
</tr>
<tr>
<td></td>
<td><img src="image" alt="Image" /></td>
</tr>
</tbody>
</table>
3.14.1.3 Preferences Dialog Box: Reaction Tab

On the Reaction tab, you can customize the appearance of reaction elements.

The tab contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Character</td>
<td>In this area, you can specify the text style for reaction pluses (for more information, refer to Section 3.6.14).</td>
</tr>
<tr>
<td>Pen</td>
<td>In this area, you can set the view for lines in the reaction arrows (refer to Section 3.6.15). Choose the required style, width, and color from the corresponding boxes.</td>
</tr>
<tr>
<td>Arrowhead Size</td>
<td>In this area, you can set the view of arrowheads in the reaction arrows (refer to Section 3.6.15). You can specify the arrowhead width and height either by clicking/dragging in the preview area or by specifying the values in the W (width) and H (height) boxes.</td>
</tr>
<tr>
<td>Double</td>
<td>In this area, you can specify the space between the lines of a double reaction arrow. Choose the required sample in the Interval box.</td>
</tr>
<tr>
<td>Standard</td>
<td>In this area, you can set the default length of a reaction arrow. Type the required value in the Length box.</td>
</tr>
<tr>
<td>Manual Mapping Color</td>
<td>In this box, you can select the appropriate color for manual mapping atom numbers (inserted using the Atom-Atom Map tool (refer to Section 3.6.18), Manual mode).</td>
</tr>
</tbody>
</table>
3.14.1.4 Preferences Dialog Box: Clean Tab

On the **Clean** tab, you can specify what method to use when applying the **Clean Structure** command.

You can choose the required method of structure representation by selecting the corresponding check boxes. If you select several check boxes, all of them will be applied one after another every time you click **Clean Structure** on the Structure toolbar, or choose the **Clean Structure** command from the **Tools** menu. For more information on this command, refer to Section 3.12.2.

If the **Use Template Library** check box is selected, the standard representation of atoms in polycyclic structures is applied.

As an example of clean methods, the structure of adamantane is given:

<table>
<thead>
<tr>
<th>Clean Method</th>
<th>Structure Representation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default Method without Template Library</td>
<td><img src="image" alt="Structure Representation" /></td>
</tr>
<tr>
<td>Default Method with Template Library</td>
<td><img src="image" alt="Structure Representation" /></td>
</tr>
<tr>
<td>Method 2</td>
<td><img src="image" alt="Structure Representation" /></td>
</tr>
<tr>
<td>Method 3</td>
<td><img src="image" alt="Structure Representation" /></td>
</tr>
</tbody>
</table>
3.14.2 Show Grid

This command allows you to display or hide grid lines in the workspace.

**Note**  To change the grid density and type, use the Preferences dialog box options (for more information, refer to Section 3.14.1.1).

**Shortcut:**

Keyboard:  CTRL+W

3.14.3 Snap on Grid

This command allows you to toggle the possibility to align objects according to the grid when moving, resizing objects, or creating new ones. Note that the grid can be enabled even if the grid lines are hidden.

In the Select/Move mode, if you click CTRL+SHIFT while moving (resizing, etc.) the objects, this command selection is ignored.

**Note**  To change the grid density and type, use the Preferences dialog box options (for more information, refer to Section 3.14.1.1).

**Shortcut:**

Keyboard:  CTRL+Q

3.14.4 Show Palette

This command allows you to switch on/off the display of the Color palette below the workspace. For more information on the Color palette options, refer to Section 2.4.

3.14.5 Show RSS

This command allows you to switch on/off the display of the RSS News bar. For more information on the RSS options, refer to Section 2.5.1.

Alternatively, you can switch on/off the display of the RSS News bar by selecting/clearing the RSS check box in the Preferences dialog box (General tab).

**Note**  You can hide RSS News bar in Commercial version only!

3.14.6 Set Structure Drawing Style Submenu

The commands on this submenu allow you to apply one of the available styles as default for drawing structures. The list of styles contains both the built-in journal styles and the user-defined styles. When choosing the required style, the message appears asking you whether or not you want to apply this style to drawn structures. If you click Yes, the selected style will be applied to all drawn structures on the active page, and to all structures that will be drawn afterwards on other pages and documents. If you click No, the already drawn structures will preserve their current view, and the selected style will be applied to the structures that will be drawn afterwards.

**Note**  You can define your own styles using the Properties panel (for more information, refer to Section 3.12.1).
3.14.7 Add-On Organizer

This command allows you to display the **Add-On Organizer** dialog box where you can specify the supplementary applications (add-ons) that are to be used to enhance the program's possibilities. The add-ons can be created by third-party developers and then added to the ACD/Labs software to enlarge its possibilities.

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>List of add-ons</strong></td>
<td>This box lists supplementary applications that can be used to enhance the program's possibilities. To edit the list, use the buttons to the right. Select the check boxes of those add-ons that are to be added to the <strong>Add-Ons</strong> menu and/or Top toolbar (if this is specified in the add-on's properties). To select/deselect all add-ons, right-click within the box, and then from the shortcut menu that appears, choose the corresponding command. Note that by default all of the commands are selected. The application of any add-on can be specified while its creation.</td>
</tr>
<tr>
<td><strong>Add...</strong></td>
<td>Displays the Open dialog box where you can specify the name and location of an ADDON file (.ADDON) that is to be added to the list.</td>
</tr>
<tr>
<td><strong>Edit...</strong></td>
<td>Displays the dialog box where you can edit the properties of the add-on selected in the list.</td>
</tr>
<tr>
<td><strong>Delete</strong></td>
<td>Removes the add-on selected in the list.</td>
</tr>
<tr>
<td><strong>Add-on location</strong></td>
<td>This box displays the location of the add-on currently selected in the list.</td>
</tr>
<tr>
<td><strong>Add-on description</strong></td>
<td>In this box, view the description of the add-on selected in the list above.</td>
</tr>
</tbody>
</table>
### 3.14.8 ChemBasic Organizer

This command allows you to manage programs written in ACD/ChemBasic (a special programming language that enables the user to customize ACD/Labs software). Choosing this command displays the **ChemBasic Organizer** dialog box where you can add ChemBasic programs to be run from the ChemSketch window, create a shortcut button for each program, and attach a hint to each button.

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Installed Programs</strong></td>
<td>Displays a list of installed ChemBasic programs. To install/uninstall programs, use the button to the right of this list. To add shortcut buttons of the corresponding programs to the ChemSketch toolbar, select their check boxes.</td>
</tr>
<tr>
<td><strong>New...</strong></td>
<td>This button allows you to install a ChemBasic program and add its name to the list. Clicking this button displays the <strong>ChemBasic Program</strong> dialog box where you can specify the program, its shortcut button, and hint. For more information, refer to Section 3.14.8.1.</td>
</tr>
<tr>
<td><strong>Modify...</strong></td>
<td>This button allows you to modify the name, shortcut, or location of the program currently highlighted in the list. Clicking this button displays the <strong>ChemBasic Program</strong> dialog box. For more information, refer to Section 3.14.8.1.</td>
</tr>
<tr>
<td><strong>Delete</strong></td>
<td>Deletes the currently highlighted program from the list and uninstalls the corresponding .BAS file.</td>
</tr>
</tbody>
</table>
3.14.8.1 ChemBasic Program Dialog Box

In this dialog box, you can define some options for running the selected ChemBasic program. The dialog box appears when, in the ChemBasic Organizer dialog box, you click either the Modify or New button.

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>In the Name area, specify the text that will appear as a yellow hint when you point to the button specified for the ChemBasic program.</td>
</tr>
<tr>
<td>File</td>
<td>In the File area, specify the name and location of a ChemBasic program to be installed.</td>
</tr>
<tr>
<td>Toolbar</td>
<td>In the Toolbar area, specify the toolbar to which the shortcut button should be placed:</td>
</tr>
<tr>
<td></td>
<td>• General toolbar (refer to Section 3.5);</td>
</tr>
<tr>
<td></td>
<td>• Additional ChemBasic toolbar (that will appear between the General and Structure toolbars);</td>
</tr>
<tr>
<td></td>
<td>• Structure toolbar (refer to Section 3.6).</td>
</tr>
<tr>
<td>Bitmap File</td>
<td>In the Bitmap File area, specify the name and location of a bitmap file (.BMP) to be used as a shortcut button for the ChemBasic program specified above. If you do not have a button image for the program, you can use the Run ChemBasic command (refer to Section 3.9.9) for running programs having no shortcut buttons.</td>
</tr>
</tbody>
</table>
3.15 Documents Menu

The commands located on this menu allow you to switch between the open documents or to close all of the open documents at once.

This menu also contains a list of currently open documents. Click a document’s name to make it the active document. Note that you may only have one document visible at a time—you cannot tile or cascade multiple document windows.

Note: You can have up to ten documents open at once.

3.15.1 Next

This command displays the next document from the Open Document list as the active document. Note that you may have only one document visible at a time—you cannot tile or cascade multiple document windows.

Note: If only one document is open, the Next function is inactive.

Shortcut:
Keyboard: CTRL+TAB

3.15.2 Previous

This command displays the previous document from the Open Document list as the active document. Note that you may only have one document visible at a time—you cannot tile or cascade multiple document windows.

Note: If only one document is open, the Previous function is inactive.

Shortcut:
Keyboard: CTRL+SHIFT+TAB

3.15.3 Close All

This command closes all of the open documents. After closing the documents, ACD/ChemSketch automatically displays a "noname" document.

Note: While closing unsaved documents, ACD/ChemSketch prompts you to save your work if you've not already done so.

3.16 Add-Ons Menu

This menu contains commands of the installed add-on applications that can be used to enhance the program possibilities (the add-ons can be created by the third-party developers).

You can install the supplementary applications through the Add-on Organizer dialog box (for more information on this dialog box, refer to Section 3.14.7).
3.17 I-Lab Menu

ACD/Labs Online (I-Lab or Interactive Laboratory) is an Internet-based service that allows you to:

- Use ACD/ChemSketch chemical drawing and import capabilities to enable structural input for the I-Lab;
- View predicted or stored CNMR and HNMR spectra (using HNMR or CNMR Viewers included with the Add-on);
- Browse databases: CNMR, HNMR, FNMR, PNMR, and NNMR;
- Attach the generated chemical names to your structures (IUPAC Name, CAS Index Name, and Name to Structure are available);
- Review and save physicochemical properties (Boiling Point, LogP, LogD, pKa, ΔH_{(vap)}, Vapor Pressure, Aqueous Solubility, BCF, and Adsorption Coefficient); and
- Browse physicochemical databases from the ChemSketch interface.

Depending on the server URL set in the ACD/I-Lab Options, you can login to **Public I-Lab** or **I-Lab: Intranet Edition**.

**Public I-Lab**: ACD/I-Lab includes free and fee-based services. ACD/I-Lab registration and membership are free. You do not have to pay anything if you only use the free services.

**I-Lab: Intranet Edition**: You pay for the package rather than for each calculation. The **I-Lab: Intranet Edition** package can include any set of the available services.

In order to get access to ACD/I-Lab resources, you should have:

- A direct Internet connection:
  - **Public I-Lab**: Access to http://ilab.acdlabs.com/ilab/perl/chsk.pl address;
- An e-mail address (for Public I-Lab only);
- ChemSketch and I-Lab Add-on for ChemSketch:
  - **Public I-Lab**: Version 4.0 or later (there are both commercial and free versions available. The free version can be downloaded from http://www.acdlabs.com/download);
  - **I-Lab: Intranet Edition**: Version 6.0 or later.

As soon as you install ACD/ChemSketch and I-Lab Add-on and start up the program, you will see the standard ChemSketch interface with the additional I-Lab menu and the status bar whose left part is modified (the number of menu commands and status bar items is different depending on the server).

For more detailed information on the functionality of the ACD/I-Lab add-on, refer to the separate ACD/I-Lab documentation.
3.18 ACD/Labs Menu

This menu displays the list of ACD/Labs programs from one package currently installed on your computer. After you have installed the first ACD/Labs package, the program’s name appears in this menu.

Note: If the ACD/Labs package is installed on the remote host, you should run any program just once to place its name into the list on your local computer.

To load any program from the list, just click its name. ACD/ChemSketch is common for all ACD/Labs programs (except for the Batch versions) and is always loaded automatically.

The list can contain programs from one package only. If you have several packages of ACD/Labs software installed on your computer, then you will not be able to run programs from one package within another.

3.18.1 Next Loaded

If you have several ACD/Labs programs installed and currently open, this command switches you to another loaded program. You may also use the SHIFT and ESC to switch between the loaded programs. Press SHIFT and, without releasing it, press ESC. Then, on the panel displaying currently loaded ACD/Labs programs, choose the required one by pressing ESC repeatedly and, when the desired program is selected, release SHIFT to switch to the chosen program.

3.18.2 Anchor—New to 12.0!

This command affects the way the buttons corresponding to the currently running ACD/Labs programs are displayed on the Windows taskbar:

- Select this command to collect all the taskbar buttons into a single button. In this case, to switch between the programs, use the Next Loaded command as described above.
- Clear the selection to expand the taskbar buttons of all the ACD/Labs programs. To switch between the programs, click these buttons. Note that the additional ACD/Labs button appears on the ChemSketch Window Switching bar in this case. Clicking it displays the shortcut menu allowing you to switch between the ChemSketch windows of the running ACD/Labs programs.

3.18.3 Exit All

This command closes all of the programs from the ACD/Labs package that are currently running.

Tip: To close only one program, from the File menu, choose Exit, or, on the title bar, click Close.

3.18.4 Setup Style—New to 12.0!

This command allows you apply a desired coloration theme to all of the ACD/Labs programs. As you choose the command, the Setup Style dialog box appears where you can choose among the available coloration themes: Windows Settings, Grey, and Blue.
3.19 Help Menu

The commands located on this menu allow you to obtain help on a required topic and to get more information about the company, software product, etc.

3.19.1 Help Topics

This command allows you to display the contents of the ACD/ChemSketch online Help.

3.19.2 Using Help

This command allows you to display instructions on how to use online Help.

3.19.3 Tip of the Day

This command displays the "Tip of the Day" help topics describing techniques and procedures more effectively.

3.19.4 Instructions for Authors

This command displays the contents of the "Instructions for Authors" help topics.

3.19.5 ChemBasic Help

This command displays the ACD/ChemBasic online Help.

ACD/ChemBasic is a special programming language that enables you to customize ACD/Labs software. It is available as a part of the ACD/ChemSketch freeware that you can download from our Web site at http://www.acdlabs.com. For more information about ACD/ChemBasic features, refer to the separate ACD/ChemBasic User’s Guide.
3.19.6 Message Box Preferences

This command allows you to display the Message Box Preferences dialog box where you can specify preferences concerning the Don't show/ask me again check boxes in program messages.

Performing some operations within ACD/Labs software displays message boxes prompting you to do something or informing you of a particular condition. At the beginning, it is helpful to consider all the information that the program proposes you. However, when a number of the same type of cases is treated, you might prefer "silent" mode. For this purpose, in such message boxes, the Don't show me again or Don't ask me again check boxes are available; selecting them will not display the corresponding message boxes each time you perform a specific action.

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Consider “Don’t show me again” Status</strong></td>
<td></td>
</tr>
<tr>
<td>Yes</td>
<td>Select this option to obey the Don’t show me again status in all the message boxes. In other words, the messages with the selected check boxes will be skipped and those with the cleared check boxes will be displayed.</td>
</tr>
<tr>
<td>Yes, Except for Today’s Choice</td>
<td>Select this option to obey the Don’t show me again status unless it was changed within the today’s calendar date. That is, the messages with the selected check boxes will be skipped and those with the cleared check boxes will be displayed; but the messages where the status of such check boxes was changed within the today’s calendar date will be displayed regardless of whether the Don’t show me again check box is selected or not. Note that enabling this option does not change the status of check boxes but only ignores them.</td>
</tr>
<tr>
<td>No (Show All Message Boxes)</td>
<td>Select this option to ignore the settings for the Don’t show me again status and display all the message boxes that occur. Note that enabling this option does not change the status of check boxes but only ignores them.</td>
</tr>
<tr>
<td><strong>Clear “Don’t show me again” Check Boxes</strong></td>
<td></td>
</tr>
<tr>
<td>Today’s Choices</td>
<td>Clears the Don’t show me again check boxes only in the message boxes for which the status of such check boxes was changed within the today’s calendar date.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>---------------------------------------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td></td>
<td>Clears the <strong>Don't show me again</strong> check boxes everywhere thus allowing you to</td>
</tr>
<tr>
<td></td>
<td>display all the message boxes that can occur.</td>
</tr>
</tbody>
</table>

**Important**  Changes in this dialog box will affect ALL of the ACD/Labs products within all the installed ACD/Labs packages (both network and local) for current user.

**EXAMPLE 1.**

When you try to export a document containing some OLE object from the ChemSketch window to Adobe PDF file, the following message appears: "Current document contains OLE objects that cannot be exported to PDF document, so they will be skipped."

If you do not want this reminder to be displayed when you do export, in the message, select the **Don't show me again** check box, and next time you export the document containing nonexportable OLE objects, this message will be skipped.

But if you then decide that you should be aware of the OLE objects that cannot be exported, you can clear the **Don't show me again** option using the **Message Box Preference** dialog box.

**EXAMPLE 2.**

When you import an MDL Molfile containing a structure of the size that the system may consider non-feasible, the **Import Warning** message box with the **Yes** and **No** choices appears asking you whether the imported structure should be resized or not.

If you want the structure to be resized now and in all the later instances, in this message, select the **Don't ask me again** check box and click **Yes**. In this case, next time a structure of non-feasible size is imported, it will be resized in a silent mode, without the message appearing, as if you have clicked **Yes** in that message box.

If you want to keep the structure size now and in all the later instances, in this message, select the **Don't ask me again** check box and click **No**. In this case, next time the structure of non-feasible size is imported, no message will appear and the structure won't be resized, as if you have clicked **No** in that message box.

And again, if you later decide that you want to choose manually whether the structures should be resized or not, you can use the required option or button in the **Message Box Preferences** dialog box to make the **Import Warning** message appear again by each import.

**3.19.7 Documents**

This command allows you to display documentation (Reference Manual, Tutorial, User’s Guide) related to current program.

**3.19.8 Visit ACD/Labs Web Site**

This command allows you to run your default Internet browser and goes to the ACD/Labs Web page at [http://www.acdlabs.com/](http://www.acdlabs.com/).

**3.19.9 Bug Report / Feature Request**

Depending on the option selected in the **Bug Report Settings** dialog box (refer to the subsequent section), this command allows you to submit a bug report and feature request either through the ACD/Labs Web site or by e-mail.
3.19.10 Bug Report Settings

This command displays the dialog box where you can choose the way you wish to submit bug reports and feature requests. Note that in both cases you are supposed to fill in a form where you can report the problems you have encountered while working with ACD/Labs software or submit a request for a new feature to be included in any of the ACD/Labs products.

The following two options are available:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Go to the ACD/Labs Bug Report Page</td>
<td>If you select this option, each time you choose the Bug Report / Feature Request command, your default Internet browser will be run and the ACD/Labs Web page (<a href="http://www.acdlabs.com/support/supportrequest.php">http://www.acdlabs.com/support/supportrequest.php</a>) will be opened.</td>
</tr>
<tr>
<td>Send E-mail to ACD/Labs Bug Processing Center</td>
<td>If you select this option, each time you choose the Bug Report / Feature Request command, your default mail client will be activated. The program will create a message according to the built-in template.</td>
</tr>
</tbody>
</table>

3.19.11 About ACD/ChemSketch

This command displays information about your copy of the ACD/Labs package, including the version number, the copyright, and your user registration information. This also contains information on how to contact ACD/Labs.

Moreover, by clicking the License ID button you can see your license ID number(s)—you will need the ID number(s) in case our technical support is required.
4. Draw Mode

4.1 Objectives

This chapter will familiarize you with the features available in the Draw mode of ACD/ChemSketch. You will also become familiar with all the parts of the ChemSketch window available in this mode and what they are aimed at.

To switch to the Draw mode, on the General toolbar, click Draw.

4.2 General Information

In the Draw mode, you can perform the following actions:

- Draw graphical objects such as lines, arrows, rectangles, ellipses, arcs, polylines, and polygons, and insert callouts, brackets, and text labels.
- Manipulate the objects: ungroup complex objects or group them into more complex objects, align, flip, rotate, resize, and fit objects to page dimensions.
- Open, close, and print documents; cut, copy, and paste the required objects; delete and zoom objects. You can also paste your work to the other Windows applications and insert the objects from other Windows applications into your work.
- Create multi-page documents, rename and delete pages, insert new pages and organize all of the pages in a document.
- Control the location of objects on the page with a ruler and gridlines. You can choose different units of measurement for a ruler and insert or remove gridlines by using the Options menu commands.
4.3 Screen

Below, you can see the ACD/ChemSketch screen with the Draw mode enabled. Names and positions of toolbars and other elements, to be used throughout this manual, are indicated.

<table>
<thead>
<tr>
<th>Interface Element</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Title bar</td>
<td>Shows the name of the program, the name and location of the currently open file, and buttons controlling the size and position of the window.</td>
</tr>
<tr>
<td>Menu bar</td>
<td>Contains the program menus of commands for working in the Draw mode of the ChemSketch window.</td>
</tr>
<tr>
<td>General toolbar</td>
<td>Includes tools that are present in both Structure and Draw modes and will help you with tasks relevant to both modes such as saving and opening .SK2 files, undoing/redoing operations, copying and pasting, zooming in and out, as well as inserting various templates.</td>
</tr>
<tr>
<td>ChemBasic toolbar</td>
<td>Includes additional tools that extend the functionality of ACD/ChemSketch. Note that the ChemBasic toolbar is present in both Structure and Draw modes only if you have the Goodies tools previously installed.</td>
</tr>
</tbody>
</table>
## Interface Element Description

**Editing toolbar**  
*For the Draw mode only*
Contains tools for changing the graphical attributes of objects in the workspace. Note that you cannot edit chemical structures with the tools of the Editing toolbar (except resizing and rotating them). For more information, refer to Section 4.6.

**Drawing toolbar**  
*For the Draw mode only*
Contains buttons used for creating graphical objects such as lines, rectangles, text boxes, etc. (for more information, refer to Section 4.7).

**Workspace**
Displays currently active page of an open ChemSketch document where you can draw and edit the required objects (structures, reactions, pictures).

**Color Palette**
Allows you to quickly change the pen and fill color of the selected objects (for more information, refer to Section 2.4).

**RSS News bar**
Lists the latest news from ACD/Labs, Reactive Reports, and any other RSS channels specified by the user (for more information, refer to Section 2.5).

**Status bar**
Contains the following actual information: name of the open file, page number, etc. It also contains a button for automatic I-Lab access. For more information, refer to Section 2.6.

---

### 4.4 Menu Bar

Right below the title bar, you will find the menu bar that contains the program menus. By clicking the menus you can access the program commands.

![ACD/ChemSketch - [noname01.sk2]](image)

For detailed information on the commands that are available from the menus of the ChemSketch window in the Draw mode, refer to Sections 4.8–4.18.

### 4.5 General Toolbar

In both Structure and Draw modes, below the menu bar, the General toolbar is displayed.

For more information on the buttons available on this toolbar, refer to Section 3.5.
4.6 Editing Toolbar

In the Draw mode, this toolbar is displayed below the General toolbar. The Editing toolbar contains buttons for changing the graphical attributes of objects in your workspace. Note that you cannot edit chemical structures with the tools of the Editing toolbar (except resizing and rotating them). Use the Structure mode for structure editing.

The Editing toolbar contains the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Select, move, resize" /></td>
<td>Allows you to select, move, and resize objects (for more information, refer to Section 4.6.1).</td>
</tr>
<tr>
<td><img src="image" alt="Select, move, rotate" /></td>
<td>Allows you to select, move, and rotate objects (for more information, refer to Section 4.6.2).</td>
</tr>
<tr>
<td><img src="image" alt="Shape editing" /></td>
<td>Allows you to change an object’s shape by editing (moving, adding, deleting) the object’s nodes. As you click this button, the right part of the Editing toolbar is replaced with the Node toolbar. For more information, refer to Section 4.6.3.</td>
</tr>
<tr>
<td><img src="image" alt="Edit text" /></td>
<td>Allows you to edit text. As you click this button, the right part of the Editing toolbar is replaced with the Text toolbar. For more information, refer to Section 4.6.4.</td>
</tr>
<tr>
<td><img src="image" alt="Bring to foreground" /></td>
<td>Brings the selected background objects to the foreground (for more information, refer to Section 4.12.2).</td>
</tr>
<tr>
<td><img src="image" alt="Send to background" /></td>
<td>Sends the selected foreground objects to the background (for more information, refer to Section 4.12.3).</td>
</tr>
<tr>
<td><img src="image" alt="Group/ungroup" /></td>
<td>Groups/ungroups the selected objects and allows you to place data into tables (for more information, refer to Section 4.12.1).</td>
</tr>
<tr>
<td><img src="image" alt="Rotate vertically" /></td>
<td>Turns the selected object(s) about the vertical axis (for more information, refer to Section 4.12.4).</td>
</tr>
<tr>
<td><img src="image" alt="Rotate horizontally" /></td>
<td>Turns the selected object(s) about the horizontal axis (for more information, refer to Section 4.12.5).</td>
</tr>
<tr>
<td><img src="image" alt="Rotate 90°" /></td>
<td>Rotates the selected object(s) by 90° (for more information, refer to Section 4.12.6).</td>
</tr>
<tr>
<td><img src="image" alt="Align left" /></td>
<td>Aligns the selected objects horizontally to the left (for more information, refer to Section 4.12.7).</td>
</tr>
<tr>
<td><img src="image" alt="Align center" /></td>
<td>Aligns the selected objects horizontally to center (for more information, refer to Section 4.12.7).</td>
</tr>
<tr>
<td><img src="image" alt="Align right" /></td>
<td>Aligns the selected objects horizontally to the right (for more information, refer to Section 4.12.7).</td>
</tr>
<tr>
<td><img src="image" alt="Align bottom" /></td>
<td>Aligns the selected objects vertically to the bottom (for more information, refer to Section 4.12.8).</td>
</tr>
<tr>
<td><img src="image" alt="Align center" /></td>
<td>Aligns the selected objects vertically to the center (for more information, refer to Section 4.12.8).</td>
</tr>
<tr>
<td><img src="image" alt="Align top" /></td>
<td>Aligns the selected objects vertically to the top (for more information, refer to Section 4.12.8).</td>
</tr>
</tbody>
</table>

**Note** To customize the toolbar contents, right-click it to display the context menu (for more information, refer to Section 2.2.1).
4.6.1 Select/Move/Resize Button

Using the Select/Move/Resize tool, you can select, move, and resize objects created in the Draw and Structure modes. If you double-click the selected object with this tool active, you can change its style using the Objects Panel that appears (for more information, refer to Section 4.11.7).

The table below summarizes the actions you can perform to select objects:

<table>
<thead>
<tr>
<th>To select…</th>
<th>You should…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single object</td>
<td>Click the object or drag around the object.</td>
</tr>
<tr>
<td>Multiple objects one by one</td>
<td>Hold down SHIFT when selecting as described in the previous action.</td>
</tr>
<tr>
<td>All objects in the workspace</td>
<td>Press CTRL+A.</td>
</tr>
</tbody>
</table>

The table below summarizes the actions you can perform to move selected objects:

<table>
<thead>
<tr>
<th>To move…</th>
<th>You should…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Object</td>
<td>Point to the object so that the gray rectangle appears around it and drag.</td>
</tr>
<tr>
<td>Object with leaving its copy behind</td>
<td>Hold down CTRL while dragging.</td>
</tr>
<tr>
<td>Object with fixing its coordinates along one of the axes</td>
<td>Drag the object while holding down SHIFT. This will move the selected object strictly horizontally (vertically) without changing its initial coordinate position along the X (Y) axis.</td>
</tr>
</tbody>
</table>

**Note** If the Informative Cursor check box is selected on the General tab of the Preferences dialog box, the object’s shift coordinates are displayed near the mouse pointer. For more information, refer to Section 3.14.1.1).

If you want to move object with/without snapping it to grid in the workspace, select/deselect the Snap on Grid command on the Options menu (refer to Section 3.14.3).

The table below summarizes the actions you can perform to resize selected objects:

<table>
<thead>
<tr>
<th>To resize…</th>
<th>You should…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Object relative to one of its sides or corners</td>
<td>Point to the required selection handle so that the mouse pointer changes to a double-headed arrow (<code>, </code>, <code> </code>, or <code> </code>, and drag. Dragging the top/bottom selection handles resizes the object’s height, dragging the left/right side handles resizes the width; and dragging the corner handles resizes the object proportionally in all directions.</td>
</tr>
<tr>
<td>Object relative to its center</td>
<td>Hold down CTRL when dragging the selection handles as described above.</td>
</tr>
<tr>
<td>Object’s width or height at certain percent</td>
<td>Point to a side selection handle while holding down SHIFT, and drag. The selected object will be resized by percent value multiple of 5.</td>
</tr>
</tbody>
</table>
To resize…

| Object so that the height and width change independently | Point to a corner selection handle while holding down SHIFT, and drag. |

**Note**

To view the percentage of resizing displayed near the mouse pointer, on the General tab of the Preferences dialog box, select the Informative Cursor check box. For more information, refer to Section 3.14.1.1.

If you want to resize object with/without snapping it to grid in the workspace, select/deselect the Snap on Grid command on the Options menu (refer to Section 3.14.3).

You can quickly switch between this tool and the Select/Move/Resize tool by right-clicking in the workspace or by clicking any selection handle.

### 4.6.2 Select/Move/Rotate Button

Using the Select/Move/Rotate tool, you can select, move, and rotate objects created in Draw and Structure modes. If you double-click the selected object with this tool active, you can change its style using the Objects Panel that appears (for more information, refer to Section 4.11.7).

The actions you can perform to select or move the required objects on the ChemSketch page are described in the corresponding tables of the previous section.

The table below summarizes the actions you can perform to rotate selected objects:

<table>
<thead>
<tr>
<th>To rotate…</th>
<th>You should…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Object around its center</td>
<td>Point to the object’s selection handle so that the mouse pointer changes to and drag.</td>
</tr>
<tr>
<td>Object in 15 degree increments</td>
<td>Hold down SHIFT when rotating as described in above.</td>
</tr>
</tbody>
</table>

**Note**

To view the angle of rotation displayed near the mouse pointer, on the General tab of the Preferences dialog box, select the Informative Cursor check box. For more information, refer to Section 3.14.1.1.

You can quickly switch between this tool and the Select/Move/Resize tool by clicking any selection handle or right-clicking in the workspace.

### 4.6.3 Edit Nodes Button

Using the Edit Nodes tool, you can modify the shape of the following objects: lines, arcs, curves, arrows, polylines, rectangles, rounded rectangles, polygons, brackets, and callouts.

When you click the Edit Nodes button, the Node toolbar replaces the right part of the Editing toolbar. To edit an object, select it so that the nodes appear:
Note: Only one object can be selected at a time when the **Edit Nodes** tool is active.

The function of the **Edit Nodes** tool varies depending on the type of object selected:

<table>
<thead>
<tr>
<th>Object Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Line/Arrow/Curve/Polygon/Curved shape</td>
<td>Changing the shape by moving nodes and control points and using the Node toolbar.</td>
</tr>
<tr>
<td>Rectangle</td>
<td>Rounding corners by moving nodes.</td>
</tr>
<tr>
<td>Rounded Rectangle</td>
<td>Changing the radius of corners by moving nodes.</td>
</tr>
<tr>
<td>Arc</td>
<td>Changing the length by moving nodes.</td>
</tr>
<tr>
<td>Brackets/Callout</td>
<td>Modifying the size and shape by moving nodes.</td>
</tr>
</tbody>
</table>

**Nodes**—the points at the ends of line and curve segments in a curve object. **Control points**—the points extending from nodes along a curve object that determine the angle at which the curve passes through the node. Control points appear when you select a node. Nodes associated with straight lines do not have control points.

**4.6.3.1 Node Toolbar**

The Node toolbar appears when you click the **Edit Nodes** button on the Editing toolbar and replaces the right part of the latter.

It contains the following buttons for manipulating nodes and control points (for more information, refer to the previous section).

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Connect" /></td>
<td>Connects end nodes of a selected free-form curve or broken line with a straight line.</td>
</tr>
<tr>
<td><img src="image" alt="Erase" /></td>
<td>Erases the segment between the two selected adjacent nodes.</td>
</tr>
<tr>
<td><img src="image" alt="Add" /></td>
<td>Adds a node between the two selected adjacent nodes. Each additional click on this button will add new nodes between the existing ones.</td>
</tr>
<tr>
<td>Button</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>![Button]</td>
<td>Deletes the selected nodes.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Converts the selected curve or curved segment into a line. If the segment is defined as a line, it has no control points and thus cannot be reshaped.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Converts the selected line segment into a curve. Once the segment is defined as a curve, you can reshape it by manipulating its nodes and control points. To see the control points, click the node.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Allows you to put a node and its both adjacent control points into line and move together with the node as you drag. Release the <strong>Smooth</strong> button to disable this function.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Equalizes the distances between the selected node and their adjacent control points. These distances will be changed equally while you drag a control point. Release the <strong>Symmet</strong> button to disable this function.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Aligns the selected nodes horizontally to the left—relative to each other.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Aligns the selected nodes horizontally to the center—relative to each other.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Aligns the selected nodes horizontally to the right—relative to each other.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Aligns the selected nodes vertically to the bottom—relative to each other.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Aligns the selected nodes vertically to the center—relative to each other.</td>
</tr>
<tr>
<td>![Button]</td>
<td>Aligns the selected nodes vertically to the top—relative to each other.</td>
</tr>
</tbody>
</table>

**Note** To select the required nodes, click them holding down SHIFT. If you do not need all of the buttons available on the toolbar, you can customize it. For more information, refer to Section 2.2.1.

### 4.6.4 Edit Text Button

Using the *Edit Text* tool, you can enter and edit the text.

With this tool enabled, click within the workspace to enter or edit the text. Modify the text as desired using the Text toolbar buttons. To leave the editing mode, click outside the text box.

Optionally, you can use the *Text* and *Artistic Text* tools (for more information, refer to Section 4.7.11).
4.6.4.1 Text Toolbar

The Text toolbar appears whenever you enter or modify text using either the Edit Text or Artistic Text tool. The Text toolbar replaces the right part of the Editing toolbar. It contains the following buttons for formatting text:

<table>
<thead>
<tr>
<th>Button/Box</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arial</td>
<td>In this box, specify the font style for the selected text or for the text to be typed.</td>
</tr>
<tr>
<td>12</td>
<td>In this box, specify the font size for the selected text or for the text to be typed.</td>
</tr>
<tr>
<td><strong>B</strong></td>
<td>Applies the bold formatting (e.g., text) to the selected text or to the text to be typed.</td>
</tr>
<tr>
<td><em>I</em></td>
<td>Applies the italic formatting (e.g., text) to the selected text or to the text to be typed.</td>
</tr>
<tr>
<td><strong>U</strong></td>
<td>Applies the underlined formatting (e.g., text) to the selected text or to the text to be typed.</td>
</tr>
<tr>
<td><strong>Ω</strong></td>
<td>Applies the strikethrough formatting (e.g., text) to the selected text or to the text to be typed.</td>
</tr>
<tr>
<td>^<em>S+</em></td>
<td>Applies the superscript formatting (e.g., text) to the selected text or to the text to be typed.</td>
</tr>
<tr>
<td>^<em>S−</em></td>
<td>Applies the subscript formatting (e.g., text) to the selected text or to the text to be typed.</td>
</tr>
<tr>
<td>²Ω</td>
<td>Transforms characters of the selected text or the text to be typed to Greek symbols.</td>
</tr>
<tr>
<td>L</td>
<td>Aligns the text to the left.</td>
</tr>
<tr>
<td>C</td>
<td>Centers the text in the text box.</td>
</tr>
<tr>
<td>R</td>
<td>Aligns the text to the right.</td>
</tr>
<tr>
<td>F</td>
<td>Stretches the text so that it fills the whole lines between the left and right borders of a text box.</td>
</tr>
<tr>
<td>Font</td>
<td>Applies the default font style specified on the Font panel (refer to Section 4.11.4) to the selected text and/or applies the default paragraph style specified on the Paragraph panel (refer to Section 4.11.5) to the paragraph where the mouse pointer is currently located.</td>
</tr>
<tr>
<td>Save</td>
<td>Saves current font and paragraph attributes as default.</td>
</tr>
</tbody>
</table>

**Note** If you do not need all of the buttons available on the toolbar, you can customize it. For more information, refer to Section 2.2.1.

4.7 Drawing Toolbar

In the Draw mode, this toolbar is displayed vertically to the left of the workspace. It contains buttons for creating graphical objects such as lines, rectangles, text boxes, etc.

**Note** To switch to the Select/Move/Resize mode, press ESC or, on the Editing toolbar, click Select/Move/Resize.
The Drawing toolbar contains the following buttons:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw straight lines (for more information, refer to Section 4.7.1).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw arcs (for more information, refer to Section 4.7.2).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw curves of a predefined shape (for more information, refer to Section 4.7.3).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw free-form curves and broken lines (for more information, refer to Section 4.7.4).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw arrows of different shape (for more information, refer to Section 4.7.5).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw rectangles (for more information, refer to Section 4.7.6).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw rectangles with rounded corners (for more information, refer to Section 4.7.7).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw ellipses and circles (for more information, refer to Section 4.7.8).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw free-form shapes (for more information, refer to Section 4.7.9).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to insert images (for more information, refer to Section 4.7.10).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to insert text into the workspace (for more information, refer to Section 4.7.11).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw table of specified size (for more information, refer to Section 4.7.12).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw brackets of different types (for more information, refer to Section 4.7.13).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to draw callouts (for more information, refer to Section 4.7.14).</td>
</tr>
<tr>
<td>![Button Image]</td>
<td>Allows you to create templates for ACD/SpecManager reports (for more information, refer to Section 4.7.15).</td>
</tr>
</tbody>
</table>

**Note** The toolbar can be customized according to your preferences; for more information, refer to Section 2.2.1.

### 4.7.1 Line Button

Using the Line tool, you can draw straight lines. Click this button and drag in the workspace to draw a line.

Holding down SHIFT while dragging draws the line at an angle multiple to 15°.

Holding down CTRL while dragging draws the line centered at the starting position of the cursor.

Objects drawn with the Line tool are automatically assigned the default attributes defined on the Pen style panel (refer to Section 4.11.1).

**Note** To change the thickness, style, and color of a drawn line without affecting defaults, double-click the line and make the required settings on the Objects Panel that appears.

If the Keep Draw Tool Active check box in the Preferences dialog box (General tab) is selected, this tool remains active until you click or right-click in the workspace (the Select/Move/Resize tool becomes active). If this check box is cleared, the Select/Move/Resize tool becomes active immediately after you have drawn a line.
4.7.2 Arc Buttons

These buttons enable the set of tools allowing you to draw arcs. Click the right bottom triangle of the button to expand it into the following buttons:

- Arc 90°
- Arc 120°
- Arc 180°
- Arc 240°
- Arc 270°

To draw an arc of the required size, click the corresponding Arc button and, as it becomes active, drag in the workspace. The direction of your mouse drag determines the arc position.

**Tip** To change the arc angle to any other value, use the Edit Nodes tool (refer to Section 4.6.3).

The default attributes defined on the Pen style panel (refer to Section 4.11.1) are automatically assigned to the objects drawn with the Arc tool.

**Note** To change the thickness, style, and color of a drawn arc without affecting defaults, double-click the arc and make the required settings on the Objects Panel that appears.

If the Keep Draw Tool Active check box in the Preferences dialog box (General tab) is selected, this tool remains active until you click or right-click in the workspace (the Select/Move/Resize tool becomes active). If this check box is cleared, the Select/Move/Resize tool becomes active immediately after you have drawn an arc.

4.7.3 Curve Button

Using the Curve tool, you can draw curves of a definite shape. Click this button and drag in the workspace to draw a curve.

Holding down SHIFT while dragging draws the curve at an angle multiple to 15°.

Holding down CTRL while dragging draws the curve centered at the starting position of the cursor.

The default attributes defined on the Pen style panel (refer to Section 4.11.1) are automatically assigned to the objects drawn with the Curve tool.

**Note** To change the thickness, style, and color of a drawn curve without affecting defaults, double-click the curve and make the required settings on the Objects Panel that appears.

If the Keep Draw Tool Active check box in the Preferences dialog box (General tab) is selected, this tool remains active until you click or right-click in the workspace (the Select/Move/Resize tool becomes active). If this check box is cleared, the Select/Move/Resize tool becomes active immediately after you have drawn a curve.

4.7.4 Polyline Button
Using the **Polyline** tool, you can draw free-form curves and broken lines.

To draw a broken line, click in the workspace several times with this tool active and right-click to finish drawing. To draw a free-formed curve, use dragging in combination with clicking.

**Note** You can edit the form of the drawn curve with the help of the **Edit Nodes** tool.

The default attributes defined on the **Pen** style panel (refer to Section 4.11.1) are automatically assigned to the objects drawn with this tool.

**Note** To change the thickness, style, and color of a drawn object without affecting defaults, double-click the polyline and make the required settings on the **Objects Panel** that appears.

If the **Keep Draw Tool Active** check box in the **Preferences** dialog box (**General** tab) is selected, this tool remains active until you click or right-click in the workspace (the **Select/Move/Resize** tool becomes active). If this check box is cleared, the **Select/Move/Resize** tool becomes active immediately after you have drawn a polyline.

### 4.7.5 Arrow Button

Using the **Draw Arrow** tool, you can draw arrows and apply arrowheads to any linear object (lines, arcs, curves, and polylines). When you click this button, the **Arrow** style panel where you can specify arrow style appears. For more information on the options on this panel, refer to Section 4.11.3.

To draw an arrow, select any of the following tools: **Line**, **Arc**, **Curve**, or **Polyline**, then click **Arrow** and drag in the workspace. As you finish drawing, the arrowhead appears at the end of the object.

To apply an arrowhead to the already drawn objects, select the object, choose this tool, and then in the **Arrow** style panel that appears, click **Apply**.

The default attributes defined on the **Pen** style panel and **Arrow** style panel (refer to Sections 4.11.1 and 4.11.3) are automatically assigned to the objects drawn with this tool.

**Note** To change the thickness, style, and color of a drawn arrow without affecting defaults, double-click the arrow and make the required settings on the **Objects Panel** that appears.

If the **Keep Draw Tool Active** check box in the **Preferences** dialog box (**General** tab) is selected, this tool remains active until you click or right-click in the workspace (the **Select/Move/Resize** tool becomes active). If this check box is cleared, the **Select/Move/Resize** tool becomes active immediately after you have drawn an arrow.
4.7.6 Rectangle Button

Using the Rectangle tool, you can draw rectangles and squares. To draw a rectangle of the desired size and form, activate this tool and drag in the workspace.

Holding down SHIFT while dragging draws a square.

Holding down CTRL while dragging draws the rectangle or square centered at the starting position of the cursor.

The default attributes defined on the Pen style panel and Fill style panel (for more information on these panels, refer to Sections 4.11.1 and 4.11.2 correspondingly) are automatically assigned to the objects drawn with this tool.

Note To change the thickness, style, and color of a drawn object without affecting defaults, double-click the rectangle and make the required settings on the Objects Panel that appears.

If the Keep Draw Tool Active check box in the Preferences dialog box (General tab) is selected, this tool remains active until you click or right-click in the workspace (the Select/Move/Resize tool becomes active). If this check box is cleared, the Select/Move/Resize tool immediately becomes active after you have drawn a rectangle.

4.7.7 Rounded Rectangle Button

Using the Rounded Rectangle tool, you can draw rounded rectangles and rounded squares. To draw a rounded rectangle of desired size and form, activate this tool and drag in the workspace.

Holding down SHIFT while dragging draws a rounded square. Holding down CTRL while dragging draws the rectangle or square centered at the starting position of the cursor.

The default attributes defined on the Pen style panel and Fill style panel (refer to Sections 4.11.1 and 4.11.2 correspondingly) are automatically assigned to the objects drawn with this tool.

Note To change the thickness, style, and color of a drawn object without affecting defaults, double-click the rounded rectangle and make the required settings on the Objects Panel that appears.

If the Keep Draw Tool Active check box in the Preferences dialog box (General tab) is selected, this tool remains active until you click or right-click in the workspace (the Select/Move/Resize tool becomes active). If this check box is cleared, the Select/Move/Resize tool immediately becomes active after you have drawn a rounded rectangle.

4.7.8 Ellipse Button

Using the Ellipse tool, you can draw ellipses and circles. To draw an ellipse of desired size and form, choose this tool and drag in the workspace.

Holding down SHIFT while dragging draws a circle.

Holding down CTRL while dragging draws the ellipse or circle centered at the starting position of the cursor.

The default attributes defined on the Pen style panel and Fill style panel (refer to Sections 4.11.1 and 4.11.2 correspondingly) are automatically assigned to the objects drawn with this tool.
4.7.9 Polygon Button

Using the Polygon tool, you can draw polygons and curved shapes.

To draw a polygon, subsequently click in the workspace with this tool active and right-click to finish drawing. To draw a curved shape, use dragging in combination with clicking.

You can then edit the form of the drawn shape with the help of the Edit Nodes tool.

The default attributes defined on the Pen style panel and Fill style panel (refer to Sections 4.11.1 and 4.11.2 correspondingly) are automatically assigned to the objects drawn with this tool.

If the Keep Draw Tool Active check box in the Preferences dialog box (General tab) is selected, this tool remains active until you click or right-click in the workspace (the Select/Move/Resize tool becomes active). If this check box is cleared, the Select/Move/Resize tool immediately becomes active after you have drawn a polygon.

4.7.10 Insert Image Button

The Insert Image tool allows you to insert external bitmap images into the body of a ChemSketch document. The following formats are available:

- Windows Bitmaps (.BMP, .DIB)
- JPEG Bitmaps (.JPG)
- GIF Bitmaps (.GIF)
- Portable Network Graphics (.PNG)

To insert a bitmap, click this button, and then click at the insertion point or select the insertion area by dragging. In the Select Bitmap dialog box that appears, specify format, name and location of a file and click Open to insert the picture.

The inserted picture retains its original size if the insertion point has been specified by clicking. In case of dragging as a selection means, however, the dimensions of the picture change in accordance with the dimensions of the selected area. You can edit the dimensions of the inserted picture using the Select/Move/Resize tool.
4.7.11 Text Button

Using the Text tool, you can insert and edit text in the workspace.

If you click the bottom right triangle of the Text button, it will be expanded into the following buttons:

- **Formatted Text**
- **Artistic Text**

ACD/ChemSketch uses two types of text: *formatted* and *artistic*. Unlike the formatted text, artistic text can be stretched or compressed to create visual effects.

To type the text, click the required text tool to make it active and click in the workspace to place the text box. Type the text and, as soon as you finish, click somewhere outside the text box.

To edit the text, click the required text tool and click the text you want to edit.

The default attributes defined on the Font panel and Paragraph panel (refer to Sections 4.11.4 and 4.11.5 correspondingly) are automatically assigned to the text written with this tool.

**Note** To change the style (font, color, etc.) of existing text, double-click the text and make the required settings on the Objects Panel that appears. You can also change the default style attributes using the tools on the Text toolbar that appears as you activate the Text tool (for more information on the toolbar, refer to Section 4.6.4.1).

To edit the existing text, use the Edit Text tool (for more information, refer to Section 4.6.4). You can rotate the text the same way as you can manipulate any graphical object using the Select/Move/Resize tool.

4.7.12 Table Button

Using the Table tool, you can insert table of required size and format. Activate this tool and then drag in the workspace to outline a box that will contain your table. As you release the mouse button, the Insert Table dialog box where you should define the number of columns and rows appears. As you click OK in this dialog box, the table is inserted and the Table toolbar appears allowing you to customize your table.

### 4.7.12.1 Table Toolbar

The Table toolbar appears on the middle part of the Editing toolbar if a table or its cell(s) is selected in the workspace and either the Select/Move/Resize or Select/Move/Rotate tool is active. This toolbar allows you to edit table rows and columns, and manipulate boxes into which a table can be arranged.

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>The following six buttons serve for the editing column(s) and row(s). Note that these buttons are available only if one or more cells of the inserted table are selected.</td>
</tr>
<tr>
<td><img src="image" alt="Add Column" /></td>
<td>Adds a column to the right of the column with the selected cell; the dimensions of a new column are the same as those of the column with the selected cell(s). Note that to view the added column(s), enlarge the table box dimensions.</td>
</tr>
<tr>
<td>Button</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td><img src="image" alt="Add Row" /></td>
<td>Adds a row under the row with the selected cell; the dimensions of a new row are the same as those of the row with the selected cell(s). Note that to view the added row(s), enlarge the table box dimensions.</td>
</tr>
<tr>
<td><img src="image" alt="Delete Column" /></td>
<td>Deletes the column containing a selected cell.</td>
</tr>
<tr>
<td><img src="image" alt="Delete Row" /></td>
<td>Deletes the row containing a selected cell.</td>
</tr>
<tr>
<td><img src="image" alt="Column Width" /></td>
<td>Displays the Column Width dialog box where you can type the appropriate width for the selected column(s). The columns containing the selected cells are considered to be selected (to select several cells, hold down SHIFT while clicking them).</td>
</tr>
<tr>
<td><img src="image" alt="Row Height" /></td>
<td>Displays the Row Height dialog box where you can type the appropriate height for the selected row(s). The rows containing the selected cells are considered selected (to select several cells, hold down SHIFT while clicking them).</td>
</tr>
</tbody>
</table>

These buttons are available only if the entire table or a table box is selected. (To select a box, point to its upper left corner so that the gray border appears around the box, and then click. To select several boxes, press SHIFT, and then select each of the boxes as described above).

- ![Add New Box](image) | Adds a new box for the selected table. |
- ![Copy Box](image) | Copies an empty box for the selected table where the rest rows of the table will be arranged, if they do not fit into one box. |
- ![Swap Boxes](image) | Swaps the contents of the selected boxes. Note that you can swap the contents of boxes within one table only. |
- ![Delete Table](image) | Deletes the selected table alongside with its content and all of the boxes referring to it. |

**Note** You can customize the toolbar using its shortcut menu. For more information, refer to Section 2.2.1.

### 4.7.13 Brackets Buttons

These buttons enable the corresponding tools allowing you to draw bracket(s), parenthes(is/es), and brace(s). Click the bottom right triangle on the button ![Bracket](image) to unfold a panel representing various types of brackets:

- ![Brackets](image)
- ![Bracket](image)
- ![Parentheses](image)
- ![Parenthesis](image)
- ![Braces](image)
- ![Brace](image)

To draw the brackets, click the button, and then drag in the workspace or point to the object and click when the brackets appear around it. To draw a right/left standalone bracket, drag from side to side horizontally to flip it left to right.
The default attributes defined on the **Pen** style panel and **Fill** style panel (refer to Sections 4.11.1 and 4.11.2 correspondingly) are automatically assigned to the brackets drawn with this tool.

**Note** To change the thickness, style, and color of a drawn object without affecting defaults, double-click the drawn brackets and specify the required options on the **Objects Panel** that appears.

If the **Keep Draw Tool Active** check box in the **Preferences** dialog box (**General** tab) is selected, this tool remains active until you click or right-click in the workspace (the **Select/Move/Resize** tool becomes active). If this check box is cleared, the **Select/Move/Resize** tool immediately becomes active after you have drawn brackets.

### 4.7.14 Callout Buttons

These buttons enable the tools allowing you to draw callouts. Click the bottom right triangle of the button to expand it into the following buttons representing various types of callouts:

- **Rounded**
- **Square**
- **Open**

To draw a callout, activate the required tool and drag in the workspace, or point to any drawn object and click when the callout appears around it.

The default attributes defined on the **Pen** style panel and **Fill** style panel (refer to Sections 4.11.1 and 4.11.2 correspondingly) are automatically assigned to the callouts drawn with this tool.

**Note** To change the thickness, style, and color of a drawn object without affecting defaults, double-click the callout and specify the required settings on the **Objects Panel** that appears.

If the **Keep draw tool active** check box in the **Preferences** dialog box (**General** tab) is selected, this tool remains active until you click or right-click in the workspace (the **Select/Move/Resize** tool becomes active). If this check box is cleared, the **Select/Move/Resize** tool immediately becomes active after you have drawn a callout.

### 4.7.15 Report Template Button

ACD/ChemSketch allows you to create report templates for data supported by 1D NMR, 2D NMR, MASS, UVIR, CURVE, and CHROM modules of ACD/SpecManager, ChemFolder, ChromGenius, PhysChemHistory, PhysChemDatabase, AutoChrom. Make sure that you are in the Draw mode, click **Report Template** on the Drawing toolbar, and then drag in the workspace to display the **ACD/ChemSketch Template** dialog box.

For more information on how to create and use report templates, refer to *ACD/Report Template Reference Manual* located in the ACD/Labs documentation folder (\DOCS\REPTEMPL.PDF).
4.8 File Menu

For detailed information on the commands that are available from this menu, refer to Section 3.9.

4.9 Edit Menu

For detailed information on the commands that are available from this menu, refer to Section 3.10.

4.10 Pages Menu

For detailed information on the commands that are available from this menu, refer to Section 3.11.

4.11 Tools Menu

The commands located on this menu allow you to change the appearance of graphical objects. These commands set the styles for lines, filling, arrows, text, paragraphs, and objects.

Default Style Panels

ACD/ChemSketch applies the default style to all new objects unless you specify otherwise by changing the default settings. You can change the default in the Draw mode either by setting another existing style as the default or by changing the default style attributes on any of the Pen, Fill, Arrow, Font, Paragraph, and Table panels from the Tools menu.

Each panel is provided with a set of buttons having common functions:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Apply</strong></td>
<td>Applies the current panel settings to selected objects.</td>
</tr>
<tr>
<td><strong>Update From</strong></td>
<td>Copies the style attributes from the drawn object(s) to the panel. When you click this button, the cursor becomes an arrow labeled <em>From</em> (ū). Click the required object to update its style attributes to the panel.</td>
</tr>
<tr>
<td><strong>Save...</strong></td>
<td>Displays the Save User Style dialog box where you can specify the name for a new style and select the style attributes to be saved. For more information, refer to Section 0.</td>
</tr>
<tr>
<td><strong>Load...</strong></td>
<td>Displays a list of styles where you can select the style whose attributes are to be added to the panel. Note that this affects all of the attributes (font, arrow, fill, etc.).</td>
</tr>
</tbody>
</table>
4.11.1 Pen Style Panel

This command displays the Pen panel where you can specify the default line style, thickness and color for drawing lines, arcs, arrows, rectangles, ellipses, brackets, and callouts.

**Note** To affect the selected objects only, without setting defaults, use the Objects Panel dialog box. For more information, refer to Section 4.11.7.

Whenever you draw a new object, ACD/ChemSketch fills it using the default style which can be specified on this panel.

The panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>In this box, select the line of the needed type.</td>
<td></td>
</tr>
<tr>
<td>In this box, select the line of desired thickness.</td>
<td></td>
</tr>
<tr>
<td>In the color palette, select the needed color for lines.</td>
<td></td>
</tr>
</tbody>
</table>

**Shortcut:**

Keyboard: CTRL+SHIFT+P
4.11.2 Fill Style Panel

This command displays the Fill panel where you can specify the default style for filling in rectangles, ellipses, polygons, and callouts.

**Note**  To affect the selected objects only, without setting defaults, use the Objects Panel dialog box. For more information, refer to Section 4.11.7.

Whenever you draw a new object, ACD/ChemSketch fills it using the default style which can be specified on this panel. Depending on the button selected at the top of this panel, it has a different view:

The panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Transparent" /></td>
<td>When this button is active, the objects will be drawn with no fill, <em>i.e.</em>, they will be transparent.</td>
</tr>
<tr>
<td><img src="image" alt="Solid" /></td>
<td>When this button is active, the objects will be drawn with the solid fill. You can specify the fill color in the color palette below.</td>
</tr>
<tr>
<td><img src="image" alt="Hatched" /></td>
<td>When this button is active, the hatched objects will be drawn. You can specify the prototype and color for hatching in the Color and Pattern boxes that appear.</td>
</tr>
<tr>
<td><img src="image" alt="Shaded" /></td>
<td>When this button is active, the object whose fill fades or becomes more intensive gradually from the basic color to one of its tones will be drawn. You can specify the prototype, color, and intensity for shading in the Color, Pattern, and Shade boxes that appear.</td>
</tr>
<tr>
<td><img src="image" alt="Color" /></td>
<td>In the color palette, choose the needed color.</td>
</tr>
<tr>
<td><img src="image" alt="Pattern" /></td>
<td>In this box, select the needed pattern for hatching.</td>
</tr>
<tr>
<td><img src="image" alt="Shade" /></td>
<td>In this box, select the required shade type.</td>
</tr>
<tr>
<td><img src="image" alt="Intensity" /></td>
<td>In this box, specify the degree of default fill shading, <em>i.e.</em>, the percentage of basic color changing in the fill.</td>
</tr>
</tbody>
</table>

**Shortcut:**

Keyboard:  CTRL+SHIFT+F
4.11.3 Arrow Style Panel

This command displays the Arrow panel where you can specify the default style for arrows.

Note To affect the selected objects only, without setting defaults, use the Objects Panel dialog box. For more information, refer to Section 4.11.7.

Whenever you draw a new arrow, the default style which can be specified on this panel is applied to it.

The panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Custom</td>
<td>In this box, specify the default arrow type. If you choose Custom, the panel expands allowing you to specify your own arrow type.</td>
</tr>
<tr>
<td>/</td>
<td>Displays/hides the right part of the panel.</td>
</tr>
<tr>
<td>Arrowhead size</td>
<td>The preview area displays the arrowhead that will be applied to your arrow. You can set the arrowhead width and height either by clicking/dragging in this area or by entering the values in the Width and Height boxes.</td>
</tr>
<tr>
<td>Arrow body style</td>
<td>In this box, specify the arrow body type.</td>
</tr>
<tr>
<td>Arrowheads shape</td>
<td>In this area, you can specify the default arrowhead shape to be applied to the right and/or to the left arrow ends.</td>
</tr>
<tr>
<td>Swap</td>
<td>Interchanges the right and the left arrowheads.</td>
</tr>
</tbody>
</table>

Shortcut:

Keyboard: CTRL+SHIFT+A
4.11.4 Font Panel

This command displays the Font panel where you can specify the default style for text.

**Note** To affect the selected objects only, without setting defaults, use **Objects Panel**. For more information, refer to Section 4.11.7.

Whenever you enter a new text, ACD/ChemSketch applies the default style which can be specified on this panel.

The panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Style</strong></td>
<td>In this box, specify the default font style.</td>
</tr>
<tr>
<td><strong>Size</strong></td>
<td>In this box, specify the default font size.</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this color palette, you can specify the default font color.</td>
</tr>
<tr>
<td><strong>B</strong></td>
<td>Applies <strong>bold</strong> formatting. You can use the bold format button in combination with other options.</td>
</tr>
<tr>
<td><strong>I</strong></td>
<td>Applies <strong>italic</strong> formatting. You can use the italic format button in combination with other options.</td>
</tr>
<tr>
<td><strong>U</strong></td>
<td>Applies <strong>underlined</strong> formatting. You can use the underline button in combination with other options.</td>
</tr>
<tr>
<td><strong>S</strong></td>
<td>Applies <strong>struck-out</strong> formatting. You can use the strikeout button in combination with other options.</td>
</tr>
<tr>
<td><strong>S+</strong></td>
<td>Sets superscript formatting. You can use the superscript button in combination with other options.</td>
</tr>
<tr>
<td><strong>S−</strong></td>
<td>Sets subscript formatting. You can use the subscript button in combination with other options.</td>
</tr>
<tr>
<td><strong>/</strong></td>
<td>Displays/hides the preview area.</td>
</tr>
<tr>
<td><strong>Preview area</strong></td>
<td>Shows how characters will look with the options selected. You can hide/display it.</td>
</tr>
</tbody>
</table>

**Shortcut:**

Keyboard: CTRL+SHIFT+T
4.11.5 Paragraph Panel

This command displays the Paragraph panel where you can specify the default style for paragraphs.

**Note** To affect the selected objects only, without setting defaults, use the Objects Panel dialog box. For more information, refer to Section 4.11.7.

Whenever you enter a new text, ACD/ChemSketch applies default paragraph attributes which can be specified on this panel.

![Paragraph panel](image)

The panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Justification</strong></td>
<td>In this area, specify the alignment for the paragraph by clicking the corresponding buttons: to the left [ ], centered [ ], to the right [ ] and justified [ ].</td>
</tr>
<tr>
<td><strong>Indentation</strong></td>
<td>On this tab, you can define the space from the left (Left) and from the right (Right) margins as well as the first line indent (First Line).</td>
</tr>
<tr>
<td><strong>Spacing</strong></td>
<td>On this tab, you can define the space above (Before) and below (After) the paragraph, as well as the distance between tab stops (Tab Step), and spacing between lines in a paragraph (Line Spacing). Note that the At option is available only if you select At Least or Exactly in the Line Spacing box.</td>
</tr>
</tbody>
</table>

**Note** In most of the boxes, you can enter values in various units (points, inches, millimeters, or centimeters) by typing the value and adding the unit you want (pt/in/mm/cm). The value will be recalculated automatically corresponding to the unit indicated in the Preferences dialog box (General tab).

**Shortcut:**

**Keyboard:** CTRL+SHIFT+R
4.11.6 Table Panel

This command displays the Table panel where you can specify the default style for tables.

**Note** To affect the selected objects only, without setting defaults, use the Objects Panel dialog box. For more information, refer to Section 4.11.7.

Whenever you draw a new table, ACD/ChemSketch applies the default style to it which can be specified on this panel.

The panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Use Header</td>
<td>If this check box is selected, the first row in the table is inserted in every box as a header.</td>
</tr>
<tr>
<td>Protect Contents</td>
<td>If this check box is selected, the program does not allow you to insert or remove objects from the table cells.</td>
</tr>
<tr>
<td>Move to the Right</td>
<td>If this check box is selected, the table rows are arranged into several groups like columns, each one is located to the right from the previous one. The table rows that do not fit in the first group are moved to the right of the first group; the table rows that do not fit in the second group are moved to the right of the second group, and so on.</td>
</tr>
<tr>
<td>Move to Next Box</td>
<td>If this check box is selected, the table rows that do not fit in the box (that is restricted as you first drag in the workspace when inserting a table), are moved to the next box.</td>
</tr>
<tr>
<td>Vertical Justify</td>
<td>If this check box is selected, numbers of rows in each group (column) are approximately equal.</td>
</tr>
</tbody>
</table>

On the **Box** tab, you can define options for table.

**Alignment**

In this area, you can specify the horizontal and vertical alignment of the content in a table.

**Fit**

In this box, select the way the table and its contents fit to each other:

- **Mixed**—various cells in the table have different Fit parameters.
- **Table to Contents**—the table dimensions are adjusted to the size of the contents (the table cells are reduced or enlarged with respect to the largest height and width of the inserted objects).
- **Contents to Table**—the inserted objects are resized to fit properly into the table cells.
- **None**—the table retains its primary dimensions irrespective of the size of the contents.

**Note** For more information on how to create a table in ACD/ChemSketch, refer to Section 4.7.12.
**Shortcut:**

Keyboard: CTRL+SHIFT+B

### 4.11.7 Update Object Style Panel

This command allows you to alter style of the selected object without affecting default settings. Clicking this command (or double-clicking the required object with the **Select/Move/Resize** or **Select/Move/Rotate** tools enabled) displays the **Objects Panel** with the options that correspond to the type of the selected object(s).

The panel may contain different buttons corresponding to the type(s) of the selected object(s); the represented screen shot is the fullest variant.

![Objects Panel](image)

Combine your choices from the tabs and the drop-down lists to create your style, and then click **Apply** to accept changes.

If no objects are selected in the workspace, this command is disabled.

**Note** To change defaults, use the **Pen**, **Fill**, **Arrow**, **Font**, **Paragraph**, and **Table** panels (for more information, refer to Sections 4.11.1–4.11.6.).

Each **Object Panel** dialog box is provided with a set of buttons having common functions:

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Apply</strong></td>
<td>Applies the specified style settings to the selected objects.</td>
</tr>
<tr>
<td><strong>Load ...</strong></td>
<td>Displays the list of the available styles. Choose the required style name to load its attributes into the panel.</td>
</tr>
<tr>
<td><strong>Set Default</strong></td>
<td>Sets the specified settings as the default.</td>
</tr>
<tr>
<td><strong>Save As...</strong></td>
<td>Displays the <strong>Save User Style</strong> dialog box where you can specify a new style name and choose which of the selected object’s attributes are to be included into the style. For more information, refer to Section 4.11.8.1.</td>
</tr>
</tbody>
</table>

ACD/ChemSketch Reference Manual 155
**Shortcuts:**

Keyboard: CTRL+SHIFT+O  
Mouse: double-click the selected object

### 4.11.7.1 Objects Panel: Common

The **Common** button displays tabs with style attributes common for different types of objects.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pen</strong></td>
<td>On the <strong>Pen</strong> tab, specify the line thickness, style, and color of the selected objects.</td>
</tr>
<tr>
<td><strong>Style</strong></td>
<td>From the list, choose the line style.</td>
</tr>
<tr>
<td><strong>Width</strong></td>
<td>In this box, specify the line thickness for the selected objects.</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this box, specify the line color to be applied to selected objects.</td>
</tr>
<tr>
<td><strong>Fill</strong></td>
<td>The <strong>Fill</strong> tab presents options for specifying the fill style, color, and pattern of selected objects.</td>
</tr>
<tr>
<td><strong>Style</strong></td>
<td>In this area, click the required button to:</td>
</tr>
<tr>
<td>✗</td>
<td>Draw the objects with no fill, i.e., they will be transparent.</td>
</tr>
<tr>
<td>■</td>
<td>Draw the objects with the solid fill (you can specify the fill color in the <strong>Color</strong> box that appears).</td>
</tr>
<tr>
<td>☐</td>
<td>Draw the hatched objects (you can specify the prototype and color for hatching in the <strong>Color</strong> and <strong>Pattern</strong> boxes that appear).</td>
</tr>
<tr>
<td>□</td>
<td>Draw the objects whose fill fades or becomes more intensive gradually from the basic color to one of its tones (you can specify the prototype, color, and intensity for shading in the <strong>Color</strong>, <strong>Pattern</strong>, and <strong>Shade</strong> boxes that appear).</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this box, specify the fill color to be applied to the selected objects.</td>
</tr>
<tr>
<td><strong>Pattern</strong></td>
<td>In this box, select the needed pattern for hatching or the required shade type.</td>
</tr>
<tr>
<td><strong>Shade</strong></td>
<td>In this box, specify the degree of default fill shading, i.e., the percentage of basic color changing in the fill.</td>
</tr>
<tr>
<td><strong>Font</strong></td>
<td>On the <strong>Font</strong> tab, specify the font and paragraph settings for the selected text.</td>
</tr>
<tr>
<td><strong>Style</strong></td>
<td>In this box, specify the font style.</td>
</tr>
<tr>
<td><strong>Size</strong></td>
<td>In this box, you can specify the font size.</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this box, you can specify the font color.</td>
</tr>
</tbody>
</table>
### Options and Description

<table>
<thead>
<tr>
<th>Attributes</th>
<th>Selecting check boxes applies the corresponding formatting:</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bold</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Italic</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Underline</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Strikeout</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Superscript</strong></td>
<td>(Superscript)</td>
</tr>
<tr>
<td><strong>Subscript</strong></td>
<td>(Subscript)</td>
</tr>
</tbody>
</table>

**Note**

If several objects are selected on the ChemSketch page, the check box of an attribute can be:
- **Cleared**, *i.e.*, this attribute will not be applied to the selected objects;
- **Selected**, *i.e.*, this attribute will be applied to the selected objects;
- **Dimmed** (if this attribute differs for the selected objects), *i.e.*, this attribute will not be changed for the selected objects.

### 4.11.7.2 Objects Panel: Structure

The **Structure** button displays tabs with style settings to be applied to the selected structures.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Font</strong></td>
<td>In this box, specify the font style to be applied to atom labels in the selected structure.</td>
</tr>
<tr>
<td><strong>Symbol Size</strong></td>
<td>In this box, specify the font size to be applied to atom labels of the selected structure.</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this box, specify the font color to be applied to atom labels of the selected structure.</td>
</tr>
<tr>
<td><strong>Style</strong></td>
<td>In this box, specify the style for atom labels: <strong>bold</strong> and/or <strong>italic</strong>. The pressed-in <strong>Mix</strong> button indicates that the corresponding attribute in the selected objects differs (<em>e.g.</em>, the selected structure has some atoms formatted just with bold and some just with italic).</td>
</tr>
</tbody>
</table>

On the **Bond** tab, specify the width and color to be used for bonds of the selected structure(s).

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Width</strong></td>
<td>In this box, specify the bond thickness for the selected structure. Note that you can enter values in various units (points, inches, millimeters, or centimeters) by typing the value and adding the unit you want (pt/in/mm/cm). The value will be recalculated automatically corresponding to the unit indicated in the <strong>Preferences</strong> dialog box (<strong>General</strong> tab).</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this box, specify the color to be applied to bonds of selected structure.</td>
</tr>
</tbody>
</table>
4.11.7.3 Objects Panel: Lines & Arrows

The Lines & Arrows button displays tabs with style settings to be applied to selected linear objects and arrows:

The following options are available:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>On the Pen tab</strong>, specify the thickness, style, and color of the line on selected linear objects.</td>
<td></td>
</tr>
<tr>
<td>Style</td>
<td>From this box, choose the line style.</td>
</tr>
<tr>
<td>Width</td>
<td>In this box, specify the line thickness for the selected objects.</td>
</tr>
<tr>
<td>Color</td>
<td>In this box, specify the line color to be applied to the selected objects.</td>
</tr>
<tr>
<td><strong>On the Arrow tab</strong>, specify the style of arrowhead and body of selected arrows.</td>
<td></td>
</tr>
<tr>
<td>Body Style</td>
<td>In this box, specify the default arrow body type.</td>
</tr>
<tr>
<td>Arrowheads shape</td>
<td>In this area, specify the default arrowhead shape to be applied to both arrow ends.</td>
</tr>
<tr>
<td>Swap</td>
<td>Interchanges the arrowheads.</td>
</tr>
<tr>
<td>Arrowheads size</td>
<td>In this area, specify the arrowhead width and height.</td>
</tr>
</tbody>
</table>
4.11.7.4 Objects Panel: Shapes

The Shapes button displays tabs with style settings to be applied to selected filling enclosures such as rectangles, ellipses, polygons and callouts.

The following options are available:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pen</strong> tab</td>
<td>Specify the thickness, style, and line color of the selected objects. These tab settings will be applied to all the selected rectangles, ellipses, polygons, and callouts.</td>
</tr>
<tr>
<td>Style</td>
<td>From this box, choose the line style.</td>
</tr>
<tr>
<td>Width</td>
<td>In this box, specify the line thickness for selected objects.</td>
</tr>
<tr>
<td>Color</td>
<td>In the color palette, you can specify the line color to be applied to the selected objects.</td>
</tr>
</tbody>
</table>

<p>| <strong>Fill</strong> tab | Specify the fill style and color of the selected objects. These settings will be applied to all the selected rectangles, ellipses, polygons, and callouts. |
| Style | In this area, click the required button to: |
| - No fill, i.e., they will be transparent. |
| - Solid fill (you can specify the fill color in the Color box that appears). |
| - Draw the hatched objects (you can specify the prototype and color for hatching in the Color and Pattern boxes that appear). |
| - Draw the objects whose fill fades or becomes more intensive gradually from the basic color to one of its tones (you can specify the prototype, color, and intensity for shading in the Color, Pattern, and Shade boxes that appear). |
| Color | In this box, specify the fill color to be applied to the selected shapes. |
| Pattern | In this box, select the needed pattern for hatching or the required shade type. |
| Shade | In this box, specify the degree of default fill shading, i.e., the percentage of basic color changing in the fill. |</p>
<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>On the Shadow tab</strong>, specify the size and color of shadow to be applied to the selected objects. These settings will be applied to all the selected rectangles, ellipses, polygons, and callouts.</td>
<td></td>
</tr>
<tr>
<td><strong>On / Off /Mixed</strong></td>
<td>Adds/removes shadow of selected shapes. Specify the shadow size and color in the other boxes. The selected Mixed option indicates that the corresponding attribute in the selected objects differs (e.g., one selected shape has a shadow and the other does not have any).</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In the color palette, specify the color of the shadow.</td>
</tr>
<tr>
<td><strong>dX / dY</strong></td>
<td>In these boxes, specify the position of a shadow relative to the object along the X and Y axes correspondingly. To enter the value in points/inches/millimeters/centimeters, type the value and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The value will be recalculated into the unit of measurement selected in the Preferences dialog box (General tab).</td>
</tr>
</tbody>
</table>

### 4.11.7.5 Objects Panel: Text

The **Text** button displays tabs with the style settings to be applied to selected text.

![Text tab](image)

The following options are available:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>On the Attr tab</strong>, you can transform the selected formatted text into the artistic one and rotate it.</td>
<td></td>
</tr>
<tr>
<td><strong>Artistic Text</strong></td>
<td>Select this check box to transform the selected Formatted text into the Artistic one. Unlike the formatted text, the artistic text can be modified like a usual graphical object (stretched, rotated, etc.).</td>
</tr>
<tr>
<td><strong>Angle of Rotation</strong></td>
<td>In this box, specify the angle at which you want to rotate the selected text.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>-------------</td>
<td>---------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Font</strong></td>
<td>On this tab, specify the font settings for the selected text.</td>
</tr>
<tr>
<td><strong>Style</strong></td>
<td>In this box, specify the font style.</td>
</tr>
<tr>
<td><strong>Size</strong></td>
<td>In this box, specify the font size.</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this box, specify the font color.</td>
</tr>
<tr>
<td><strong>Attributes</strong></td>
<td>Selecting check boxes applies the corresponding formatting: <strong>Bold</strong>, <strong>Italic</strong>, <strong>Underline</strong>, <strong>Strikeout</strong>, <strong>Superscript</strong> (<strong>Superscript</strong>), <strong>Subscript</strong> (<strong>Subscript</strong>)</td>
</tr>
<tr>
<td><strong>Paragraph</strong></td>
<td>On this tab, you can specify the style for paragraphs of selected text.</td>
</tr>
<tr>
<td><strong>Justification</strong></td>
<td>In this area, specify the alignment for the paragraph by clicking the corresponding buttons: to the left (<strong>left</strong>), centered (<strong>centered</strong>), to the right (<strong>right</strong>), and justified (<strong>justified</strong>). Text will be aligned relative to the current indents that can be specified in the Indentation area below. The active <strong>Mix</strong> button (<strong>Mix</strong>) indicates that the justification of the selected objects differs and will not be changed.</td>
</tr>
<tr>
<td><strong>Indentation</strong></td>
<td>In this area, specify the left and the right indentation of the paragraph in the text box as well as the indent of the first line in the paragraph.</td>
</tr>
<tr>
<td><strong>Spacing</strong></td>
<td>In this area, define the space above (<strong>Before</strong>) and below (<strong>After</strong>) the paragraph, as well as the distance between tab stops (<strong>Tab Step</strong>), and spacing between lines in a paragraph (<strong>Line Spacing</strong>). Note that the <strong>At</strong> option is available only if you select <strong>At Least</strong> or <strong>Exactly</strong> in the <strong>Line Spacing</strong> box. In most of the boxes, you can enter values in various units (points, inches, millimeters, or centimeters) by typing the value and adding the unit you want (pt/in/mm/cm). The value will be recalculated automatically corresponding to the unit indicated in the <strong>Preferences</strong> dialog box (<strong>General</strong> tab).</td>
</tr>
<tr>
<td><strong>Note</strong></td>
<td>If several objects are selected on the ChemSketch page, the check box of an attribute can be: <strong>Cleared</strong>, i.e., this attribute will not be applied to the selected objects; <strong>Selected</strong>, i.e., this attribute will be applied to the selected objects; <strong>Dimmed</strong> (if this attribute differs for the selected objects), i.e., this attribute will not be changed for the selected objects. The units of measurement in most of the boxes correspond to those set in the <strong>Preferences</strong> dialog box (<strong>General</strong> tab). To enter the value in points/inches/millimeters/centimeters, type the value and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The value will be recalculated into the corresponding unit of measurement.</td>
</tr>
</tbody>
</table>
4.11.7.6 Objects Panel: NMR Spectrum

The NMR Spectrum button displays tabs with style settings to be applied to the selected 1D NMR spectra copied from the ACD/CNMR or ACD/HNMR applications.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>On the View tab, specify the objects to be displayed with the spectrum.</td>
<td></td>
</tr>
<tr>
<td>Spectrum display options</td>
<td>In this area, select the check boxes of the elements to be displayed on the spectrum: gridlines, integral curves, lines' labels, confidence limits. If several spectra are selected on the ChemSketch page, the check box of an element can be dimmed, i.e., the state of the current element differs for these spectra.</td>
</tr>
<tr>
<td>Scale display options</td>
<td>In this area, select/clear the Vertical Scale / Horizontal Scale check boxes to display/hide the corresponding scales of the spectrum. If several spectra are selected on the ChemSketch page, the check box of an element can be dimmed, i.e., the state of the current element differs for these spectra.</td>
</tr>
<tr>
<td>On the Spectrum tab, specify the spectrum lines style and labels font style.</td>
<td></td>
</tr>
<tr>
<td>Spectrum Lines Styles</td>
<td>In this area, specify the style, thickness, and color to be applied to the spectrum lines (solute, solvent, and overlapped lines).</td>
</tr>
<tr>
<td>Labels Font Style</td>
<td>In this area, specify the style, size, and color for spectrum labels.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>-----------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Scale Line Style</strong></td>
<td>In this area, specify the style, thickness, and color to be applied to the scale lines.</td>
</tr>
<tr>
<td><strong>Scale Font Style</strong></td>
<td>In this area, define the font style, size, and color for scale values.</td>
</tr>
</tbody>
</table>

### 4.11.7.7 Objects Panel: Spectrum

The **Spectrum** button displays tabs with style settings to be applied to the spectra copied from ACD/SpecManager.

The following options are available:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>On the View tab</strong>, specify the objects to be displayed with the spectrum: labels, integral curves, gridlines, vertical scale, and horizontal scale.</td>
<td></td>
</tr>
<tr>
<td><strong>On the Spectrum tab</strong>, specify the style for spectrum and scales.</td>
<td></td>
</tr>
<tr>
<td><strong>Spectrum Line Style</strong></td>
<td>In this area, specify the ordinal number of the line for which the style, width, and color should be specified in the <strong>Lines</strong> boxes below.</td>
</tr>
<tr>
<td><strong>Scale Style</strong></td>
<td>In this area, define the font style, size, and color for scale values (<strong>Values</strong> boxes), also specify the style, width, and color for scale lines (<strong>Lines</strong> boxes).</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>---------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>On the <strong>Labels</strong> tab, specify the style, position, and orientation of peak labels.</td>
<td></td>
</tr>
<tr>
<td><strong>Labels Style</strong></td>
<td>In this area, specify the style, size, and color for spectrum labels.</td>
</tr>
<tr>
<td><strong>Position</strong></td>
<td>In this area, specify the position of peak labels on the spectrum. The selected <strong>Mixed</strong> option indicates that the position of labels in several selected spectra differs and will not be changed.</td>
</tr>
<tr>
<td><strong>Orientation</strong></td>
<td>In this area, specify the orientation of peak labels. The selected <strong>Mixed</strong> option indicates that the orientation of labels in several selected spectra differs and will not be changed.</td>
</tr>
<tr>
<td>On the <strong>Integrals</strong> tab, specify the styles for integral lines and integral values.</td>
<td></td>
</tr>
<tr>
<td><strong>Note</strong></td>
<td>If several objects are selected on the ChemSketch page, the check box of an attribute can be:</td>
</tr>
<tr>
<td></td>
<td>— <strong>Cleared</strong>, <em>i.e.</em>, this attribute will not be applied to the selected objects;</td>
</tr>
<tr>
<td></td>
<td>— <strong>Selected</strong>, <em>i.e.</em>, this attribute will be applied to the selected objects;</td>
</tr>
<tr>
<td></td>
<td>— <strong>Dimmed</strong> (if this attribute differs for the selected objects), <em>i.e.</em>, this attribute will not be changed for the selected objects.</td>
</tr>
</tbody>
</table>
4.11.7.8 Objects Panel: 2D Spectrum

The 2D Spectrum button displays tabs with style settings to be applied to the selected 2D NMR spectra copied from ACD/SpecManager.

The following options are available:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>On the Spectrum tab</td>
<td>Specify the style for 2D spectrum and 1D curves.</td>
</tr>
<tr>
<td>2D Spectrum Colors</td>
<td>In this area, specify the color settings for peaks of current spectrum and background. As you click the Coloration Scheme box, the dialog box appears allowing you to choose the coloration scheme (either Polychromatic or Dichromatic) you want to apply, set the additional color gradient for better visualization of a spectrum, and specify the colors to be used for displaying plot layers. You can select colors for up to ten overlaid spectra: in the No. box, choose the spectrum number and set the desired colors. Using this option helps you to distinguish between the collected 2D NMR spectra.</td>
</tr>
</tbody>
</table>
### Option Description

**Plots and Contours**
In this area, specify a form of the plot to be used for the spectrum representation. If several spectra are selected and they are represented with different types of plots, the **Mixed Plot** button is pressed in.

For **Contour Plot** you can also set the number of **Contours** to be used for each peak display.

**Spectrum Bitmap Resolution**
In this area, choose **Low** or **High** resolution depending on your requirements. Note that the higher resolution provides the better image quality, but also the larger file size.

**1D spectra**
In this area, select the check boxes of those 1D spectra that should be inserted together with the 2D spectrum. Note that these check boxes are enabled when you have 1D spectra attached. Moreover, in this area you can specify the color and width of the 1D spectrum lines.

On the **Labels** tab, specify the labels’ components, units of measurement, color and style of the labels’ text and lines.

**Show Labels**
Select this check box to display the labels on the spectrum. In the section below you can specify the elements to be included into a label. If several spectra are selected on the ChemSketch page, this check box can be dimmed, **i.e.,** the state of the elements differs in these spectra.

**Include in Label**
In this area, select check boxes of the elements to be included in peak labels: F2 / F1 shifts, intensities, volumes, assignments, annotations, diagonal line, and gridlines. If several spectra are selected on the ChemSketch page, the check box of an element can be dimmed, **i.e.,** state of the current element differs for these spectra.

**F2 Units / F1 Units**
In these areas, specify the units of measurement for the F2 and F1 scales. The pressed **Mix** button indicates that the units of measurement in several selected spectra differ and will not be changed.

**Style**
In this area, you can specify the display preferences for up to ten overlaid spectra. In the **No.** box, select the number of the spectrum, and then select the appropriate style attributes (label font style, size, and color, as well as the line style and color) in the boxes to the right.

On the **Scales** tab, specify the units of measurement, position of scales, color and style of the scales’ text and lines.

**Show**
In this area, select the check boxes of those elements that should be displayed together with the spectrum. If several spectra are selected on the ChemSketch page, the check box of an element can be dimmed, **i.e.,** state of the current element differs for these spectra.

**Position of Scales**
In this area, select the location of the axes: right and bottom; left and bottom; right and top; left and top.

If several spectra are selected and they have different display of scales, the **Mixed Scales** button is active.

**Style**
In this area, define the font style, size, and color for the scale values (**Text** boxes); also specify the style and color for scale lines (**Lines** boxes).
### 4.11.7.9 Objects Panel: Table

The **Table** button displays the tabs with style settings for table:

![Table buttons](image)

The following options are available:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Box</strong></td>
<td>On the <strong>Box</strong> tab, specify the general table options including arrangement of table rows in the box in the various ways.</td>
</tr>
<tr>
<td>Use Header</td>
<td>If this check box is selected, the first row in the table is inserted in every box as a header.</td>
</tr>
<tr>
<td>Protect Contents</td>
<td>If this check box is selected, the program does not allow you to insert or remove objects from the table cells until you clear this check box.</td>
</tr>
<tr>
<td>Move to the Right</td>
<td>If this check box is selected, the table rows are arranged into several groups like columns, each one is located to the right from the previous one. The table rows that do not fit in the first group are moved to the right of the first group; the table rows that do not fit in the second group are moved to the right of the second group, and so on.</td>
</tr>
<tr>
<td>Move to Next Box</td>
<td>If this check box is selected, the table rows that do not fit in the box (that is restricted as you first drag in the workspace when inserting a table), are moved to the next box.</td>
</tr>
<tr>
<td>Vertical Justify</td>
<td>If this check box is selected, numbers of rows in each group (column) are approximately equal.</td>
</tr>
<tr>
<td><strong>Cell</strong></td>
<td>On the <strong>Cell</strong> tab, you can define options for content alignment and manipulation within the table.</td>
</tr>
<tr>
<td>Alignment</td>
<td>In this area, specify the horizontal and vertical alignment of the content in a table.</td>
</tr>
<tr>
<td>Fit</td>
<td>In this box, select the way the table and its contents fit to each other:</td>
</tr>
<tr>
<td>Mixed</td>
<td>various cells in the table have different Fit parameters.</td>
</tr>
<tr>
<td>Table to Contents</td>
<td>the table dimensions are adjusted to the size of the contents (the table cells are reduced or enlarged with respect to the largest height and width of the inserted objects).</td>
</tr>
<tr>
<td>Contents to Table</td>
<td>the inserted objects are resized to fit properly into the table cells.</td>
</tr>
<tr>
<td>None</td>
<td>the table retains its primary dimensions irrespective of the size of the contents.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td><strong>On the Pen tab, specify the line style, width, and color of the table borders.</strong></td>
<td></td>
</tr>
<tr>
<td><strong>On the Fill tab, specify the fill style and color of table cells.</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Style</strong></td>
<td>In this area, click the required button to:</td>
</tr>
<tr>
<td></td>
<td>Draw the objects with no fill, <em>i.e.</em>, they will be transparent.</td>
</tr>
<tr>
<td></td>
<td>Draw the objects with the solid fill (<em>you can specify the fill color in the Color box that appears</em>).</td>
</tr>
<tr>
<td></td>
<td>Draw the hatched objects (<em>you can specify the prototype and color for hatching in the Color and Pattern boxes that appear</em>).</td>
</tr>
<tr>
<td></td>
<td>Draw the objects whose fill fades or becomes more intensive gradually from the basic color to one of its tones (<em>you can specify the prototype, color, and intensity for shading in the Color, Pattern, and Shade boxes that appear</em>).</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>In this box, specify the fill color to be applied to the table cells.</td>
</tr>
<tr>
<td><strong>Pattern</strong></td>
<td>In this box, select the needed pattern for hatching or the required shade type.</td>
</tr>
<tr>
<td><strong>Shade</strong></td>
<td>In this box, specify the degree of default fill shading, <em>i.e.</em>, the percentage of basic color changing in the fill.</td>
</tr>
</tbody>
</table>

**Note** If several objects are selected on the ChemSketch page, the check box of an attribute can be:

- **Cleared**, *i.e.*, this attribute will not be applied to the selected objects;
- **Selected**, *i.e.*, this attribute will be applied to the selected objects;
- **Dimmed** (if this attribute differs for the selected objects), *i.e.*, this attribute will not be changed for the selected objects.
4.11.8 Style Organizer Panel

This command allows you to manage styles. It displays the **Style Panel** containing a list of all saved styles and attributes (pen, arrow, fill, font, paragraph, and table) included in each style.

Using this panel you can apply any of the existing styles to the selected object, set any style from the list as the default one, rename or delete an existing style, and save the current default settings as a new style.

If you choose one or several attributes from the row at the top of the panel, the list of styles which include the chosen attributes will appear.

Choose all of the attributes to see the whole list of styles.

This panel contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Attributes</strong></td>
<td>Click the required button to view the styles containing the corresponding attribute. The following attributes are available:</td>
</tr>
<tr>
<td>Pen</td>
<td>(for more information on this attribute, refer to Section 4.11.1)</td>
</tr>
<tr>
<td>Arrow</td>
<td>(for more information on this attribute, refer to Section 4.11.3)</td>
</tr>
<tr>
<td>Fill</td>
<td>(for more information on this attribute, refer to Section 4.11.2)</td>
</tr>
<tr>
<td>Font</td>
<td>(for more information on this attribute, refer to Section 4.11.4)</td>
</tr>
<tr>
<td>Paragraph</td>
<td>(for more information on this attribute, refer to Section 4.11.5)</td>
</tr>
<tr>
<td>Table</td>
<td>(for more information on this attribute, refer to Section 4.11.6)</td>
</tr>
<tr>
<td><strong>List of Styles</strong></td>
<td>Displays a list of all saved styles and attributes (pen, arrow, fill, font, paragraph, and table) included in each style. Click the style to highlight it. You can then delete, rename, apply, and set as default the highlighted style. Built-in styles are shown in gray in the list and cannot be modified or deleted.</td>
</tr>
<tr>
<td>Apply</td>
<td>Applies the style highlighted in the list to the selected object(s).</td>
</tr>
<tr>
<td>Set Default</td>
<td>Sets the style highlighted in the list as the default.</td>
</tr>
</tbody>
</table>
4.11.8.1 Save User Style Dialog Box

In this dialog box, you can specify current default attributes to be saved as a new user-defined style.

You can open this dialog box from any of the default style panels (Tools menu) by clicking Save or from the Style Panel dialog box by clicking New.

The dialog box contains the following options:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Style Name</td>
<td>Specify a new name for the style or choose the one from the list and modify it.</td>
</tr>
<tr>
<td>Pen Style</td>
<td>Select this check box to include current default pen style attributes (specified in the Pen panel) in a user-defined style.</td>
</tr>
<tr>
<td>Arrow Style</td>
<td>Select this check box to include current default arrow style attributes (specified in the Arrow panel) in a user-defined style.</td>
</tr>
<tr>
<td>Fill Style</td>
<td>Select this check box to include current default fill style attributes (specified in the Fill panel) in a user-defined style.</td>
</tr>
<tr>
<td>Font Style</td>
<td>Select this check box to include current default font style attributes (specified in the Font panel) in a user-defined style.</td>
</tr>
<tr>
<td>Paragraph Style</td>
<td>Select this check box to include current default paragraph style attributes (specified in the Paragraph panel) in a user-defined style.</td>
</tr>
<tr>
<td>Table Style</td>
<td>Select this check box to include current default table style attributes (specified in the Table panel) in a user-defined style.</td>
</tr>
<tr>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>OK</td>
<td>Click this button to save the specified attributes into the user-defined style with specified name.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Click this button to close the dialog box without saving any changes you have made.</td>
</tr>
</tbody>
</table>

4.11.9 Generate Submenu

For detailed information on the commands that are available from this submenu, refer to Sections 3.12.16–3.12.24.

4.11.10 Search for Structure

*Commercial version only!*

For detailed information on this command, refer to Section 3.12.25.

4.12 Object Menu

The commands located on this menu allow you to control the location of the graphical objects on the page. These commands group, layer, rotate, and align selected objects, connect lines and convert selected objects to polylines. Most of the commands on this menu are also available on the Editing toolbar (refer to Section 4.6).

4.12.1 Group/Ungroup

This command allows you to do the following:

- Group all of the selected objects together so that they can be selected and manipulated as a single object.
- Break up the selected group into its individual objects. If you have grouped several groups together, **Ungroup** breaks up one level of grouping at a time.
- Place/extract the selected object to the selected table's cell.

**Note**  
The **Group** and **Ungroup** commands automatically replace each other on the **Object** menu depending on current selection.

This command is unavailable if there is only one selected object or no selected objects in the workspace.

**Shortcuts:**

- **Keyboard:**  
  \[\text{CTRL}+G\]
- **Editing toolbar:**
4.12.2 Bring to Front

This command brings the selected background objects to the foreground. Select the object(s) and choose this command. To reverse Bring to Front, use the Send to Back command.

To select objects that are completely covered by foreground objects, you can apply the Send to Back command to the front object(s).

Shortcuts:

- Keyboard: CTRL+F
- Editing toolbar:

4.12.3 Send to Back

This command allows you to move objects from the foreground to the background. Select the object(s) and choose this command. To reverse Send to Back, use the Bring to Front command.

Shortcuts:

- Keyboard: CTRL+K
- Editing toolbar:

4.12.4 Flip Left to Right

This command allows you to turn the selected object(s) about the vertical plane.

If the Select Graphics check box in the Preferences dialog box (Structure tab) is selected, you can apply some of the selecting, rotating, and flipping tools available on the Structure toolbar to the objects created in the Draw mode.

Shortcut:

- Editing toolbar:

4.12.5 Flip Top to Bottom

This command allows you to turn the selected object(s) about the horizontal plane.

If the Select Graphics check box in the Preferences dialog box (Structure tab) is selected, you can apply some of the selecting, rotating, and flipping tools available on the Structure toolbar to the objects created in the Draw mode.

Shortcut:

- Editing toolbar:
4.12.6 Rotate 90°

This command rotates the selected objects anticlockwise by 90°.

Tip You can also use the Select/Move/Rotate tool for rotating objects (for more information, refer to Section 4.6.2).

Shortcut:

Editing toolbar:

4.12.7 Align Horizontally > Left/Center/Right

These commands allow you to align the selected objects horizontally to the left, to the center, or to the right correspondingly.

- If a single object is selected, it is aligned to the center, left, or right margin of the whole page.
- If a group of objects is selected, objects are aligned to the center, left, or right edge of the whole group relative each other.

Shortcuts:

Editing toolbar:

4.12.8 Align Vertically > Top/Center/Bottom

These commands allow you to align the selected objects vertically to the top, to the center, or to the bottom correspondingly.

- If a single object is selected, it is aligned to the top, center, or bottom margin of the page.
- If a group of objects is selected, objects are aligned to the top, center, or bottom edge of the whole group relative each other.

Shortcuts:

Editing toolbar:

4.12.9 Fit Horizontally

This command stretches the selected object(s) horizontally to the left and right margins of the page.

Unlike the Fit All option that only changes the display of objects, this command changes the actual size of objects.
4.12.10  Fit Vertically

This command stretches the selected object(s) vertically to the top and bottom margins of the page.

Unlike the Fit All and Fit Selected options that only change the display of objects, this command changes the actual size of objects.

4.12.11  Convert to Polyline

This command converts the selected objects drawn with the Rectangle, Rounded Rectangle, Arc, and Ellipse tools to polyline so that you can change their shape using the Edit Nodes tool.

**Shortcut:**

Keyboard:   CTRL+Y

4.12.12  Connect Lines

This command draws connecting lines between two or more selected graphical objects drawn with the Line, Curve, Arrow, or Polyline tools. The nearest end points of the selected objects are joined together.

To be able to apply this tool to objects drawn with the Arc tool, you can convert the drawn arcs into polyline using the Convert to Polyline command from the Object menu.

4.13  Templates Menu

For detailed information on the commands that are available from this menu, refer to Section 3.13.

4.14  Options Menu

For detailed information on the commands that are available from this menu, refer to Section 3.14.

4.15  Documents Menu

For detailed information on the commands that are available from this menu, refer to Section 0.
4.16 I-Lab Menu

For detailed information on the commands that are available from this menu, refer to Section 3.17.

4.17 ACD/Labs Menu

For detailed information on the commands that are available from this menu, refer to Section 3.18.

4.18 Help Menu

For detailed information on the commands that are available from this menu, refer to Section 3.19.
Appendix A. Running ACD/ChemSketch from Command Line

There may be circumstances (such as a call from another program) in which you need to run ACD/ChemSketch in the command-line mode instead of the Windows graphical user interface.

The following command arguments are available to be issued from the command line:

<table>
<thead>
<tr>
<th>Command</th>
<th>This command…</th>
</tr>
</thead>
<tbody>
<tr>
<td>chemsk</td>
<td>Runs ACD/ChemSketch.</td>
</tr>
<tr>
<td>chemsk PathFilename.SupportedFormat</td>
<td>Opens the specified file in the ChemSketch window (if possible).</td>
</tr>
<tr>
<td>where PathFilename.SupportedFormat can be a file of any format supported by current version of ACD/ChemSketch (for the list of supported formats, refer to Section 3.9.8).</td>
<td>If there are spaces in the file or folder name, its name should be enclosed in double quotation marks.</td>
</tr>
<tr>
<td>/print</td>
<td>Prints the file open in ACD/ChemSketch.</td>
</tr>
<tr>
<td>/exportpdf</td>
<td>Exports the file open in ACD/ChemSketch into PDF format.</td>
</tr>
<tr>
<td>/exportpdf:Filename.pdf</td>
<td>Exports the file into PDF format with the specified name.</td>
</tr>
<tr>
<td>/norestore</td>
<td>If this switch is added to the command line, all of the specified actions will be executed without opening ACD/ChemSketch.</td>
</tr>
<tr>
<td>/quit</td>
<td>Quits ACD/ChemSketch.</td>
</tr>
</tbody>
</table>

**Note** The command line length is limited to 260 characters.

For example, the following line:

```bash
cemsk "e:\my examples\poster.sk2" /print /exportpdf /quit
```

opens POSTER.SK2 from E:\EXAMPLES in the ChemSketch window, prints it, exports it into the POSTER.PDF file, and quits the program;

and the following line

```bash
cemsk c:\temp\borneol.mol /exportpdf:example.pdf /norestore /quit
```

loads the BORNEOL.MOL file located in C:\TEMP, exports it into the EXAMPLE.PDF file, and quits the program without opening it.
Appendix B. Calculated Properties

Overview

In addition to the drawing capabilities, ACD/ChemSketch offers predictions of numerous properties for your compounds. These include prediction of

- Molecular formula
- Formula weight
- Composition
- Molar refractivity
- Molar volume
- Parachor
- Index of refraction
- Surface tension
- Density
- Dielectric constant
- Polarizability
- Monoisotopic, nominal, and average mass
- \( M^+ \)
- \( M^- \)
- \([M+H]^+\)
- \([M+H]^-\)
- \([M-H]^+\)
- \([M-H]^-\)

In this chapter, the simple means to calculate these properties and the calculation algorithms are briefly described. An agreement between calculated and experimental values is shown for several hundreds of compounds.

Algorithms for Calculating Properties

At the heart of the additive-constitutive calculation algorithm of all physicochemical properties in ACD/ChemSketch lies the presumption that these properties can be estimated using additive atomic or group increments. Apart from molecular weight (MW), which is trivial to calculate, the algorithms may be divided into three general groups:

- Basic macroscopic properties: molar volume (MV), molar refractivity (MR), and parachor \( (P_r) \)
• Derived macroscopic properties: density (\(d\)), refractive index (\(n\)), and surface tension (\(\gamma\))
• The dielectric constant \(\varepsilon\) (Permittivity)

Basic macroscopic properties such as molar volume (MV), molar refractivity (MR), and the parachor (\(P_r\)) are calculated first for the input structure. The atomic additive increments in such an algorithm depend on the bonds (single, double, aromatic, etc.) of this atom and on neighboring atoms. ACD/ChemSketch rapidly analyzes the input structure to determine the class of each atom, i.e., whether it is cyclic, aromatic, aliphatic, etc.

The prediction algorithms for density (\(d\)), refractive index (\(n\)) and surface tension (\(\gamma\)) are founded on well-known physicochemical formula which can be found in literature on physicochemical properties of compounds. They express \(d\), \(n\), and \(\gamma\) as functions of MV, MR, or \(P_r\). Once the MV, MR, or \(P_r\), have been predicted by additive means, it is straightforward to predict \(d\), \(n\), and \(\gamma\) using these formula.

The determination of the additive-constitutive atomic increments for MV, MR, and \(P_r\), were obtained internally by ACD/Labs scientists using large experimental databases relating structure to density, refractive index, and surface tension. The MV, MR, and \(P_r\), were recalculated from \(d\), \(n\), and \(\gamma\). These parameters are proprietary information of ACD/Labs, Inc.

The prediction of the dielectric constant \(\varepsilon\) (permittivity) resembles very closely the prediction of boiling point, which is a separate ACD/Labs product available from ACD/ChemSketch. Senior scientists at ACD/Labs discovered an additive function, which relates the dielectric constant to other macroscopic properties which can be additively treated, such as MV. Once this relationship was discovered, the additive-constitutive atomic increments for this function were obtained using large databases consisting of molecular structures and their observed dielectric constants. Using the function and estimated MV for the input structure, its dielectric constant can be quickly predicted.

**Molar Volume, MV**

By definition, 
\[
MV = \frac{MW}{d}.
\]

ACD/ChemSketch calculates molar volume from additive increments. The additive atomic increments were obtained using a database of density and calculated MW.

**Molar Refractivity, MR**

The Lorentz-Lorenz equation relates refractive index, density, and refractive index:
\[
MR = \frac{n^2 - 1}{n^2 + 2} \cdot \frac{MW}{d}
\]

ACD/ChemSketch calculates molar refractivity from additive increments. The additive atomic increments were obtained using a database of density, refractive index, and calculated MW.

**Parachor, \(P_r\)**

By definition,
Appendix B. Calculated Properties

\[ P_r = \left( \frac{MW}{d} \right)^{\gamma/4} \]

ACD/ChemSketch calculates the parachor from additive increments. The additive atomic increments were obtained using a database of density, surface tension, and calculated MW.

**Density, d**

By definition,

\[ d = \frac{MW}{MV} \]

ACD/ChemSketch calculates the density from MW and the calculated molar volume (see above).

**Refractive Index, n**

By the Lorentz-Lorenz equation,

\[ n = \sqrt{\frac{2 \cdot MR + MV}{MV - MR}} \]

ACD/ChemSketch calculates the refractive index from the molar volume and molar refractivity, both of which are calculated as above.

**Surface Tension, \( \gamma \)**

By definition,

\[ \gamma = \left( \frac{P_r}{MV} \right)^4 \]

ACD/ChemSketch calculates the surface tension from calculated MV (see above) and calculated \( P_r \) (see above).

**Dielectric Constant, \( \varepsilon \) (Permittivity)**

By definition,

\[ f(\varepsilon) = f(MV, AdditiveFunction) \]

ACD/ChemSketch calculates the dielectric constant from calculated MV (see above) and a proprietary empirical additive function.

**Polarizability**

This property is calculated from the Molar Refractivity (MR) as follows:

\[ \text{Polarizability} = 0.3964308 \cdot MR \]
Appendix B. Calculated Properties

Monoisotopic, Nominal, Average Masses and other Mass Values

Monoisotopic mass ($M_{mi}$) is the exact mass of the most abundant stable isotope that can occur naturally.

Nominal Mass ($M_n$) is the sum of the approximated monoisotopic masses of the elements forming the structure.

Average Mass ($M_{av}$) is the calculated mass of a particle based on the atomic weights of the elements from which it is composed.

$M^+$, $M^-$, $[M+H]^+$, $[M+H]^-$, $[M-H]^+$, $[M-H]^-$ mass values are calculated by addition or subtraction of proton and electron masses from Monoisotopic mass. These mass values are used for identification of molecules in mass-spectra at different ionization conditions.

Correlation Statistics with Experimental Data

Distribution of Molar Refractivity Prediction Error

Vertical scale: Number of Tested Structures
Horizontal scale: ACD Molar Refractivity Estimation Error
Number of tested structures: 592

$MR_{exp} = 0.99901(±0.00067) \times MR_{calc} + 0.026(±0.025)$  \( R=0.999867 \), \( StD=0.23 \)
Appendix B. Calculated Properties

Distribution of Molar Volume Prediction Error

Vertical scale: Number of Tested Structures
Horizontal scale: ACD/Molar Volume Estimation Error
Number of tested structures: 671

\[ MV_{\text{exp}} = 0.9989(\pm 0.0020) \times MV_{\text{calc}} + 0.18(\pm 0.29) \]
\[ R = 0.998626, \text{ StD} = 2.74 \]

Distribution of the Parachor Prediction Error

Vertical scale: Number of Tested Structures
Horizontal scale: ACD/Parachor Estimation Error
Number of tested structures: 377

\[ Pr_{\text{exp}} = 0.9978(\pm 0.0015) \times Pr_{\text{calc}} + 0.68(\pm 0.46) \]
\[ R = 0.99958, \text{ StD} = 3.11 \]
Appendix B. Calculated Properties

Distribution of the Refractive Index Prediction Error

\[ n^{20 \text{exp}} = 0.98035(\pm 0.0073) \, n^{20 \text{calc}} + 0.028(\pm 0.011) \quad R=0.982, \text{StD}=0.012 \]

Distribution of the Density Prediction Error

\[ d^{20 \text{exp}} = 0.9947(\pm 0.0036) \, d^{20 \text{calc}} + 0.0052(\pm 0.0036) \quad R=0.995683, \text{StD}=0.028 \]
Appendix B. Calculated Properties

### Distribution of the Surface Tension Prediction Error

Vertical scale: Number of Tested Structures  
Horizontal scale: ACD/Surface Tension Estimation Error  
Number of tested structures: 432

\[ s_{\text{t}^{20}}^{\text{exp}} = 0.998(\pm0.018) s_{\text{t}^{20}}^{\text{calc}} + 0.08(\pm0.53) \]  
\( R=0.934720, \text{Std}=2.84 \)

### Distribution of the Dielectric Constant (Permittivity) Estimation Error

Vertical scale: Number of Tested Structures  
Horizontal scale: Dielectric constant (Permittivity) Estimation Error  
Number of tested structures: 85

\[ \varepsilon^{\text{exp}} = 1.005(0.033)\varepsilon^{\text{exp}} - 0.013(0.072) \]  
\( R=0.9588, \text{Std}=0.079 \)  

**Note:** Derived only for hydrocarbons
Appendix C. Goodies

What are “Goodies”? Goodies are additional tools that extend the functionality of ACD/ChemSketch. They are, actually, implemented as ACD/ChemBasic programs associated with the 22 supplementary ChemSketch buttons. ACD/ChemBasic is a special programming language that enables you to customize ACD/Labs software, and we think this is a great way to show off how useful it is—and at the same time make your ACD/ChemSketch even more versatile!

Note that you do not need to know anything about ACD/ChemBasic (although, if you wish, you can learn it by using the Goodies' code as example).

Where Can I Get Them? Goodies are included into ACD/ChemSketch package. Look for all .BAS files within your ACD/Labs example folder (\EXAMPLES\CHEMBAS\GOODIES). They are easy to install and to use. After installation, the Goodies tools are available as buttons on a toolbar you have specified; later you can customize the toolbar (refer to Section 2.2.1).

Note ChemBasic Goodies buttons are only available when you are in the Structure mode.

Goodies This chapter will familiarize you with the list of Goodies tools that are available at the moment at our Web site:

Insert Page

This tool allows you to insert a blank page at any place within your ChemSketch document. Note that the usual way—through New (Pages menu)—adds a page at the end of document.

How to use:
Go to the page before which you want to insert a blank page and click Insert Page.
Clone Page

This tool allows you to clone current page (together with its contents) a specified number of times—it is very useful for filling in the document with page templates, tables, titles, etc. New pages are added at the end of a document.

*How to use:*  
Make the page which you wish to clone active and click **Clone Page**. In the dialog box that appears, specify the number of clones and click **OK**.

Move/Copy Page

This tool allows you to move and copy pages—*i.e.*, changes page order in your document.

*How to use:*  
Go to the page which you wish to move or copy and click **Move/Copy Page**. In the dialog box that appears, type the number of the page after which you wish to place the current page, and then define the required action: **Copy** or **Move**. Click **OK**.

Reorder Pages

This tool allows you to cut-and-paste or copy-and-paste a sequence of pages to a new position within the same document.

*How to use:*  
Click **Reorder Pages** and, in the dialog box that appears, type the numbers of the pages to be moved or copied to a new position. Then, type the page number after which you want to place the selected range of pages. Specify the required action (**Copy** or **Move**) and click **OK**.

Delete Pages

This tool allows you to delete a range of pages at a time.

*Note*  
The pages you have deleted cannot be recovered with the **Undo** command from the **Edit** menu.

*How to use:*  
Click **Delete Pages**. In the dialog box that appears, type the sequence of pages to be deleted and click **OK**.

Rename Pages

This tool allows you to change the name of pages.

*Note*  
The names of the pages will be shown when you click Page 1/1 on the status bar.

*How to use:*  
Click **Rename Pages** and, in the dialog box that appears, type the number of the page to be (re)named, a new name of the page, and then click **OK**. In the message that appears, click **Yes** and repeat the previous action if you want to rename the next page; if it is not required to rename the next page, click **No**.
Appendix C. Goodies

Insert Page Numbers/ Annotations

This tool allows you to insert page numbers or complex annotations in your document.

| Note | An annotation will be inserted at the bottom right corner of the page. |

How to use:

Click Insert Page Numbers/ Annotations and, in the dialog box that appears, type a page annotation template, and then click OK.

Annotation template keys:

- $P$—inserts page numbers;
- $N$—inserts pages names (that can be inserted by clicking Rename Pages or by using Rename (Pages menu)).

Tip: You can also include any fixed text into your annotation template (for example, template: Page $P$: $N$ will insert “Page 1: Page Name”, etc. annotations). If a template contains no keys, just a fixed text for each page will be inserted; for example, you can sign all of the pages with your name.

Annotate Document

This tool allows you to annotate your documents based on the content of the leftmost top text box on each page. This is very convenient for managing large documents and presentations.

How to use:

Click Annotate Document to annotate all of the pages containing any text. After program execution click the page counter on the status bar to see page names.

Document Browse

This tool allows you to look through the folders to find the specified ChemSketch documents as well as to search ChemSketch documents for the text string without opening them.

How to use:

Click Document Browse and follow the instructions that appear in the dialog box.

Create HTML

This tool allows you to export all selected pages of a current document into an HTML file, which you can later view with your favorite web-browser. Note that this option requires ChemSketch 4.01 or later.

How to use:

Click Create HTML. In the dialog box that appears, enter a sequence of ChemSketch pages or select a whole document. Specify an output directory and the name of file that contains your lines of template. (All the details may be found in FILLTMP.DOC file provided in the Goodies folder (\EXAMPLES\CHEMBAS\GOODIES)).
**Sketch-to-VRML Converter**

This tool allows you to export all structures from current page into a VRML 2.0 file, which you may then view with Cosmo, GLView, or any other VRML browser.

*How to use:*

Draw structures which you wish to export on the same page, and then click **Sketch-to-VRML Converter**. In the dialog box that appears, type the name and location of .WRL file to which structures are to be exported. (If you have typed the filename only, the program will place the resulting WRL file in the same folder with SK2VRML.BAS.) Specify the desired structure presentation by selecting the corresponding option and click **OK**.

**SDF-to-Sketch Converter**

This tool allows you to import the data (structures, text, etc.) from a file of MDL's SDfile format into ChemSketch document.

*How to use:*

Click **SDF-to-Sketch Converter** and, in the dialog box that appears, specify the name and location of the SDfile which you want to import. (If you type the filename without specifying the full path, the program will search your SDfile in the folder where ACD/ChemBasic programs are located. So, if you placed the needed SDfile in the same folder with SDF2SK.BAS, then simply specify the file name without a path.) Specify the number of structures per page and an SDfile field containing structures, then click **OK**.

**Sketch-To-SDF Converter**

This tool allows you to export all structures from current page or from the whole document to an SDfile.

*How to use:*

Open the page with the structures you want to export (if required). Click **Sketch-To-SDF Converter** and, in the dialog box that appears, choose what you want to import—the current page or the whole document; specify whether the formula, FW, and ID are to be exported along with the structures. Specify the name and the path for an SDfile and click **OK**. (Note that if you type the filename only, the program will place the resulting SDfile in the same folder where EXPSDF.BAS resides.)

**Table Wizard**

This tool allows you to create tables or/and align objects according to the specified number of rows and columns.

*How to use:*

Click **Table Wizard**, you will be informed about the number of objects on the page and some suggestions on how to align them. Specify the number of rows and columns for the table, choose whether to create borders (the **Mark-up table** check box) in the table, and then click **OK**. To create an empty table, run the **Table Wizard** with the blank page active.
Replace Element

This tool allows you to replace all of the atoms of a given type with atoms of another type in a chemical structure. This is very useful for drawing, for example, perfluorinated structures.

**Note**  The program execution is possible only with a single structure on the page.

*How to use:*

Draw or leave only one structure on the page and click **Replace Element**. In the dialog box that appears, specify the element to be replaced and the element that should replace the one specified before, and then click **OK**.

**Note**  The hydrogen atoms should be drawn explicitly (use **Add Explicit Hydrogens** from the **Tools** menu).

Solution Calculator

This tool allows you to calculate the weight of a compound required for preparing an aqueous solution of the user-defined volume and molar concentration.

**Note**  The program execution is possible only with a single structure on the page.

*How to use:*

Draw or leave one structure on the page and click **Solution Calculator**. In the dialog box that appears, specify the required molar concentration and aqueous solution volume, then click **OK**.

Label Printer

This tool allows you to quickly create labels for chemicals and print them according to the Avery Standard (45 templates included) or according to your own template.

*How to use:*

Draw structures for which you want to create labels and click **Label Printer**. Note that you can create labels for structures from an SD file if you run this program with an empty active page. For more information, see LPRINTER.TXT provided in the Goodies folder (\EXAMPLES\CHEMBAS\GOODIES\LPRINTER).

Peptide Builder

This tool allows you to build a 3D peptide structure from the amino acids sequence.

*How to use:*

Select the text box with peptide short-hand formula and click **Peptide Builder**. For more information, refer to the PEPBUILD.SK2 file provided in the Goodies folder (\EXAMPLES\CHEMBAS\GOODIES\PEPBUILD) as a guide to using this tool.
**Carbohydrate Builder**

This tool allows you to build a structure from carbohydrate abbreviated names.

*How to use:*

Select the text box with carbohydrate abbreviated name and click **Carbohydrate Builder**.

For more detailed information, refer to the SUGARSK.TXT file that you can find in the Goodies folder (\EXAMPLES\CHEMBAS\GOODIES\SUGARSK).

**Remove Spectator Ions (Desalt)**

An SDfile that contains one or more salt structure entries can be changed to a "one-molecule-per-entry" SDfile. This tool removes the smallest ion, either by MW or by number of atoms. For example, sodium acetate will have the sodium atom removed, and acetic acid will remain behind. (Note that the structure left behind is put into neutral form.)

*How to use:*

Click **Desalt** and in the dialog box that appears, specify the name and the path for an SDfile. Note that if you type the filename only, the program will look for a file in the Goodies folder (\EXAMPLES\CHEMBAS\GOODIES). Then, define a criterion for smallest part: mass or atom. The resultant SDfile will be saved in the same folder with the original file under NEWFILE.SDF name. A special sample file, SALTS.SDF with 5 salts in it is placed in the Goodies folder (\EXAMPLES\CHEMBAS\GOODIES) for testing.

**Nucleic Acid Builder**

This tool allows you to build a 3D nucleic acid (DNA, RNA) structure (one or two chains) from your input sequence.

*How to use:*

Click **Nucleic Acid Builder** and follow the instructions in the dialog box that appears.

**Column Selector**

This tool lets the chromatographer search a knowledge base of the most utilized columns in order to locate the ones that have the properties best suited to the separation at hand.

*How to use:*

Click **Column Selector** and, in the dialog box that appears, specify whether to compare the selected column with the list or two selected columns between themselves, and then click **OK**. In the next dialog box, choose the proper column(s) from the drop-down list and set the weighting coefficients to be applied to all six column parameters, then click **OK**. (For information on how to work with this tool, refer to the COLSEL_W.PDF file that you can find in the (\DOCS) folder.)